Emilio Benfenati

List of Publications by Year
in descending order

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506 papers	14,495 citations	31976 53 h-index	45317 90 g-index
536 all docs	536 docs citations	536 times ranked	9674 citing authors

#	Article	IF	Citations
1	CAESAR models for developmental toxicity. Chemistry Central Journal, 2010, 4, S4.	2.6	1,099
2	Alternative (non-animal) methods for cosmetics testing: current status and future prospectsâ€”2010. Archives of Toxicology, 2011, 85, 367-485.	4.2	488
3	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	6.0	264
4	Guidance on the use of the weight of evidence approach in scientific assessments. EFSA Journal, 2017, 15, e04971.	1.8	221
5	Guidance on harmonised methodologies for human health, animal health and ecological risk assessment of combined exposure to multiple chemicals. EFSA Journal, 2019, 17, e05634.	1.8	201
6	Genotoxicity of metal oxide nanomaterials: review of recent data and discussion of possible mechanisms. Nanoscale, 2015, 7, 2154-2198.	5.6	163
7	Green Chemistry in the Synthesis of Pharmaceuticals. Chemical Reviews, 2022, 122, 3637-3710.	47.7	155
8	A European perspective on alternatives to animal testing for environmental hazard identification and risk assessment. Regulatory Toxicology and Pharmacology, 2013, 67, 506-530.	2.7	139
9	QSAR as a random event: Modeling of nanoparticles uptake in PaCa2 cancer cells. Chemosphere, 2013, 92, 31-37.	8.2	133
10	A combined approach to investigate the toxicity of an industrial landfillâ€™s leachate: Chemical analyses, risk assessment and in vitro assays. Environmental Research, 2011, 111, 603-613.	7.5	126
11	Automatic knowledge extraction from chemical structures: the case of mutagenicity prediction. SAR and QSAR in Environmental Research, 2013, 24, 365-383.	2.2	121
12	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
13	Determination of aromatic amines by solid-phase microextraction and gas chromatographyâ€“mass spectrometry in water samples. Journal of Chromatography A, 1997, 791, 221-230.	3.7	113
14	In vivo exposure of carp to graded concentrations of bisphenol A. General and Comparative Endocrinology, 2007, 153, 15-24.	1.8	111
15	Interpretation of Quantitative Structureâ^'Property and â^'Activity Relationships. Journal of Chemical Information and Computer Sciences, 2001, 41, 679-685.	2.8	110
16	Androgenic and antiandrogenic activities in water and sediment samples from the river Lambro, Italy, detected by yeast androgen screen and chemical analyses. Chemosphere, 2007, 67, 1080-1087.	8.2	106
17	New public QSAR model for carcinogenicity. Chemistry Central Journal, 2010, 4, S3.	2.6	105
18	Exposure to PFOA and PFOS and fetal growth: a critical merging of toxicological and epidemiological data. Critical Reviews in Toxicology, 2017, 47, 489-515.	3.9	104

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19	The Expanding Role of Predictive Toxicology: An Update on the (Q)SAR Models for Mutagens and Carcinogens. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2007, 25, 53-97.	2.9	103
20	Predictive Models for Carcinogenicity and Mutagenicity: Frameworks, State-of-the-Art, and Perspectives. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2009, 27, 57-90.	2.9	99
21	Computational predictive programs (expert systems) in toxicology. Toxicology, 1997, 119, 213-225.	4.2	97
22	Novel application of the CORAL software to model cytotoxicity of metal oxide nanoparticles to bacteria Escherichia coli. Chemosphere, 2012, 89, 1098-1102.	8.2	96
23	Investigating landfill leachate toxicity in vitro: A review of cell models and endpoints. Environment International, 2019, 122, 21-30.	10.0	96
24	Predicting logP of pesticides using different software. Chemosphere, 2003, 53, 1155-1164.	8.2	94
25	CORAL: Quantitative structureâ€“activity relationship models for estimating toxicity of organic compounds in rats. Journal of Computational Chemistry, 2011, 32, 2727-2733.	3.3	94
