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	Paradox of â€˜ideal correlationsâ€™: improved model for air half-life of persistent organic pollutants. Environmental Technology (United Kingdom), 2022, 43, 2510-2515.	2.2	7
2	QSAR models for soil ecotoxicity: Development and validation of models to predict reproductive toxicity of organic chemicals in the collembola Folsomia candida. Journal of Hazardous Materials, 2022, 423, 127236.	12.4	22
3	Patent Toxicity. Research Policy, 2022, 51, 104329.	6.4	11
4	Skin sensitization quantitative QSAR models based on mechanistic structural alerts. Toxicology, 2022, 468, 153111.	4.2	2
5	The system of self-consistent models for vapour pressure. Chemical Physics Letters, 2022, 790, 139354.	2.6	9
6	Green Chemistry in the Synthesis of Pharmaceuticals. Chemical Reviews, 2022, 122, 3637-3710.	47.7	155
7	In Silico Methods for Carcinogenicity Assessment. Methods in Molecular Biology, 2022, 2425, 201-215.	0.9	4
8	Using VEGAHUB Within a Weight-of-Evidence Strategy. Methods in Molecular Biology, 2022, 2425, 479-495.	0.9	2
9	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, 2022, 2425, 241-258.	0.9	3
10	In Silico Prediction of Chemically Induced Mutagenicity: A Weight of Evidence Approach Integrating Information from QSAR Models and Read-Across Predictions. Methods in Molecular Biology, 2022, 2425, 149-183.	0.9	5
11	In Silico Models for Developmental Toxicity. Methods in Molecular Biology, 2022, 2425, 217-240.	0.9	3
12	Prediction of the Neurotoxic Potential of Chemicals Based on Modelling of Molecular Initiating Events Upstream of the Adverse Outcome Pathways of (Developmental) Neurotoxicity. International Journal of Molecular Sciences, 2022, 23, 3053.	4.1	9
13	The VEGAHUB Platform: The Philosophy and the Tools. ATLA Alternatives To Laboratory Animals, 2022, 50, 121-135.	1.0	10
14	Exploration of structural requirements for azole chemicals towards human aromatase CYP19A1 activity: Classification modeling, structure-activity relationships and read-across study. Toxicology in Vitro, 2022, 81, 105332.	2.4	4
15	A regression-based QSAR-model to predict acute toxicity of aromatic chemicals in tadpoles of the Japanese brown frog (Rana japonica): Calibration, validation, and future developments to support risk assessment of chemicals in amphibians. Science of the Total Environment, 2022, 830, 154795.	8.0	10
16	Development of new QSAR models for water, sediment, and soil half-life. Science of the Total Environment, 2022, 838, 156004.	8.0	5
17	Modeling the migration of chemicals from food contact materials to food: The MERLIN-expo/VERMEER toolbox. Food and Chemical Toxicology, 2022, 166, 113118.	3.6	3
18	Carcinogenicity prediction using the index of ideality of correlation. SAR and QSAR in Environmental Research, 2022, 33, 419-428.	2.2	4

#	Article	IF	Citations
19	Monte Carlo Models for Sub-Chronic Repeated-Dose Toxicity: Systemic and Organ-Specific Toxicity. International Journal of Molecular Sciences, 2022, 23, 6615.	4.1	6
20	Pesticides, cosmetics, drugs: identical and opposite influences of various molecular features as measures of endpoints similarity and dissimilarity. Molecular Diversity, 2021, 25, 1137-1144.	3.9	2
21	Integrated In Silico Models for the Prediction of No-Observed-(Adverse)-Effect Levels and Lowest-Observed-(Adverse)-Effect Levels in Rats for Sub-chronic Repeated-Dose Toxicity. Chemical Research in Toxicology, 2021, 34, 247-257.	3.3	13
22	Towards a systematic use of effect biomarkers in population and occupational biomonitoring. Environment International, 2021, 146, 106257.	10.0	48
23	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
24	First report on chemometric modeling of hydrolysis half-lives of organic chemicals. Environmental Science and Pollution Research, 2021, 28, 1627-1642.	5.3	4
25	SpheraCosmolife: a new tool for the risk assessment of cosmetic products. ALTEX: Alternatives To Animal Experimentation, 2021, 38, 565-579.	1.5	4
26	Maintenance, update and further development of EFSA's Chemical Hazards: OpenFoodTox 2.0. EFSA Supporting Publications, 2021, 18, 6476E.	0.7	2
27	Defining the Human-Biota Thresholds of Toxicological Concern for Organic Chemicals in Freshwater: The Proposed Strategy of the LIFE VERMEER Project Using VEGA Tools. Molecules, 2021, 26, 1928.	3.8	1
28	The Monte Carlo method to build up models of the hydrolysis half-lives of organic compounds. SAR and QSAR in Environmental Research, 2021, 32, 463-471.	2.2	8
29	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	6.0	63
30	The self-organizing vector of atom-pairs proportions: use to develop models for melting points. Structural Chemistry, 2021, 32, 967-971.	2.0	7
31	A descriptor-based analysis to highlight the mechanistic rationale of mutagenicity. Journal of Environmental Science and Health, Part C: Toxicology and Carcinogenesis, 2021, , 1-24.	0.7	0
32	Safer chemicals using less animals: kick-off of the European ONTOX project. Toxicology, 2021, 458, 152846.	4.2	33
33	The index of ideality of correlation improves the predictive potential of models of the antioxidant activity of tripeptides from frog skin (Litoria rubella). Computers in Biology and Medicine, 2021, 133, 104370.	7.0	13
34	The QSAR-search of effective agents towards coronaviruses applying the Monte Carlo method. SAR and QSAR in Environmental Research, 2021, 32, 689-698.	2.2	6
35	Quantitative Structure-Activity Relationship Modeling of the Amplex Ultrared Assay to Predict Thyroperoxidase Inhibitory Activity. Frontiers in Pharmacology, 2021, 12, 713037.	3.5	4
36	Ecotoxicological QSAR modeling of the acute toxicity of organic compounds to the freshwater crustacean Thamnocephalus platyurus. Chemosphere, 2021, 280, 130652.	8.2	14

