Kunal Roy

List of Publications by Year
in descending order

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348	13,164	44444	38517
papers	citations	50 h-index	99 g-index

374	374	374	7923
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	In silico modeling for quick prediction of inhibitory activity against 3CL^{pro} enzyme in SARS CoV diseases. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1010-1036.	2.0	23
2	Exploring CIP2A modulators using multiple molecular modeling approaches. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1048-1063.	2.0	3
3	Chemometric Modelling of Heat Release Capacity, Total Heat Release and Char Formation of Polymers to Assess Their Flammability Characteristics. Molecular Informatics, 2022, 41, .	1.4	5
4	QSAR modelling of inhalation toxicity of diverse volatile organic molecules using no observed adverse effect concentration (NOAEC) as the endpoint. Chemosphere, 2022, 287, 131954.	4.2	9
5	Chemometric modeling of plant protection products (PPPs) for the prediction of acute contact toxicity against honey bees (A. mellifera): A 2D-QSAR approach. Journal of Hazardous Materials, 2022, 423, 127230.	6.5	16
6	QSPR modeling of absorption maxima of dyes used in dye sensitized solar cells (DSSCs). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 265, 120387.	2.0	11
7	A novel quantitative read-across tool designed purposefully to fill the existing gaps in nanosafety data. Environmental Science: Nano, 2022, 9, 189-203.	2.2	41
8	Ecotoxicological risk assessment of organic compounds against various aquatic and terrestrial species: application of interspecies i-QSTTR and species sensitivity distribution techniques. Green Chemistry, 2022, 24, 2160-2178.	4.6	8
9	Nitroaromatics as hypoxic cell radiosensitizers: A 2D-QSAR approach to explore structural features contributing to radiosensitization effectiveness. European Journal of Medicinal Chemistry Reports, 2022, , 100035.	0.6	3
10	Green Chemistry in the Synthesis of Pharmaceuticals. Chemical Reviews, 2022, 122, 3637-3710.	23.0	155
11	Computational Modeling of Mixture Toxicity. Methods in Molecular Biology, 2022, 2425, 561-587.	0.4	2
12	In Silico Tools and Software to Predict ADMET of New Drug Candidates. Methods in Molecular Biology, 2022, 2425, 85-115.	0.4	15
13	QSAR modelling of organic dyes for their acute toxicity in Daphnia magna using 2D-descriptors. SAR and QSAR in Environmental Research, 2022, 33, 111-139.	1.0	10
14	Modeling and mechanistic understanding of cytotoxicity of metal oxide nanoparticles (MeOxNPs) to Escherichia coli: categorization and data gap filling for untested metal oxides. Nanotoxicology, 2022, 16, 152-164.	1.6	7
15	Recent Advances on Modelling the Toxicity of Environmental Pollutants for Risk Assessment: from Single Pollutants to Mixtures. Current Pollution Reports, 2022, 8, 81-97.	3.1	6
16	Prediction reliability of QSAR models: an overview of various validation tools. Archives of Toxicology, 2022, 96, 1279-1295.	1.9	49
17	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
18	Ecotoxicological QSTR and QSTTR Modeling for the Prediction of Acute Oral Toxicity of Pesticides against Multiple Avian Species. Environmental Science & Technology, 2022, 56, 335-348.	4.6	29

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19	Application of cross-validation strategies to avoid overestimation of performance of 2D-QSAR models for the prediction of aquatic toxicity of chemical mixtures. SAR and QSAR in Environmental Research, 2022, 33, 463-484.	1.0	17
20	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
21	First report of q-RASAR modeling toward an approach of easy interpretability and efficient transferability. Molecular Diversity, 2022, 26, 2847-2862.	2.1	51