26	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.	6.0	93
27	Improvement of quantitative structureâ€“activity relationship (QSAR) tools for predicting Ames mutagenicity: outcomes of the Ames/QSAR International Challenge Project. Mutagenesis, 2019, 34, 3-16.	2.6	93
28	A new hybrid system of QSAR models for predicting bioconcentration factors (BCF). Chemosphere, 2008, 73, 1701-1707.	8.2	92
29	Comparison ofin silicotools for evaluating rat oral acute toxicity. SAR and QSAR in Environmental Research, 2015, 26, 1-27.	2.2	87
30	Ecotoxicological assessment of pharmaceuticals and personal care products using predictive toxicology approaches. Green Chemistry, 2020, 22, 1458-1516.	9.0	86
31	Comparison of In Silico Models for Prediction of Mutagenicity. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2013, 31, 45-66.	2.9	84
32	Aquatic toxicity of several textile dye formulations: Acute and chronic assays with Daphnia magna and Raphidocelis subcapitata. Ecotoxicology and Environmental Safety, 2017, 144, 79-87.	6.0	84
33	Volatile organic compounds produced during the aerobic biological processing of municipal solid waste in a pilot plant. Chemosphere, 2005, 59, 423-430.	8.2	82
34	Screening of endocrine-disrupting phenols, herbicides, steroid estrogens, and estrogenicity in drinking water from the waterworks of 35 Italian cities and from PET-bottled mineral water. Environmental Science and Pollution Research, 2013, 20, 1649-1660.	5.3	82
35	Estrogenicity profile and estrogenic compounds determined in river sediments by chemical analysis, ELISA and yeast assays. Chemosphere, 2008, 73, 1078-1089.	8.2	77
36	A generalizable definition of chemical similarity for read-across. Journal of Cheminformatics, 2014, 6, 39.	6.1	75

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37	Analysis of some pesticides in water samples using solid-phase microextractionâ€“gas chromatography with different mass spectrometric techniques. Journal of Chromatography A, 1999, 859, 193-201.	3.7	74
38	In silico methods to predict drug toxicity. Current Opinion in Pharmacology, 2013, 13, 802-806.	3.5	72
39	Predictive Carcinogenicity:â€‰ A Model for Aromatic Compounds, with Nitrogen-Containing Substituents, Based on Molecular Descriptors Using an Artificial Neural Network. Journal of Chemical Information and Computer Sciences, 1999, 39, 1076-1080.	2.8	71
40	SAR and QSAR modeling of a large collection of LD50 rat acute oral toxicity data. Journal of Cheminformatics, 2019, 11, 58.	6.1	71
41	QSAR modeling of Daphnia magna and fish toxicities of biocides using 2D descriptors. Chemosphere, 2019, 229, 8-17.	8.2	71
42	REACH and in silico methods: an attractive opportunity for medicinal chemists. Drug Discovery Today, 2014, 19, 1757-1768.	6.4	70
43	Sterols in sediment samples from Venice Lagoon, Italy. Chemosphere, 1996, 33, 2383-2393.	8.2	68
44	Integrating in silico models and read-across methods for predicting toxicity of chemicals: A step-wise strategy. Environment International, 2019, 131, 105060.	10.0	68
45	Simultaneous analysis of 50 pesticides in water samples by solid phase extraction and GC-MS. Chemosphere, 1990, 21, 1411-1421.	8.2	66
46	Automated sample preparation with extraction columns followed by liquid chromatography-ionspray mass spectrometry interferences, determination and degradation of polar organophosphorus pesticides in water samples. Journal of Chromatography A, 1996, 737, 47-58.	3.7	65
47	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	6.0	63
48	QSAR Modeling of ToxCast Assays Relevant to the Molecular Initiating Events of AOPs Leading to Hepatic Steatosis. Journal of Chemical Information and Modeling, 2018, 58, 1501-1517.	5.4	61
49	Patterns and Sources of Polychlorinated Dibenzo-p-dioxins and Dibenzofurans in Sediments from the Venice Lagoon, Italy. Environmental Science & Technology, 1997, 31, 1777-1784.	10.0	58
50	Levels of PCDD/F and dioxin-like PCB in Baltic fish of different age and gender. Chemosphere, 2008, 71, 369-378.	8.2	57