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37	Semi-correlations as a tool to model for skin sensitization. Food and Chemical Toxicology, 2021, 157, 112580.	3.6	4
38	QSAR Models for Human Carcinogenicity: An Assessment Based on Oral and Inhalation Slope Factors. Molecules, 2021, 26, 127.	3.8	13
39	The system of self-consistent semi-correlations as one of the tools of cheminformatics for designing antiviral drugs. New Journal of Chemistry, 2021, 45, 20713-20720.	2.8	7
40	New Models to Predict the Acute and Chronic Toxicities of Representative Species of the Main Trophic Levels of Aquatic Environments. Molecules, 2021, 26, 6983.	3.8	17
41	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
42	Structures of Endocrine-Disrupting Chemicals Correlate with the Activation of 12 Classic Nuclear Receptors. Environmental Science & Technology, 2021, 55, 16552-16562.	10.0	20
43	Chemometric modeling to predict air half-life of persistent organic pollutants (POPs). Journal of Hazardous Materials, 2020, 382, 121035.	12.4	15
44	The index of ideality of correlation: models for flammability of binary liquid mixtures. Chemical Papers, 2020, 74, 601-609.	2.2	18
45	QSAR-Models, Validation, and IIC-Paradox for Drug Toxicity. International Journal of Quantitative Structure-Property Relationships, 2020, 5, 22-43.	0.5	1
46	Ecotoxicological assessment of pharmaceuticals and personal care products using predictive toxicology approaches. Green Chemistry, 2020, 22, 1458-1516.	9.0	86
47	Exploring QSAR modeling of toxicity of chemicals on earthworm. Ecotoxicology and Environmental Safety, 2020, 190, 110067.	6.0	25
48	Use of the index of ideality of correlation to improve aquatic solubility model. Journal of Molecular Graphics and Modelling, 2020, 96, 107525.	2.4	14
49	First report on a classification-based QSAR model for chemical toxicity to earthworm. Journal of Hazardous Materials, 2020, 386, 121660.	12.4	29
50	New in silico models to predict in vitro micronucleus induction as marker of genotoxicity. Journal of Hazardous Materials, 2020, 385, 121638.	12.4	25
51	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
52	Evaluation of non-commercial models for genotoxicity and carcinogenicity in the assessment of EFSAâ€™s databases. SAR and QSAR in Environmental Research, 2020, 31, 33-48.	2.2	3
53	Zebrafish AC modelling: (Q)SAR models to predict developmental toxicity in zebrafish embryo. Ecotoxicology and Environmental Safety, 2020, 202, 110936.	6.0	13
54	QSAR model for pesticides toxicity to Rainbow Trout based on â€œideal correlationsâ€• Aquatic Toxicology, 2020, 227, 105589.	4.0	14

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55	Ecosystem ecology: Models for acute toxicity of pesticides towards Daphnia magna. Environmental Toxicology and Pharmacology, 2020, 80, 103459.	4.0	13
56	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
57	â€˜Ideal correlationsâ€™ for the predictive toxicity to Tetrahymena pyriformis. Toxicology Mechanisms and Methods, 2020, 30, 605-610.	2.7	6
58	Comparing in vivo data and in silico predictions for acute effects assessment of biocidal active substances and metabolites for aquatic organisms. Ecotoxicology and Environmental Safety, 2020, 205, 111291.	6.0	4
59	Modelling quantitative structure activityâ€“activity relationships (QSAARs): auto-pass-pass, a new approach to fill data gaps in environmental risk assessment under the REACH regulation. SAR and QSAR in Environmental Research, 2020, 31, 785-801.	2.2	6
60	Prediction of No Observed Adverse Effect Concentration for inhalation toxicity using Monte Carlo approach. SAR and QSAR in Environmental Research, 2020, 31, 1-12.	2.2	8
61	Maintenance,update and further development of EFSA's Chemical Hazards: OpenFoodTox 2.0. EFSA Supporting Publications, 2020, 17, 1822E.	0.7	4
62	New QSAR models to predict chromosome damaging potential based on the in vivo micronucleus test. Toxicology Letters, 2020, 329, 80-84.	0.8	7
63	Integrating QSAR models predicting acute contact toxicity and mode of action profiling in honey bees (A. mellifera): Data curation using open source databases, performance testing and validation. Science of the Total Environment, 2020, 735, 139243.	8.0	22
64	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
65	Review and priority setting for substances that are listed without a specific migration limit in TableÂ1 of Annex 1 of Regulation 10/2011 on plastic materials and articles intended to come into contact with food. EFSA Journal, 2020, 18, e06124.	1.8	7
66	The using of the Index of Ideality of Correlation (IIC) to improve predictive potential of models of water solubility for pesticides. Environmental Science and Pollution Research, 2020, 27, 13339-13347.	5.3	21
67	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
68	Ecotoxicological effects of atmospheric particulate produced by braking systems on aquatic and edaphic organisms. Environment International, 2020, 137, 105564.	10.0	23
69	Value and limitation of structure-based profilers to characterize developmental and reproductive toxicity potential. Archives of Toxicology, 2020, 94, 939-954.	4.2	5
70	Towards an Understanding of the Mode of Action of Human Aromatase Activity for Azoles through Quantum Chemical Descriptors-Based Regression and Structure Activity Relationship Modeling Analysis. Molecules, 2020, 25, 739.	3.8	8
71	QSAR models for biocides: The example of the prediction of Daphnia magna acute toxicity. SAR and QSAR in Environmental Research, 2020, 31, 227-243.	2.2	22
72	The index of ideality of correlation and the variety of molecular rings as a base to improve model of HIV-1 protease inhibitors activity. Structural Chemistry, 2020, 31, 1441-1448.	2.0	6