22	Applications of chem-bioinformatic, chemometric and machine learning approaches for COVID-19 related research. Structural Chemistry, 2022, 33, 1389-1390.	1.0	1
23	First report on soil ecotoxicity prediction against Folsomia candida using intelligent consensus predictions and chemical read-across. Environmental Science and Pollution Research, 2022, 29, 88302-88317.	2.7	10
24	Quantitative predictions from chemical read-across and their confidence measures. Chemometrics and Intelligent Laboratory Systems, 2022, 227, 104613.	1.8	32
25	Chemometric modeling of acute toxicity of diverse aromatic compounds against Rana japonica. Toxicology in Vitro, 2022, 83, 105427.	1.1	5
26	QSPR modeling of octanol-water partition coefficient and organic carbon normalized sorption coefficient of diverse organic chemicals using Extended Topochemical Atom (ETA) indices. Ecotoxicology and Environmental Safety, 2021, 208, 111411.	2.9	7
27	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
28	First report on chemometric modeling of hydrolysis half-lives of organic chemicals. Environmental Science and Pollution Research, 2021, 28, 1627-1642.	2.7	4
29	Computational Modeling of RdRp Inhibitors for the Development of Drugs against Novel Coronavirus (nCoV). Methods in Pharmacology and Toxicology, 2021, , 541.	0.1	0
30	Chemometric Modeling of Absorption Maxima of Carbazole Dyes Used in Dye-Sensitized Solar Cells. Challenges and Advances in Computational Chemistry and Physics, 2021, , 207-232.	0.6	1
31	Assessment of toxicity of metal oxide and hydroxide nanoparticles using the QSAR modeling approach. Environmental Science: Nano, 2021, 8, 3395-3407.	2.2	13
32	Computational Modeling of ACE2-Mediated Cell Entry Inhibitors for the Development of Drugs Against Coronaviruses. Methods in Pharmacology and Toxicology, 2021, , 495.	0.1	1
33	QSAR and QSAAR modeling of nitroimidazole sulfonamide radiosensitizers: application of small dataset modeling. Structural Chemistry, 2021, 32, 631-642.	1.0	11
34	Prediction of aquatic toxicity of chemical mixtures by the QSAR approach using 2D structural descriptors. Journal of Hazardous Materials, 2021, 408, 124936.	6.5	28
35	QSPR modelling for investigation of different properties of aminoglycoside-derived polymers using 2D descriptors. SAR and QSAR in Environmental Research, 2021, 32, 595-614.	1.0	4
36	Special issue of molecular diversity on â€œAI and ML for small molecule drug discovery in the big data eraâ€• Molecular Diversity, 2021, 25, 1259-1260.	2.1	1

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37	In silico modelling of acute toxicity of 1, 2, 4-triazole antifungal agents towards zebrafish (Danio) Tj ETQq1 1 0.784314 rgBT /Overloc	1.1	3
38	Application of QSAR for the identification of key molecular fragments and reliable predictions of effects of textile dyes on growth rate and biomass values of Raphidocelis subcapitata. Aquatic Toxicology, 2021, 238, 105925.	1.9	9
39	Ecotoxicological QSAR modeling of the acute toxicity of organic compounds to the freshwater crustacean Thamnocephalus platyurus. Chemosphere, 2021, 280, 130652.	4.2	14
40	QSTR and interspecies-QSTR modelling for aquatic toxicity data gap filling of cationic polymers. Computational Toxicology, 2021, 20, 100181.	1.8	3
41	Computational Modeling of Chloroquine Analogues for Development of Drugs Against Novel Coronavirus (nCoV). Methods in Pharmacology and Toxicology, 2021, , 579-614.	0.1	1
42	Recent advances in quantitative structureâ€“activity relationship models of antimalarial drugs. Expert Opinion on Drug Discovery, 2021, 16, 659-695.	2.5	13
43	Target prioritization of novel substituted 5-aryl-2-oxo-/thioxo-2,3-dihydro-1H-benzo[6,7]chromeno[2,3-d]pyrimidine-4,6,11(5H)-triones as anticancer agents using in-silico approach. Journal of Biomolecular Structure and Dynamics, 2020, 38, 1415-1424.	2.0	2