51	CORAL: Building up the model for bioconcentration factor and defining itâ€™s applicability domain. European Journal of Medicinal Chemistry, 2011, 46, 1400-1403.	5.5	57
52	CORAL: QSAR modeling of toxicity of organic chemicals towards Daphnia magna. Chemometrics and Intelligent Laboratory Systems, 2012, 110, 177-181.	3.5	57
53	Evaluation of QSAR Models for the Prediction of Ames Genotoxicity: A Retrospective Exercise on the Chemical Substances Registered Under the EU REACH Regulation. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2014, 32, 273-298.	2.9	57
54	A new semi-automated workflow for chemical data retrieval and quality checking for modeling applications. Journal of Cheminformatics, 2018, 10, 60.	6.1	56

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55	Increased concentrations of nitrophenols in leaves from a damaged forestal site. Chemosphere, 1999, 38, 1495-1503.	8.2	54
56	Assessment and validation of the CAESAR predictive model for bioconcentration factor (BCF) in fish. Chemistry Central Journal, 2010, 4, S1.	2.6	54
57	ToxRead: A tool to assist in read across and its use to assess mutagenicity of chemicals. SAR and QSAR in Environmental Research, 2014, 25, 999-1011.	2.2	54
58	Investigating combined toxicity of binary mixtures in bees: Meta-analysis of laboratory tests, modelling, mechanistic basis and implications for risk assessment. Environment International, 2019, 133, 105256.	10.0	54
59	Ecotoxicological QSAR modeling of endocrine disruptor chemicals. Journal of Hazardous Materials, 2019, 369, 707-718.	12.4	54
60	Comparison of SMILES and molecular graphs as the representation of the molecular structure for QSAR analysis for mutagenic potential of polyaromatic amines. Chemometrics and Intelligent Laboratory Systems, 2011, 109, 94-100.	3.5	53
61	SMILES as an alternative to the graph in QSAR modelling of bee toxicity. Computational Biology and Chemistry, 2007, 31, 57-60.	2.3	52
62	PCDD/Fs and PCBs in ambient air in a highly industrialized city in Northern Italy. Chemosphere, 2013, 90, 2352-2357.	8.2	52
63	QSAR models for predicting acute toxicity of pesticides in rainbow trout using the CORAL software and EFSAâ€™s OpenFoodTox database. Environmental Toxicology and Pharmacology, 2017, 53, 158-163.	4.0	52
64	Description of the Electronic Structure of Organic Chemicals Using Semiempirical and Ab Initio Methods for Development of Toxicological QSARs. Journal of Chemical Information and Modeling, 2005, 45, 106-114.	5.4	51
65	Validation of counter propagation neural network models for predictive toxicology according to the OECD principles: a case study. SAR and QSAR in Environmental Research, 2006, 17, 265-284.	2.2	50
66	SMILES in QSPR/QSAR Modeling: Results and Perspectives. Current Drug Discovery Technologies, 2007, 4, 77-116.	1.2	50
67	Polychlorinated dibenzo-p-dioxins (PCDD) and polychlorinated dibenzofurans (PCDF) in emissions from an urban incineratop. 1. Average and peak values. Chemosphere, 1982, 11, 577-583.	8.2	49
68	Investigating the Estrogenic Risk Along the River Po and Its Intermediate Section. Archives of Environmental Contamination and Toxicology, 2006, 51, 641-651.	4.1	49
69	Predicting acute contact toxicity of pesticides in honeybees (Apis mellifera) through a k-nearest neighbor model. Chemosphere, 2017, 166, 438-444.	8.2	49
70	Towards a systematic use of effect biomarkers in population and occupational biomonitoring. Environment International, 2021, 146, 106257.	10.0	48
71	Internationalization of read-across as a validated new approach method (NAM) for regulatory toxicology. ALTEX: Alternatives To Animal Experimentation, 2020, 37, 579-606.	1.5	48
72	SMILESâ€based optimal descriptors: QSAR analysis of fullereneâ€based HIVâ€1 PR inhibitors by means of balance of correlations. Journal of Computational Chemistry, 2010, 31, 381-392.	3.3	47

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73	In silico models for predicting ready biodegradability under REACH: A comparative study. Science of the Total Environment, 2013, 463-464, 161-168.	8.0	47