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73	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
74	Automated Integration of Structural, Biological and Metabolic Similarities to Sustain Read-Across. ALTEX: Alternatives To Animal Experimentation, 2020, 37, 469-481.	1.5	10
75	CORAL: Building up QSAR models for the chromosome aberration test. Saudi Journal of Biological Sciences, 2019, 26, 1101-1106.	3.8	25
76	QSPR as a random event: solubility of fullerenes C[60] and C[70]. Fullerenes Nanotubes and Carbon Nanostructures, 2019, 27, 816-821.	2.1	8
77	Ensemble-Based Modeling of Chemical Compounds with Antimalarial Activity. Current Topics in Medicinal Chemistry, 2019, 19, 957-969.	2.1	8
78	In silico model for mutagenicity (Ames test), taking into account metabolism. Mutagenesis, 2019, 34, 41-48.	2.6	10
79	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
80	SAR and QSAR modeling of a large collection of LD50 rat acute oral toxicity data. Journal of Cheminformatics, 2019, 11, 58.	6.1	71
81	Integrating in silico models for the prediction of mutagenicity (Ames test) of botanical ingredients of cosmetics. Computational Toxicology, 2019, 12, 100108.	3.3	10
82	Could deep learning in neural networks improve the QSAR models?. SAR and QSAR in Environmental Research, 2019, 30, 617-642.	2.2	28
83	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
84	QSAR Development for Plasma Protein Binding: Influence of the Ionization State. Pharmaceutical Research, 2019, 36, 28.	3.5	11
85	Idealization of correlations between optimal simplified molecular input-line entry system-based descriptors and skin sensitization. SAR and QSAR in Environmental Research, 2019, 30, 447-455.	2.2	19
86	Integrating QSAR, Read-Across, and Screening Tools: The VEGAHUB Platform as an Example. Challenges and Advances in Computational Chemistry and Physics, 2019, , 365-381.	0.6	11
87	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
88	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
89	QSAR modeling of Daphnia magna and fish toxicities of biocides using 2D descriptors. Chemosphere, 2019, 229, 8-17.	8.2	71
90	Methodology of aiQSAR: a group-specific approach to QSAR modelling. Journal of Cheminformatics, 2019, 11, 27.	6.1	16

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91	The Index of Ideality of Correlation: QSAR Model of Acute Toxicity for Zebrafish (Danio rerio) Embryo. International Journal of Environmental Research, 2019, 13, 387-394.	2.3	7
92	Ecotoxicological QSAR modeling of endocrine disruptor chemicals. Journal of Hazardous Materials, 2019, 369, 707-718.	12.4	54
93	Chemometric modeling of Daphnia magna toxicity of agrochemicals. Chemosphere, 2019, 224, 470-479.	8.2	37
94	On the uses of predictive toxicology to approve the use of engineered nanomaterials as biocidal active substances under the Biocidal Products Regulation. IOP Conference Series: Materials Science and Engineering, 2019, 499, 012007.	0.6	1
95	Development, validation and integration of in silico models to identify androgen active chemicals. Chemosphere, 2019, 220, 204-215.	8.2	23
96	Impact of REACH legislation on the production and importation of CMR (carcinogen, mutagen and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 Pharmacology, 2019, 101, 166-171.	2.7	1
97	Investigating landfill leachate toxicity in vitro: A review of cell models and endpoints. Environment International, 2019, 122, 21-30.	10.0	96
98	Semi-correlations as a tool to build up categorical (active/inactive) model of GABAA receptor modulator activity. Structural Chemistry, 2019, 30, 853-861.	2.0	7
99	Phytotoxicity of wear debris from traditional and innovative brake pads. Environment International, 2019, 123, 156-163.	10.0	30
100	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
101	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
102	Virtual Screening of Anti-Cancer Compounds: Application of Monte Carlo Technique. Anti-Cancer Agents in Medicinal Chemistry, 2019, 19, 148-153.	1.7	4
103	Mutagenicity, anticancer activity and blood brain barrier: similarity and dissimilarity of molecular alerts. Toxicology Mechanisms and Methods, 2018, 28, 321-327.	2.7	12
104	QSPR analysis of threshold of odor for the large number of heterogenic chemicals. Molecular Diversity, 2018, 22, 397-403.	3.9	3
105	Use of quasi-SMILES to model biological activity of â€œmicelleâ€“polymerâ€•samples. Structural Chemistry, 2018, 29, 1213-1223.	2.0	10
106	Performance of In Silico Models for Mutagenicity Prediction of Food Contact Materials. Toxicological Sciences, 2018, 163, 632-638.	3.1	14
107	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
108	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