44	Chemometric modeling to predict air half-life of persistent organic pollutants (POPs). Journal of Hazardous Materials, 2020, 382, 121035.	6.5	15
45	Exploration of nitroimidazoles as radiosensitizers: application of multilayered feature selection approach in QSAR modeling. Structural Chemistry, 2020, 31, 1043-1055.	1.0	7
46	Application of QSARs in identification of mutagenicity mechanisms of nitro and amino aromatic compounds against Salmonella typhimurium species. Toxicology in Vitro, 2020, 65, 104768.	1.1	11
47	Ecotoxicological assessment of pharmaceuticals and personal care products using predictive toxicology approaches. Green Chemistry, 2020, 22, 1458-1516.	4.6	86
48	Exploring QSAR modeling of toxicity of chemicals on earthworm. Ecotoxicology and Environmental Safety, 2020, 190, 110067.	2.9	25
49	Exploring 2D-QSAR for prediction of beta-secretase 1 (BACE1) inhibitory activity against Alzheimerâ€™s disease. SAR and QSAR in Environmental Research, 2020, 31, 87-133.	1.0	21
50	First report on a classification-based QSAR model for chemical toxicity to earthworm. Journal of Hazardous Materials, 2020, 386, 121660.	6.5	29
51	QSAR modeling of algal low level toxicity values of different phenol and aniline derivatives using 2D descriptors. Aquatic Toxicology, 2020, 228, 105627.	1.9	18
52	QSAR modeling of PET imaging agents for the diagnosis of Parkinsonâ€™s disease targeting dopamine receptor. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	7
53	In silico modeling for dual inhibition of acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE) enzymes in Alzheimerâ€™s disease. Computational Biology and Chemistry, 2020, 88, 107355.	1.1	31
54	Development of a simple, interpretable and easily transferable QSAR model for quick screening antiviral databases in search of novel 3C-like protease (3CLpro) enzyme inhibitors against SARS-CoV diseases. SAR and QSAR in Environmental Research, 2020, 31, 511-526.	1.0	54

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55	QSAR modeling with ETA indices for cytotoxicity and enzymatic activity of diverse chemicals. Journal of Hazardous Materials, 2020, 394, 122498.	6.5	12
56	Exploring QSAR models for assessment of acute fish toxicity of environmental transformation products of pesticides (ETPPs). Chemosphere, 2020, 252, 126508.	4.2	32
57	Cheminformatic modelling of Î²-amyloid aggregation inhibitory activity against Alzheimer's disease. Computers in Biology and Medicine, 2020, 118, 103658.	3.9	5
58	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
59	Ecotoxicological QSARs of Personal Care Products and Biocides. Methods in Pharmacology and Toxicology, 2020, , 357-386.	0.1	5
60	Ecotoxicological QSARs of Mixtures. Methods in Pharmacology and Toxicology, 2020, , 437-475.	0.1	4
61	A Brief Introduction to Quantitative Structure-Activity Relationships as Useful Tools in Predictive Ecotoxicology. Methods in Pharmacology and Toxicology, 2020, , 27-53.	0.1	5
62	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
63	Chemometric modeling of PET imaging agents for diagnosis of Parkinsonâ€™s disease: a QSAR approach. Structural Chemistry, 2020, 31, 1969-1981.	1.0	2
64	In silico modeling of small molecule carboxamides as inhibitors of SARS-CoV 3CL protease: An approach towards combating COVID-19. Combinatorial Chemistry and High Throughput Screening, 2020, 23, .	0.6	6
65	A Multi-layered Variable Selection Strategy for QSAR Modeling of Butyrylcholinesterase Inhibitors. Current Topics in Medicinal Chemistry, 2020, 20, 1601-1627.	1.0	20
66	QSPR Modeling of Adsorption of Pollutants by Carbon Nanotubes (CNTs). Methods in Pharmacology and Toxicology, 2020, , 477-511.	0.1	0
67	Ecotoxicological QSAR modelling of organic chemicals against Pseudokirchneriella subcapitata using consensus predictions approach. SAR and QSAR in Environmental Research, 2019, 30, 665-681.	1.0	25