74	Modeling Toxicity by Using Supervised Kohonen Neural Networks. Journal of Chemical Information and Computer Sciences, 2003, 43, 485-492.	2.8	46
75	Additive SMILES-based optimal descriptors in QSAR modelling bee toxicity: Using rare SMILES attributes to define the applicability domain. Bioorganic and Medicinal Chemistry, 2008, 16, 4801-4809.	3.0	46
76	QSAR modeling of measured binding affinity for fullerene-based HIV-1 PR inhibitors by CORAL. Journal of Mathematical Chemistry, 2010, 48, 959-987.	1.5	46
77	Acute phytotoxicity of seven metals alone and in mixture: Are Italian soil threshold concentrations suitable for plant protection?. Environmental Research, 2015, 140, 102-111.	7.5	46
78	â€œDe novoâ€•synthesis of PCDD, PCDF, PCB, PCN and PAH in a pilot incinerator. Chemosphere, 1991, 22, 1045-1052.	8.2	45
79	Comparative studies of the leachate of an industrial landfill by gas chromatographyâ€“mass spectrometry, liquid chromatographyâ€“nuclear magnetic resonance and liquid chromatographyâ€“mass spectrometry. Journal of Chromatography A, 1999, 831, 243-256.	3.7	45
80	Meta-analysis of toxicity and teratogenicity of 133 chemicals from zebrafish developmental toxicity studies. Reproductive Toxicology, 2013, 41, 98-108.	2.9	45
81	Structures of Endocrine-Disrupting Chemicals Determine Binding to and Activation of the Estrogen Receptor Î± and Androgen Receptor. Environmental Science & Technology, 2020, 54, 11424-11433.	10.0	45
82	QSAR Model for Predicting Pesticide Aquatic Toxicity. Journal of Chemical Information and Modeling, 2005, 45, 1767-1774.	5.4	44
83	The acceptance of in silicomodels for REACH: Requirements, barriers, and perspectives. Chemistry Central Journal, 2011, 5, 58.	2.6	44
84	GCâ€“MS analysis of dichlobenil and its metabolites in groundwater. Talanta, 2005, 68, 146-154.	5.5	43
85	Binary classification models for endocrine disrupter effects mediated through the estrogen receptor. SAR and QSAR in Environmental Research, 2008, 19, 697-733.	2.2	43
86	SMILES-based optimal descriptors: QSAR modeling of carcinogenicity by balance of correlations with ideal slopes. European Journal of Medicinal Chemistry, 2010, 45, 3581-3587.	5.5	42
87	A comparative survey of chemistry-driven in silico methods to identify hazardous substances under REACH. Regulatory Toxicology and Pharmacology, 2013, 66, 301-314.	2.7	42
88	Individual breast milk consumption and exposure to PCBs and PCDD/Fs in Hungarian infants: A time-course analysis of the first three months of lactation. Science of the Total Environment, 2013, 449, 336-344.	8.0	42
89	Evaluation and comparison of benchmark QSAR models to predict a relevant REACH endpoint: The bioconcentration factor (BCF). Environmental Research, 2015, 137, 398-409.	7.5	42
90	The Importance of Scaling in Data Mining for Toxicity Prediction. Journal of Chemical Information and Computer Sciences, 2002, 42, 1250-1255.	2.8	41

#	Article	IF	Citations
91	Quantitative consensus of bioaccumulation models for integrated testing strategies. Environment International, 2012, 45, 51-58.	10.0	41
92	Optimal nano-descriptors as translators of eclectic data into prediction of the cell membrane damage by means of nano metal-oxides. Environmental Science and Pollution Research, 2015, 22, 745-757.	5.3	41
93	An alternative QSAR-based approach for predicting the bioconcentration factor for regulatory purposes. ALTEX: Alternatives To Animal Experimentation, 2014, 31, 23-36.	1.5	41
94	Comparison of genistein metabolism in rats and humans using liver microsomes and hepatocytes. Food and Chemical Toxicology, 2008, 46, 939-948.	3.6	40
95	Comparison ofin silicomodels for prediction ofDaphnia magnaacute toxicity. SAR and QSAR in Environmental Research, 2014, 25, 673-694.	2.2	40
96	QSAR model for predicting cell viability of human embryonic kidney cells exposed to SiO2 nanoparticles. Chemosphere, 2016, 144, 995-1001.	8.2	40