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109	Harmonised risk assessment for human health, animal health and ecological risk assessment of combined exposure to multiple chemicals: a food and feed safety perspective. Toxicology Letters, 2018, 295, S37-S38.	0.8	0
110	A new semi-automated workflow for chemical data retrieval and quality checking for modeling applications. Journal of Cheminformatics, 2018, 10, 60.	6.1	56
111	Role of in silico tools and text mining in the risk assessment of selected alkaloids. Toxicology Letters, 2018, 295, S159.	0.8	0
112	Prediction of antimicrobial activity of large pool of peptides using quasi-SMILES. BioSystems, 2018, 169-170, 5-12.	2.0	13
113	SAR for gastro-intestinal absorption and blood-brain barrier permeation of pesticides. Chemico-Biological Interactions, 2018, 290, 1-5.	4.0	10
114	QSARpy: A new flexible algorithm to generate QSAR models based on dissimilarities. The log Kow case study. Science of the Total Environment, 2018, 637-638, 1158-1165.	8.0	8
115	CORAL: Predictive models for cytotoxicity of functionalized nanozeolites based on quasi-SMILES. Chemosphere, 2018, 210, 52-56.	8.2	15
116	Criteria and Application on the Use of Nontesting Methods within a Weight of Evidence Strategy. Methods in Molecular Biology, 2018, 1800, 199-218.	0.9	0
117	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
118	Prediction of Biochemical Endpoints by the CORAL Software: Prejudices, Paradoxes, and Results. Methods in Molecular Biology, 2018, 1800, 573-583.	0.9	6
119	A large comparison of integrated SAR/QSAR models of the Ames test for mutagenicity[$]. SAR and QSAR in Environmental Research, 2018, 29, 591-611.	2.2	21
120	Quasi-SMILES as a tool to predict removal rates of pharmaceuticals and dyes in sewage. Chemical Engineering Research and Design, 2018, 118, 227-233.	5.6	11
121	(Eco)toxicological maps: A new risk assessment method integrating traditional and in silico tools and its application in the Ledra River (Italy). Environment International, 2018, 119, 275-286.	10.0	11
122	Classification of a NaÃ¯ve Bayesian Fingerprint model to predict reproductive toxicity[$]. SAR and QSAR in Environmental Research, 2018, 29, 631-645.	2.2	9
123	Genotoxicity induced by metal oxide nanoparticles: a weight of evidence study and effect of particle surface and electronic properties. Nanotoxicology, 2018, 12, 1113-1129.	3.0	22
124	Integrated strategy for mutagenicity prediction applied to food contact chemicals. ALTEX: Alternatives To Animal Experimentation, 2018, 35, 169-178.	1.5	9
125	Air quality in the Olona Valley and in vitro human health effects. Science of the Total Environment, 2017, 579, 1929-1939.	8.0	13
126	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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127	(Q)SAR tools for priority setting: A case study with printed paper and board food contact material substances. Food and Chemical Toxicology, 2017, 102, 109-119.	3.6	21
128	Compilation of Data and Modelling of Nanoparticle Interactions and Toxicity in the NanoPUZZLES Project. Advances in Experimental Medicine and Biology, 2017, 947, 303-324.	1.6	8
129	Nano-QSAR Model for Predicting Cell Viability of Human Embryonic Kidney Cells. Methods in Molecular Biology, 2017, 1601, 275-290.	0.9	11
130	VOC exposures in California early childhood education environments. Indoor Air, 2017, 27, 609-621.	4.3	36
131	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
132	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
133	Fragment Prioritization on a Large Mutagenicity Dataset. Molecular Informatics, 2017, 36, 1600133.	2.5	10
134	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
135	Guidance on the use of the weight of evidence approach in scientific assessments. EFSA Journal, 2017, 15, e04971.	1.8	221
136	Developing innovative in silico models with EFSA's OpenFoodTox database. EFSA Supporting Publications, 2017, 14, 1206E.	0.7	10
137	Predicting acute contact toxicity of pesticides in honeybees (Apis mellifera) through a k-nearest neighbor model. Chemosphere, 2017, 166, 438-444.	8.2	49
138	Role of in silico tools and text mining in the safety assessment of selected plant coumarins. Toxicology Letters, 2017, 280, S96.	0.8	0
139	QSPR/QSAR Analyses by Means of the CORAL Software. , 2017, , 929-955.		0
140	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	6.0	264
141	QSAR as a Random Event: Selecting of the Molecular Structure for Potential Anti-tuberculosis Agents. Anti-Infective Agents, 2016, 14, 3-10.	0.4	7
142	A New Structure-Activity Relationship (SAR) Model for Predicting Drug-Induced Liver Injury, Based on Statistical and Expert-Based Structural Alerts. Frontiers in Pharmacology, 2016, 7, 442.	3.5	26
143	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
144	QSAR Model for Cytotoxicity of Silica Nanoparticles on Human Embryonic Kidney Cells1. Materials Today: Proceedings, 2016, 3, 847-854.	1.8	10