68	New Workflow for QSAR Model Development from Small Data Sets: Small Dataset Curator and Small Dataset Modeler. Integration of Data Curation, Exhaustive Double Cross-Validation, and a Set of Optimal Model Selection Techniques. Journal of Chemical Information and Modeling, 2019, 59, 4070-4076.	2.5	46
69	Predictive quantitative structureâ€“property relationship (QSPR) modeling for adsorption of organic pollutants by carbon nanotubes (CNTs). Environmental Science: Nano, 2019, 6, 224-247.	2.2	23
70	Application of multilayered strategy for variable selection in QSAR modeling of PET and SPECT imaging agents as diagnostic agents for Alzheimerâ€™s disease. Structural Chemistry, 2019, 30, 2429-2445.	1.0	9
71	Consensus QSPR modelling for the prediction of cellular response and fibrinogen adsorption to the surface of polymeric biomaterials. SAR and QSAR in Environmental Research, 2019, 30, 363-382.	1.0	4
72	Ecotoxicological QSAR modeling of organic compounds against fish: Application of fragment based descriptors in feature analysis. Aquatic Toxicology, 2019, 212, 162-174.	1.9	39

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73	QSAR modeling of Daphnia magna and fish toxicities of biocides using 2D descriptors. Chemosphere, 2019, 229, 8-17.	4.2	71
74	Exploring QSPR modeling for adsorption of hazardous synthetic organic chemicals (SOCs) by SWCNTs. Chemosphere, 2019, 228, 545-555.	4.2	18
75	Exploration of synthetic antioxidant flavonoid analogs as acetylcholinesterase inhibitors: an approach towards finding their quantitative structureâ€“activity relationship. Medicinal Chemistry Research, 2019, 28, 723-741.	1.1	23
76	Risk assessment of heterogeneous TiO₂-based engineered nanoparticles (NPs): a QSTR approach using simple periodic table based descriptors. Nanotoxicology, 2019, 13, 701-716.	1.6	20
77	Ecotoxicological QSAR modeling of endocrine disruptor chemicals. Journal of Hazardous Materials, 2019, 369, 707-718.	6.5	54
78	Chemometric modeling of Daphnia magna toxicity of agrochemicals. Chemosphere, 2019, 224, 470-479.	4.2	37
79	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
80	Toward comprehension of multiple human cells uptake of engineered nano metal oxides: quantitative inter cell line uptake specificity (QICLUS) modeling. Nanotoxicology, 2019, 13, 14-34.	1.6	23
81	Consensus QSAR modeling of toxicity of pharmaceuticals to different aquatic organisms: Ranking and prioritization of the DrugBank database compounds. Ecotoxicology and Environmental Safety, 2019, 168, 287-297.	2.9	93
82	Design of antimalarial transmission blocking agents: Pharmacophore mapping of ligands active against stage-V mature gametocytes of Plasmodium falciparum. Journal of Biomolecular Structure and Dynamics, 2019, 37, 3660-3673.	2.0	3
83	Identifying natural compounds as multi-target-directed ligands against Alzheimerâ€™s disease: an in silico approach. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1282-1306.	2.0	60
84	Computational Approaches as Rational Decision Support Systems for Discovering Next-Generation Antitubercular Agents: Mini-Review. Current Computer-Aided Drug Design, 2019, 15, 369-383.	0.8	1
85	On Error Measures for Validation and Uncertainty Estimation of Predictive QSAR Models. , 2019, , 437-493.		1
86	Greener chemicals for the future: QSAR modelling of the PBT index using ETA descriptors. SAR and QSAR in Environmental Research, 2018, 29, 319-337.	1.0	12
87	Chemometric modeling of odor threshold property of diverse aroma components of wine. RSC Advances, 2018, 8, 4750-4760.	1.7	12
88	Chemometric modeling of larvicidal activity of plant derived compounds against zika virus vectorAedes aegypti: application of ETA indices. RSC Advances, 2018, 8, 4662-4670.	1.7	23
89	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