97	Nano-QSAR: Model of mutagenicity of fullerene as a mathematical function of different conditions. Ecotoxicology and Environmental Safety, 2016, 124, 32-36.	6.0	40
98	QSAR in Ecotoxicity:â€‰ An Overview of Modern Classification Techniques. Journal of Chemical Information and Computer Sciences, 2004, 44, 105-112.	2.8	39
99	QSAR models for Daphnia toxicity of pesticides based on combinations of topological parameters of molecular structures. Bioorganic and Medicinal Chemistry, 2006, 14, 2779-2788.	3.0	39
100	Additive SMILES-Based Carcinogenicity Models: Probabilistic Principles in the Search for Robust Predictions. International Journal of Molecular Sciences, 2009, 10, 3106-3127.	4.1	39
101	Co-evolutions of correlations for QSAR of toxicity of organometallic and inorganic substances: An unexpected good prediction based on a model that seems untrustworthy. Chemometrics and Intelligent Laboratory Systems, 2011, 105, 215-219.	3.5	39
102	Integrating in silico models to enhance predictivity for developmental toxicity. Toxicology, 2016, 370, 127-137.	4.2	39
103	Ecotoxicological QSAR modeling of organic compounds against fish: Application of fragment based descriptors in feature analysis. Aquatic Toxicology, 2019, 212, 162-174.	4.0	39
104	PCDD, PCDF, PCB, PAH, cadmium and lead in roadside soil: relationship between road distance and concentration. Chemosphere, 1992, 24, 1077-1083.	8.2	38
105	Predicting acute contact toxicity of organic binary mixtures in honey bees (A. mellifera) through innovative QSAR models. Science of the Total Environment, 2020, 704, 135302.	8.0	38
106	Screening of 21 pesticides in water by single extraction with C18 silica bonded phase columns and HRGC-MS. Chemosphere, 1988, 17, 59-65.	8.2	37
107	Chemometric modeling of Daphnia magna toxicity of agrochemicals. Chemosphere, 2019, 224, 470-479.	8.2	37
108	Physicochemical and Analytical Characteristics ofAmiodarone. Journal of Pharmaceutical Sciences, 1984, 73, 829-831.	3.3	36

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109	Additive InChI-based optimal descriptors: QSPR modeling of fullerene C 60 solubility in organic solvents. Journal of Mathematical Chemistry, 2009, 46, 1232-1251.	1.5	36
110	<scp>coral</scp> Software: QSAR for Anticancer Agents. Chemical Biology and Drug Design, 2011, 77, 471-476.	3.2	36
111	QSAR model as a random event: A case of rat toxicity. Bioorganic and Medicinal Chemistry, 2015, 23, 1223-1230.	3.0	36
112	VOC exposures in California early childhood education environments. Indoor Air, 2017, 27, 609-621.	4.3	36
113	EFSAâ€™s OpenFoodTox: An open source toxicological database on chemicals in food and feed and its future developments. Environment International, 2021, 146, 106293.	10.0	36
114	Combining Unsupervised and Supervised Artificial Neural Networks to PredictAquatic Toxicity. Journal of Chemical Information and Computer Sciences, 2004, 44, 1897-1902.	2.8	35
115	Directions in QSAR Modeling for Regulatory Uses in OECD Member Countries, EU and in Russia. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2008, 26, 201-236.	2.9	35
116	The ToxBank Data Warehouse: Supporting the Replacement of In Vivo Repeated Dose Systemic Toxicity Testing. Molecular Informatics, 2013, 32, 47-63.	2.5	35
117	Identification of structural alerts for liver and kidney toxicity using repeated dose toxicity data. Chemistry Central Journal, 2015, 9, 62.	2.6	35
118	Homology Modeling of the Human P-glycoprotein (ABCB1) and Insights into Ligand Binding through Molecular Docking Studies. International Journal of Molecular Sciences, 2020, 21, 4058.	4.1	35
119	Guidance Document on Scientific criteria for grouping chemicals into assessment groups for human risk assessment of combined exposure to multiple chemicals. EFSA Journal, 2021, 19, e07033.	1.8	35
120	CORAL: QSPR model of water solubility based on local and global SMILES attributes. Chemosphere, 2013, 90, 877-880.	8.2	34
121	A new in silico classification model for ready biodegradability, based on molecular fragments. Chemosphere, 2014, 108, 10-16.	8.2	34