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145	Quasi-SMILES as a tool to utilize eclectic data for predicting the behavior of nanomaterials. NanoImpact, 2016, 1, 60-64.	4.5	24
146	Results of a round-robin exercise on read-across. SAR and QSAR in Environmental Research, 2016, 27, 371-384.	2.2	18
147	Classification nano-SAR modeling of metal oxides nanoparticles genotoxicity based on comet assay data. Toxicology Letters, 2016, 258, S271.	0.8	3
148	Integrating in silico models to enhance predictivity for developmental toxicity. Toxicology, 2016, 370, 127-137.	4.2	39
149	3D human hepatic organoids for testing Fibrosis, Cholestasis and Phospholipidosis. Toxicology Letters, 2016, 258, S129.	0.8	0
150	Odor threshold prediction by means of the Monte Carlo method. Ecotoxicology and Environmental Safety, 2016, 133, 390-394.	6.0	9
151	Integrated in silico strategy for PBT assessment and prioritization under REACH. Environmental Research, 2016, 151, 478-492.	7.5	32
152	New Quantitative Structureâ€“Activity Relationship Models Improve Predictability of Ames Mutagenicity for Aromatic Azo Compounds. Toxicological Sciences, 2016, 153, 316-326.	3.1	23
153	In Silico Methods for Carcinogenicity Assessment. Methods in Molecular Biology, 2016, 1425, 107-119.	0.9	10
154	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
155	Use of Read-Across Tools. Methods in Molecular Biology, 2016, 1425, 305-322.	0.9	10
156	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.	2.2	6
157	Novel chemical hazard characterisation approaches. EFSA Journal, 2016, 14, e00506.	1.8	3
158	In Silico Prediction of Chemically Induced Mutagenicity: How to Use QSAR Models and Interpret Their Results. Methods in Molecular Biology, 2016, 1425, 87-105.	0.9	8
159	In Silico Model for Developmental Toxicity: How to Use QSAR Models and Interpret Their Results. Methods in Molecular Biology, 2016, 1425, 139-161.	0.9	7
160	A new integrated in silico strategy for the assessment and prioritization of persistence of chemicals under REACH. Environment International, 2016, 88, 250-260.	10.0	22
161	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
162	In silicotools and transcriptomics analyses in the mutagenicity assessment of cosmetic ingredients: a proof-of-principle on how to add weight to the evidence. Mutagenesis, 2016, 31, 453-461.	2.6	9

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163	New clues on carcinogenicity-related substructures derived from mining two large datasets of chemical compounds. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2016, 34, 97-113.	2.9	24
164	QSAR model for predicting cell viability of human embryonic kidney cells exposed to SiO2 nanoparticles. Chemosphere, 2016, 144, 995-1001.	8.2	40
165	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
166	QSAR Methods to Screen Endocrine Disruptors. Nuclear Receptor Research, 2016, 3, .	2.5	6
167	Toxicology is IN: in silico, in vitro, integrated testing strategy. ALTEX: Alternatives To Animal Experimentation, 2016, 33, 187-188.	1.5	1
168	Use of (Q)SAR tools as a first step in a strategy to assign priority to substances migrating from printed paper and board food contact materials based on genotoxic potential. Toxicology Letters, 2015, 238, S66.	0.8	0
169	A quasi-QSPR modelling for the photocatalytic decolourization rate constants and cellular viability (CV%) of nanoparticles by CORAL. SAR and QSAR in Environmental Research, 2015, 26, 29-40.	2.2	23
170	QSAR model as a random event: A case of rat toxicity. Bioorganic and Medicinal Chemistry, 2015, 23, 1223-1230.	3.0	36
171	Synthesis, biological evaluation, and docking studies of PAR2-AP-derived pseudopeptides as inhibitors of kallikrein 5 and 6. Biological Chemistry, 2015, 396, 45-52.	2.5	4
172	Assessment ofin silicomodels for acute aquatic toxicity towards fish under REACH regulation. SAR and QSAR in Environmental Research, 2015, 26, 977-999.	2.2	17
173	In silicoexploratory study using structureâ€“activity relationship models and metabolic information for prediction of mutagenicity based on the Ames test and rodent micronucleus assay. SAR and QSAR in Environmental Research, 2015, 26, 1017-1031.	2.2	8
174	Identification of structural alerts for liver and kidney toxicity using repeated dose toxicity data. Chemistry Central Journal, 2015, 9, 62.	2.6	35
175	Comparison ofin silicotools for evaluating rat oral acute toxicity. SAR and QSAR in Environmental Research, 2015, 26, 1-27.	2.2	87
176	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
177	Physiologically based pharmacokinetic modeling of perfluoroalkyl substances in the human body. Toxicological and Environmental Chemistry, 2015, 97, 814-827.	1.2	16
178	Chemical characterization and ecotoxicity of three soil foaming agents used in mechanized tunneling. Journal of Hazardous Materials, 2015, 296, 210-220.	12.4	32
179	CORAL: Model for octanol/water partition coefficient. Fluid Phase Equilibria, 2015, 397, 44-49.	2.5	15
180	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