90	PLS regression-based chemometric modeling of odorant properties of diverse chemical constituents of black tea and coffee. RSC Advances, 2018, 8, 2293-2304.	1.7	14

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91	Development of a robust and validated 2D-QSPR model for sweetness potency of diverse functional organic molecules. Food and Chemical Toxicology, 2018, 112, 551-562.	1.8	39
92	Molecular dynamics simulation study reveals polar nature of pathogenic mutations responsible for stabilizing active conformation of kinase domain in leucine-rich repeat kinase II. Structural Chemistry, 2018, 29, 657-666.	1.0	8
93	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
94	QSPR modelling for prediction of glass transition temperature of diverse polymers. SAR and QSAR in Environmental Research, 2018, 29, 935-956.	1.0	18
95	Chemometric modeling of aquatic toxicity of contaminants of emerging concern (CECs) in Dugesia japonica and its interspecies correlation with daphnia and fish: QSTR and QSTTR approaches. Ecotoxicology and Environmental Safety, 2018, 166, 92-101.	2.9	47
96	QSPR Modeling of the Refractive Index for Diverse Polymers Using 2D Descriptors. ACS Omega, 2018, 3, 13374-13386.	1.6	36
97	Current approaches for choosing feature selection and learning algorithms in quantitative structureâ€“activity relationships (QSAR). Expert Opinion on Drug Discovery, 2018, 13, 1075-1089.	2.5	83
98	How Precise Are Our Quantitative Structureâ€“Activity Relationship Derived Predictions for New Query Chemicals?. ACS Omega, 2018, 3, 11392-11406.	1.6	88
99	Impact of Pharmaceuticals on the Environment: Risk Assessment Using QSAR Modeling Approach. Methods in Molecular Biology, 2018, 1800, 395-443.	0.4	32
100	Applicability Domain: A Step Toward Confident Predictions and Decidability for QSAR Modeling. Methods in Molecular Biology, 2018, 1800, 141-169.	0.4	61
101	Molecular diversity: at a crossroads. Molecular Diversity, 2018, 22, 543-543.	2.1	0
102	A Comparative Study on Selective PPAR Modulators through Quantitative Structure-activity Relationship, Pharmacophore and Docking Analyses. Current Computer-Aided Drug Design, 2018, 14, 54-67.	0.8	2
103	QSPR/QSAR-based Perturbation Theory approach and mechanistic electrochemical assays on carbon nanotubes with optimal properties against mitochondrial Fenton reaction experimentally induced by Fe2+-overload. Carbon, 2017, 115, 312-330.	5.4	11
104	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
105	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
106	Development of a temperature dependent 2D-QSPR model for viscosity of diverse functional ionic liquids. Journal of Molecular Liquids, 2017, 240, 454-467.	2.3	18
107	Exploring the structural requirements in multiple chemical scaffolds for the selective inhibition of Plasmodium falciparum calcium-dependent protein kinase-1 (PfCDPK-1) by 3D-pharmacophore modelling, and docking studies. SAR and QSAR in Environmental Research, 2017, 28, 390-414.	1.0	20
108	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

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109	Ecotoxicological modelling of cosmetics for aquatic organisms: A QSTR approach. SAR and QSAR in Environmental Research, 2017, 28, 567-594.	1.0	32
110	Structural exploration of PPARÎ³ modulators through pharmacophore mapping, fragment-based design, docking, and molecular dynamics simulation analyses. Medicinal Chemistry Research, 2017, 26, 52-63.	1.1	2
111	Multilayered Variable Selection in QSPR. International Journal of Quantitative Structure-Property Relationships, 2017, 2, 106-124.	1.1	10
112	CADD Modeling of Multi-Target Drugs Against Alzheimer's Disease. Current Drug Targets, 2017, 18, 522-533.	1.0	17
113	The â€œETAâ€•Indices in QSAR/QSPR/QSTR Research. , 2017, , 978-1011.		5