122	In silico-aided prediction of biological properties of chemicals: oestrogen receptor-mediated effects. Chemical Society Reviews, 2008, 37, 441-450.	38.1	33
123	The application of new HARD-descriptor available from the CORAL software to building up NOAEL models. Food and Chemical Toxicology, 2018, 112, 544-550.	3.6	33
124	Safer chemicals using less animals: kick-off of the European ONTOX project. Toxicology, 2021, 458, 152846.	4.2	33
125	Factors Influencing Predictive Models for Toxicology. SAR and QSAR in Environmental Research, 2001, 12, 593-603.	2.2	32
126	PCDD/Fs in ambient air in north-east Italy: The role of a MSWI inside an industrial area. Chemosphere, 2009, 77, 1224-1229.	8.2	32

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127	Comparing In Vivo, In Vitro and In Silico Methods and Integrated Strategies for Chemical Assessment: Problems and Prospects. ATLA Alternatives To Laboratory Animals, 2010, 38, 153-166.	1.0	32
128	Chemical characterization and ecotoxicity of three soil foaming agents used in mechanized tunneling. Journal of Hazardous Materials, 2015, 296, 210-220.	12.4	32
129	Integrated in silico strategy for PBT assessment and prioritization under REACH. Environmental Research, 2016, 151, 478-492.	7.5	32
130	A POLARIZATION FLUORESCENCE IMMUNOASSAY FOR THE HERBICIDE PROPANIL. Analytical Letters, 2001, 34, 2285-2301.	1.8	31
131	The proposal of architecture for chemical splitting to optimize QSAR models for aquatic toxicity. Chemosphere, 2008, 72, 772-780.	8.2	31
132	CORAL: QSPR models for solubility of [C60] and [C70] fullerene derivatives. Molecular Diversity, 2011, 15, 249-256.	3.9	31
133	Predicting persistence in the sediment compartment with a new automatic software based on the k-Nearest Neighbor (k-NN) algorithm. Chemosphere, 2016, 144, 1624-1630.	8.2	31
134	Involvement of a serine protease in the synthesis of platelet-activating factor by endothelial cells stimulated by tumor necrosis factor-Î± or interleukin-1Î±. European Journal of Immunology, 1994, 24, 3131-3139.	2.9	30
135	Metabolites of Alachlor in Water:Â Identification by Mass Spectrometry and Chemical Synthesis. Environmental Science & Technology, 1997, 31, 3637-3646.	10.0	30
136	Comparative Quantitative Structureâ€“Activityâ€“Activity Relationships for Toxicity to Tetrahymena pyriformis and Pimephales promelas. ATLA Alternatives To Laboratory Animals, 2007, 35, 15-24.	1.0	30
137	QSPR modeling for enthalpies of formation of organometallic compounds by means of SMILES-based optimal descriptors. Chemical Physics Letters, 2008, 461, 343-347.	2.6	30
138	Coral: QSPR modeling of rate constants of reactions between organic aromatic pollutants and hydroxyl radical. Journal of Computational Chemistry, 2012, 33, 1902-1906.	3.3	30
139	Docking-based classification models for exploratory toxicology studies on high-quality estrogenic experimental data. Future Medicinal Chemistry, 2015, 7, 1921-1936.	2.3	30
140	In Silico Models for Repeated-Dose Toxicity (RDT): Prediction of the No Observed Adverse Effect Level (NOAEL) and Lowest Observed Adverse Effect Level (LOAEL) for Drugs. Methods in Molecular Biology, 2016, 1425, 163-176.	0.9	30
141	Phytotoxicity of wear debris from traditional and innovative brake pads. Environment International, 2019, 123, 156-163.	10.0	30
142	EVALUATION OF SOLID PHASE MICROEXTRACTIONâ€“GAS CHROMATOGRAPHY IN THE ANALYSIS OF SOME PESTICIDES WITH DIFFERENT MASS SPECTROMETRIC TECHNIQUES: APPLICATION TO ENVIRONMENTAL WATERS AND FOOD SAMPLES. Analytical Letters, 2002, 35, 327-338.	1.8	29
143	Accelerated solvent extraction then liquid chromatography coupled with mass spectrometry for determination of 4-t-octylphenol, 4-nonylphenols, and bisphenol A in fish liver. Chromatographia, 2002, 56, 463-467.	1.3	29
144	Emerging organic contaminants in leachates from industrial waste landfills and industrial effluent. TrAC - Trends in Analytical Chemistry, 2003, 22, 757-765.	11.4	29