#	Article	IF	Citations
181	CORAL: model for no observed adverse effect level (NOAEL). Molecular Diversity, 2015, 19, 563-575.	3.9	20
182	Hierarchical Rules for Read-Across and In Silico Models of Mutagenicity. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2015, 33, 385-403.	2.9	7
183	Evaluation of QSAR models for predicting the partition coefficient (logP) of chemicals under the REACH regulation. Environmental Research, 2015, 143, 26-32.	7.5	21
184	Comparison between bioconcentration factor (BCF) data provided by industry to the European Chemicals Agency (ECHA) and data derived from QSAR models. Environmental Research, 2015, 142, 529-534.	7.5	24
185	Docking-based classification models for exploratory toxicology studies on high-quality estrogenic experimental data. Future Medicinal Chemistry, 2015, 7, 1921-1936.	2.3	30
186	Integrating QSAR and read-across for environmental assessment. SAR and QSAR in Environmental Research, 2015, 26, 605-618.	2.2	17
187	CORAL: Prediction of binding affinity and efficacy of thyroid hormone receptor ligands. European Journal of Medicinal Chemistry, 2015, 101, 452-461.	5.5	17
188	Genotoxicity of metal oxide nanomaterials: review of recent data and discussion of possible mechanisms. Nanoscale, 2015, 7, 2154-2198.	5.6	163
189	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
190	QSPR/QSAR Analyses by Means of the CORAL Software. Advances in Chemical and Materials Engineering Book Series, 2015, , 560-585.	0.3	10
191	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
192	A generalizable definition of chemical similarity for read-across. Journal of Cheminformatics, 2014, 6, 39.	6.1	75
193	Soil quality in the Lomellina area using in vitro models and ecotoxicological assays. Environmental Research, 2014, 133, 220-231.	7.5	16
194	Building up QSAR model for toxicity of psychotropic drugs by the Monte Carlo method. Structural Chemistry, 2014, 25, 1067-1073.	2.0	7
195	A new in silico classification model for ready biodegradability, based on molecular fragments. Chemosphere, 2014, 108, 10-16.	8.2	34
196	QSAR model for cytotoxicity of SiO2 nanoparticles on human lung fibroblasts. Journal of Nanoparticle Research, 2014, 16, 1.	1.9	21
197	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
198	Optimizing the aquatic toxicity assessment under REACH through an integrated testing strategy (ITS). Environmental Research, 2014, 135, 156-164.	7.5	11

#	Article	IF	Citations
199	REACH and in silico methods: an attractive opportunity for medicinal chemists. Drug Discovery Today, 2014, 19, 1757-1768.	6.4	70
200	Comparison ofin silicomodels for prediction ofDaphnia magnaacute toxicity. SAR and QSAR in Environmental Research, 2014, 25, 673-694.	2.2	40
201	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
202	Immunofluorescence detection and localization of B[a]P and TCDD in earthworm tissues. Chemosphere, 2014, 107, 282-289.	8.2	21
203	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
204	A k-NN algorithm for predicting oral sub-chronic toxicity in the rat. ALTEX: Alternatives To Animal Experimentation, 2014, 31, 423-432.	1.5	13
205	Optimal descriptor as a translator of eclectic information into the prediction of thermal conductivity of micro-electro-mechanical systems. Journal of Mathematical Chemistry, 2013, 51, 2230-2237.	1.5	12
206	Validation of quantitative structureâ€“activity relationship models to predict water-solubility of organic compounds. Science of the Total Environment, 2013, 463-464, 781-789.	8.0	16
207	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
208	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
209	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
210	QSAR models for inhibitors of physiological impact of Escherichia coli that leads to diarrhea. Biochemical and Biophysical Research Communications, 2013, 432, 214-225.	2.1	11
211	In silico methods to predict drug toxicity. Current Opinion in Pharmacology, 2013, 13, 802-806.	3.5	72
212	The definition of the molecular structure for potential anti-malaria agents by the Monte Carlo method. Structural Chemistry, 2013, 24, 1369-1381.	2.0	22
213	Meta-analysis of toxicity and teratogenicity of 133 chemicals from zebrafish developmental toxicity studies. Reproductive Toxicology, 2013, 41, 98-108.	2.9	45
214	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
215	Application of ERICA index to evaluation of soil ecosystem health according to sustainability threshold for chemical impact. Science of the Total Environment, 2013, 443, 134-142.	8.0	13
216	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

#	Article	IF	Citations
217	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
218	PCDD/Fs and PCBs in ambient air in a highly industrialized city in Northern Italy. Chemosphere, 2013, 90, 2352-2357.	8.2	52
219	Automatic knowledge extraction from chemical structures: the case of mutagenicity prediction. SAR and QSAR in Environmental Research, 2013, 24, 365-383.	2.2	121
220	CORAL: QSPR model of water solubility based on local and global SMILES attributes. Chemosphere, 2013, 90, 877-880.	8.2	34
221	Development of QSAR models for predicting anti-HIV-1 activity using the Monte Carlo method. Open Chemistry, 2013, 11, 371-380.	1.9	4
222	The ToxBank Data Warehouse: Supporting the Replacement of In Vivo Repeated Dose Systemic Toxicity Testing. Molecular Informatics, 2013, 32, 47-63.	2.5	35
223	Integration of QSAR models for bioconcentration suitable for REACH. Science of the Total Environment, 2013, 456-457, 325-332.	8.0	27
224	QSAR as a random event: Modeling of nanoparticles uptake in PaCa2 cancer cells. Chemosphere, 2013, 92, 31-37.	8.2	133
225	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
226	Genistein and dicarboximide fungicides in infant formulae from the EU market. Food Chemistry, 2013, 136, 116-119.	8.2	10
227	CORAL: QSPRs of enthalpies of formation of organometallic compounds. Journal of Mathematical Chemistry, 2013, 51, 1684-1693.	1.5	7
228	CORAL: Monte Carlo Method as a Tool for the Prediction of the Bioconcentration Factor of Industrial Pollutants. Molecular Informatics, 2013, 32, 145-154.	2.5	21
229	Using toxicological evidence from QSAR models in practice. ALTEX: Alternatives To Animal Experimentation, 2013, 30, 19-40.	1.5	27
230	CORAL: Classification Model for Predictions of Anti-Sarcoma Activity. Current Topics in Medicinal Chemistry, 2013, 12, 2741-2744.	2.1	7
231	OCWLGI Descriptors: Theory and Praxis. Current Computer-Aided Drug Design, 2013, 9, 226-232.	1.2	9
232	CORAL: Binary Classifications (Active/Inactive) for Liver-Related Adverse Effects of Drugs. Current Drug Safety, 2012, 7, 257-261.	0.6	14
233	CORAL: Quantitative models for estimating bioconcentration factor of organic compounds. Chemometrics and Intelligent Laboratory Systems, 2012, 118, 70-73.	3.5	6
234	CORAL: Models of toxicity of binary mixtures. Chemometrics and Intelligent Laboratory Systems, 2012, 119, 39-43.	3.5	23