114	Importance of Applicability Domain of QSAR Models. , 2017, , 1012-1043.		1
115	Can Toxicity for Different Species be Correlated?. International Journal of Quantitative Structure-Property Relationships, 2016, 1, 23-51.	1.1	20
116	Understanding the structural requirements of cyclic sulfone hydroxyethylamines as hBACE1 inhibitors against AÎ² plaques in Alzheimer's disease: a predictive QSAR approach. RSC Advances, 2016, 6, 28171-28186.	1.7	29
117	Exploring structural requirements for the inhibition of Plasmodium falciparum calcium-dependent protein kinase-4 (PfCDPK-4) using multiple in silico approaches. RSC Advances, 2016, 6, 51957-51982.	1.7	9
118	Development of predictive QSAR models for Vibrio fischeri toxicity of ionic liquids and their true external and experimental validation tests. Toxicology Research, 2016, 5, 1388-1399.	0.9	33
119	The â€œdouble cross-validationâ€•software tool for MLR QSAR model development. Chemometrics and Intelligent Laboratory Systems, 2016, 159, 108-126.	1.8	72
120	In Silico Models for Ecotoxicity of Pharmaceuticals. Methods in Molecular Biology, 2016, 1425, 237-304.	0.4	15
121	Be aware of error measures. Further studies on validation of predictive QSAR models. Chemometrics and Intelligent Laboratory Systems, 2016, 152, 18-33.	1.8	536
122	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
123	Pharmacophore generation, atom-based 3D-QSAR, HQSAR and activity cliff analyses of benzothiazine and deazaxanthine derivatives as dual A2Aantagonists/MAOâ€‘B inhibitors. SAR and QSAR in Environmental Research, 2016, 27, 183-202.	1.0	19
124	Computation of chromatographic lipophilicity parameter logk0 of ionic liquid cations from â€œETAâ€• descriptors: Application in modeling of toxicity of ionic liquids to pathogenic bacteria. Journal of Molecular Liquids, 2016, 216, 754-763.	2.3	16
125	Scoring Functions in Docking Experiments. Advances in Medical Technologies and Clinical Practice Book Series, 2016, , 54-98.	0.3	2
126	Development of Energy-based Pharmacophore Model and Stepwise Virtual Screening of LRRK2 Inhibitors Through Molecular Dynamics and Mechanics. Letters in Drug Design and Discovery, 2015, 13, 24-32.	0.4	2

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127	Editorial (Thematic Issue: Application of Chemometrics and Cheminformatics in Antimalarial Drug) Tj ETQq1 1 0.784314 rgBT /Overlock	0.6	4
128	Exploring molecular fingerprints of selective PPARÎ´ agonists through comparative and validated chemometric techniques. SAR and QSAR in Environmental Research, 2015, 26, 363-382.	1.0	2
129	QSAR/QSPR Modeling: Introduction. Springer Briefs in Molecular Science, 2015, , 1-36.	0.1	20
130	In vitro evaluation and in silico screening of synthetic acetylcholinesterase inhibitors bearing functionalized piperidine pharmacophores. Bioorganic and Medicinal Chemistry, 2015, 23, 4567-4575.	1.4	50
131	A Primer on QSAR/QSPR Modeling. Springer Briefs in Molecular Science, 2015, , .	0.1	197
132	Interspecies quantitative structureâ€“toxicityâ€“toxicity (QSTTR) relationship modeling of ionic liquids. Toxicity of ionic liquids to V. fischeri, D. magna and S. vacuolatus. Ecotoxicology and Environmental Safety, 2015, 122, 497-520.	2.9	32
133	Exploring simple, transparent, interpretable and predictive QSAR models for classification and quantitative prediction of rat toxicity of ionic liquids using OECD recommended guidelines. Chemosphere, 2015, 139, 163-173.	4.2	25
134	â€œNanoBRIDGESâ€•software: Open access tools to perform QSAR and nano-QSAR modeling. Chemometrics and Intelligent Laboratory Systems, 2015, 147, 1-13.	1.8	129
135	On a simple approach for determining applicability domain of QSAR models. Chemometrics and Intelligent Laboratory Systems, 2015, 145, 22-29.	1.8	534
136	Newer QSAR Techniques. , 2015, , 319-356.		7