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145	Classification of Potential Endocrine Disrupters on the Basis of Molecular Structure Using a Nonlinear Modeling Methodâ€. Journal of Chemical Information and Computer Sciences, 2004, 44, 300-309.	2.8	29
146	QSPR modeling bioconcentration factor (BCF) by balance of correlations. European Journal of Medicinal Chemistry, 2009, 44, 2544-2551.	5.5	29
147	InChI-based optimal descriptors: QSAR analysis of fullerene[C60]-based HIV-1 PR inhibitors by correlation balance. European Journal of Medicinal Chemistry, 2010, 45, 1387-1394.	5.5	29
148	A new bioconcentration factor model based on SMILES and indices of presence of atoms. European Journal of Medicinal Chemistry, 2010, 45, 4399-4402.	5.5	29
149	QSAR modeling of endpoints for peptides which is based on representation of the molecular structure by a sequence of amino acids. Structural Chemistry, 2012, 23, 1891-1904.	2.0	29
150	First report on a classification-based QSAR model for chemical toxicity to earthworm. Journal of Hazardous Materials, 2020, 386, 121660.	12.4	29
151	Tuning Neural and Fuzzy-Neural Networks for Toxicity Modeling. Journal of Chemical Information and Computer Sciences, 2003, 43, 513-518.	2.8	28
152	QSAR modelling of aldehyde toxicity by means of optimisation of correlation weights of nearest neighbouring codes. Computational and Theoretical Chemistry, 2004, 676, 165-169.	1.5	28
153	A QSAR Study of Avian Oral Toxicity using Support Vector Machines and Genetic Algorithms. QSAR and Combinatorial Science, 2006, 25, 616-628.	1.4	28
154	QSAR models of quail dietary toxicity based on the graph of atomic orbitals. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 1941-1943.	2.2	28
155	Chemical-based risk assessment and in vitro models of human health effects induced by organic pollutants in soils from the Olona valley. Science of the Total Environment, 2013, 463-464, 790-801.	8.0	28
156	A knowledge-based expert rule system for predicting mutagenicity (Ames test) of aromatic amines and azo compounds. Toxicology, 2016, 370, 20-30.	4.2	28
157	Could deep learning in neural networks improve the QSAR models?. SAR and QSAR in Environmental Research, 2019, 30, 617-642.	2.2	28
158	Polychlorinated dibenzo-p-dioxins (PCDD) and polychlorinated dibenzofurans (PCDF) in emissions from an urban incinerator. 2. Correlation between concentration of micropollutants and combustion conditions. Chemosphere, 1983, 12, 1151-1157.	8.2	27
159	Concentrations of PCDD and PCDF in different points of a modern refuse incinerator. Chemosphere, 1990, 21, 507-517.	8.2	27
160	A GC-MS method for the analysis of fecal and plant sterols in sediment samples. Chemosphere, 1994, 29, 1393-1405.	8.2	27
161	Virtual Screening for Aryl Hydrocarbon Receptor Binding Prediction. Journal of Medicinal Chemistry, 2006, 49, 5702-5709.	6.4	27
162	Predicting toxicity through computers: a changing world. Chemistry Central Journal, 2007, 1, 32.	2.6	27

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163	Concentrations of PCDD/PCDF in soil close to a secondary aluminum smelter. Chemosphere, 2011, 85, 1719-1724.	8.2	27
164	QSAR models for ACE-inhibitor activity of tri-peptides based on representation of the molecular structure by graph of atomic orbitals and SMILES. Structural Chemistry, 2012, 23, 1873-1878.	2.0	27
165	Integration of QSAR models for bioconcentration suitable for REACH. Science of the Total Environment, 2013, 456-457, 325-332.	8.0	27
166	Optimal descriptor as a translator of eclectic information into the prediction of membrane damage: The case of a group of ZnO and TiO2 nanoparticles. Ecotoxicology and Environmental Safety, 2014, 108, 203-209.	6.0	27
167	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.	3.6	27
168	Using toxicological evidence from QSAR models in practice. ALTEX: Alternatives To Animal Experimentation, 2013, 30, 19-40.	1.5	27
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