#	Article	IF	Citations
235	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
236	The average numbers of outliers over groups of various splits into training and test sets: A criterion of the reliability of a QSPR? A case of water solubility. Chemical Physics Letters, 2012, 542, 134-137.	2.6	4
237	Quantitative consensus of bioaccumulation models for integrated testing strategies. Environment International, 2012, 45, 51-58.	10.0	41
238	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
239	Use and perceived benefits and barriers of QSAR models for REACH: findings from a questionnaire to stakeholders. Chemistry Central Journal, 2012, 6, 159.	2.6	8
240	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
241	Toxicological and Ecotoxicological Studies for Additives. Handbook of Environmental Chemistry, 2012, , 73-89.	0.4	0
242	Toxicological Characterization of Waste-Related Products Using Alternative Methods: Three Case Studies. Handbook of Environmental Chemistry, 2012, , 171-205.	0.4	0
243	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
244	QSAR Models for Toxicity of Organic Substances to Daphnia magna Built up by Using the CORAL Freeware. Chemical Biology and Drug Design, 2012, 79, 332-338.	3.2	18
245	CORAL: QSAR modeling of toxicity of organic chemicals towards Daphnia magna. Chemometrics and Intelligent Laboratory Systems, 2012, 110, 177-181.	3.5	57
246	CORAL: Predictions of rate constants of hydroxyl radical reaction using representation of the molecular structure obtained by combination of SMILES and Graph approaches. Chemometrics and Intelligent Laboratory Systems, 2012, 112, 65-70.	3.5	23
247	CORAL: the prediction of biodegradation of organic compounds with optimal SMILES-based descriptors. Open Chemistry, 2012, 10, 1042-1048.	1.9	7
248	Coral: QSAR models for acute toxicity in fathead minnow (Pimephales promelas). Journal of Computational Chemistry, 2012, 33, 1218-1223.	3.3	23
249	SMILES-based optimal descriptors: QSAR modeling of estrogen receptor binding affinity by correlation balance. Structural Chemistry, 2012, 23, 529-544.	2.0	8
250	Calculation of Molecular Features with Apparent Impact on Both Activity of Mutagens and Activity of Anticancer Agents. Anti-Cancer Agents in Medicinal Chemistry, 2012, 12, 807-817.	1.7	10
251	International workshop on safety assessment of consumer goods coming from recovered materials in a global scale perspective. Journal of Vietnamese Environment, 2012, 2, 20-26.	0.2	0
252	Mining toxicity structural alerts from SMILES: A new way to derive Structure Activity Relationships. , 2011, , .		17

#	Article	IF	Citations
253	Identification of Toxifying and Detoxifying Moieties for Mutagenicity Prediction by Priority Assessment. Journal of Chemical Information and Modeling, 2011, 51, 1564-1574.	5.4	3
254	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
255	1-(â„´o-Methoxyphenyl)piperazine is a metabolite of drugs bearing a methoxyphenylpiperazine side-chain. Journal of Pharmacy and Pharmacology, 2011, 39, 312-313.	2.4	4
256	Simplified Molecular Inputâ€Line Entry System and International Chemical Identifier in the QSAR Analysis of Styrylquinoline Derivatives as HIVâ€1 Integrase Inhibitors. Chemical Biology and Drug Design, 2011, 77, 343-360.	3.2	9
257	<scp>coral</scp> Software: QSAR for Anticancer Agents. Chemical Biology and Drug Design, 2011, 77, 471-476.	3.2	36
258	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
259	Concentrations of PCDD/PCDF in soil close to a secondary aluminum smelter. Chemosphere, 2011, 85, 1719-1724.	8.2	27
260	QSAR modelling toxicity toward rats of inorganic substances by means of CORAL. Open Chemistry, 2011, 9, 75-85.	1.9	17
261	Analysis of the co-evolutions of correlations as a tool for QSAR-modeling of carcinogenicity: an unexpected good prediction based on a model that seems untrustworthy. Open Chemistry, 2011, 9, 165-174.	1.9	26
262	QSAR modeling of anxiolytic activity taking into account the presence of keto- and enol-tautomers by balance of correlations with ideal slopes. Open Chemistry, 2011, 9, 846-854.	1.9	5
263	Evaluating the applicability domain in the case of classification predictive models for carcinogenicity based on the counter propagation artificial neural network. Journal of Computer-Aided Molecular Design, 2011, 25, 1147-1158.	2.9	16
264	CORAL: QSPR models for solubility of [C60] and [C70] fullerene derivatives. Molecular Diversity, 2011, 15, 249-256.	3.9	31
265	Alternative (non-animal) methods for cosmetics testing: current status and future prospectsâ€”2010. Archives of Toxicology, 2011, 85, 367-485.	4.2	488
266	The acceptance of in silicomodels for REACH: Requirements, barriers, and perspectives. Chemistry Central Journal, 2011, 5, 58.	2.6	44
267	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
268	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
269	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
270	SMILES-based QSAR Approaches for Carcinogenicity and Anticancer Activity: Comparison of Correlation Weights for Identical SMILES Attributes. Anti-Cancer Agents in Medicinal Chemistry, 2011, 11, 974-982.	1.7	26