137	Future Avenues. , 2015, , 455-462.		3
138	Topological QSAR. , 2015, , 103-149.		0
139	Chemical Information and Descriptors. , 2015, , 47-80.		15
140	Selected Statistical Methods in QSAR. , 2015, , 191-229.		22
141	Validation of QSAR Models. , 2015, , 231-289.		36
142	Background of QSAR and Historical Developments. , 2015, , 1-46.		21
143	Classical QSAR. , 2015, , 81-102.		5
144	First report on exploring classification and regression based QSAR modelling ofPlasmodium falciparumglycogen synthase kinase (PfGSK-3) inhibitors. SAR and QSAR in Environmental Research, 2015, 26, 959-976.	1.0	9

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145	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
146	Cytotoxicity towards CCO cells of imidazolium ionic liquids with functionalized side chains: Preliminary QSTR modeling using regression and classification based approaches. Ecotoxicology and Environmental Safety, 2015, 112, 22-28.	2.9	37
147	Predictive QSAR modelling of algal toxicity of ionic liquids and its interspecies correlation with Daphnia toxicity. Environmental Science and Pollution Research, 2015, 22, 6634-6641.	2.7	41
148	Statistical Methods in QSAR/QSPR. Springer Briefs in Molecular Science, 2015, , 37-59.	0.1	75
149	Application of GFA-MLR and G/PLS Techniques in QSAR/QSPR Studies with Application in Medicinal Chemistry and Predictive Toxicology. , 2015, , 501-529.		1
150	Understanding the Structural Requirements in Diverse Scaffolds for the Inhibition of P. falciparum Dihydroorotate Dehydrogenase (PfDHODH) Using 2D-QSAR, 3D-Pharmacophore and Structure-Based Energy- Optimized Pharmacophore Models. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 217-226.	0.6	4
151	The Current Status of Antimalarial Drug Research with Special Reference to Application of QSAR Models. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 91-128.	0.6	10
152	Exploring Structural Requirements of Imaging Agents Against AÎ² Plaques in Alzheimerâ€™s Disease: A QSAR Approach. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 411-419.	0.6	7
153	In silico Modeling of Antimalarial Protein Kinase Inhibitors. Letters in Drug Design and Discovery, 2015, 13, 129-134.	0.4	2
154	The â€œETAâ€•Indices in QSAR/QSPR/QSTR Research. Advances in Chemical and Materials Engineering Book Series, 2015, , 48-83.	0.2	6
155	Importance of Applicability Domain of QSAR Models. Advances in Chemical and Materials Engineering Book Series, 2015, , 180-211.	0.2	11
156	QSAR/QSPR Methods. Springer Briefs in Molecular Science, 2015, , 61-103.	0.1	0
157	Cytotoxic and Antioxidant Activity of a Set of Hetero Bicylic Methylthiadiazole Hydrazones: A Structure-Activity Study. International Journal of Molecular and Cellular Medicine, 2015, 4, 128-37.	1.1	7
158	QSPR Modeling of Odor Threshold of Aliphatic Alcohols Using Extended Topochemical Atom (ETA) Indices. Croatica Chemica Acta, 2014, 87, 29-37.	0.1	9
159	Chemometric modelling of triphenylmethyl derivatives as potent anticancer agents. Molecular Simulation, 2014, 40, 1218-1235.	0.9	1
160	Chemometric modeling of the chromatographic lipophilicity parameter logk0 of ionic liquid cations with ETA and QTMS descriptors. Journal of Molecular Liquids, 2014, 200, 223-228.	2.3	11
161	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
162	Exploring structural requirement, pharmacophore modeling, and de novo design of LRRK2 inhibitors using homology modeling approach. Medicinal Chemistry Research, 2014, 23, 3705-3713.	1.1	7

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163	Modeling bioconcentration factor (BCF) using mechanistically interpretable descriptors computed from open source tool â€œPaDEL-Descriptorâ€. Environmental Science and Pollution Research, 2014, 21, 2955-2965.	2.7	22
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