#	Article	IF	Citations
271	Comparison and Possible Use ofIn SilicoTools for Carcinogenicity Within REACH Legislation. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2011, 29, 300-323.	2.9	24
272	In Silico Approaches to Screening Dietary Endocrine Disruptors. Issues in Toxicology, 2011, , 170-183.	0.1	0
273	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
274	QSPR modelling of normal boiling points and octanol/water partition coefficient for acyclic and cyclic hydrocarbons using SMILES-based optimal descriptors. Open Chemistry, 2010, 8, 1047-1052.	1.9	6
275	QSPR modeling of octanol/water partition coefficient of antineoplastic agents by balance of correlations. European Journal of Medicinal Chemistry, 2010, 45, 1639-1647.	5.5	14
276	Use of the international chemical identifier for constructing QSPR-model of normal boiling points of acyclic carbonyl substances. Journal of Mathematical Chemistry, 2010, 47, 355-369.	1.5	6
277	QSAR analysis of 1,4-dihydro-4-oxo-1-(2-thiazolyl)-1,8-naphthyridines exhibiting anticancer activity by optimal SMILES-based descriptors. Journal of Mathematical Chemistry, 2010, 47, 647-666.	1.5	10
278	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
279	QSAR-modeling of toxicity of organometallic compounds by means of the balance of correlations for InChI-based optimal descriptors. Molecular Diversity, 2010, 14, 183-192.	3.9	20
280	QSAR modelling of the toxicity to Tetrahymena pyriformis by balance of correlations. Molecular Diversity, 2010, 14, 821-827.	3.9	18
281	Endocrine modulation, inhibition of ovarian development and hepatic alterations in rainbow trout exposed to polluted river water. Environmental Pollution, 2010, 158, 3675-3683.	7.5	17
282	Assessing the environmental risks associated with contaminated sites: Definition of an Ecotoxicological Classification index for landfill areas (ECRIS). Chemosphere, 2010, 80, 60-66.	8.2	15
283	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
284	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
285	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
286	The CAESAR project for in silico models for the REACH legislation. Chemistry Central Journal, 2010, 4, I1.	2.6	25
287	Assessment and validation of the CAESAR predictive model for bioconcentration factor (BCF) in fish. Chemistry Central Journal, 2010, 4, S1.	2.6	54
288	New public QSAR model for carcinogenicity. Chemistry Central Journal, 2010, 4, S3.	2.6	105

#	Article	IF	Citations
289	CAESAR models for developmental toxicity. Chemistry Central Journal, 2010, 4, S4.	2.6	1,099
290	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
291	QSAR model for the prediction of bio-concentration factor using aqueous solubility and descriptors considering various electronic effects. SAR and QSAR in Environmental Research, 2010, 21, 711-729.	2.2	18
292	ERICA: A multiparametric toxicological risk index for the assessment of environmental healthiness. Environment International, 2010, 36, 665-674.	10.0	15
293	Computer-aided methodologies to predict endocrine-disrupting potency of chemicals. , 2009, , 306-321.		0
294	Food contamination control in European new Member States and associated candidate countries: Data collected within the SAFEFOODNET project. Journal of Environmental Science and Health - Part B Pesticides, Food Contaminants, and Agricultural Wastes, 2009, 44, 407-414.	1.5	6
295	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
296	QSPR modeling of enthalpies of formation for organometallic compounds by SMARTâ€based optimal descriptors. Journal of Computational Chemistry, 2009, 30, 2576-2582.	3.3	10
297	QSPR modeling bioconcentration factor (BCF) by balance of correlations. European Journal of Medicinal Chemistry, 2009, 44, 2544-2551.	5.5	29
298	QSAR modelling of carcinogenicity by balance of correlations. Molecular Diversity, 2009, 13, 367-373.	3.9	22
299	QSPR modeling of octanol water partition coefficient of platinum complexes by InChI-based optimal descriptors. Journal of Mathematical Chemistry, 2009, 46, 1060-1073.	1.5	15
300	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
301	QSAR Modelling for Mutagenic Potency of Heteroaromatic Amines by Optimal SMILESâ€based Descriptors. Chemical Biology and Drug Design, 2009, 73, 301-312.	3.2	17
302	Simplified Molecular Input Line Entry Systemâ€Based Optimal Descriptors: Quantitative Structureâ€“Activity Relationship Modeling Mutagenicity of Nitrated Polycyclic Aromatic Hydrocarbons. Chemical Biology and Drug Design, 2009, 73, 515-525.	3.2	22
303	QSPR modelling of the octanol/water partition coefficient of organometallic substances by optimal SMILES-based descriptors. Open Chemistry, 2009, 7, 846-856.	1.9	6
304	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
305	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
306	Support vector machines in the prediction of mutagenicity of chemical compounds. , 2009, , .		5

#	Article	IF	Citations
307	QSAR Models for Regulatory Purposes: Experiences and Perspectives. , 2009, , 183-200.		0
308	A combination of 3D-QSAR, docking, local-binding energy (LBE) and GRID study of the species differences in the carcinogenicity of benzene derivatives chemicals. Journal of Molecular Graphics and Modelling, 2008, 27, 147-160.	2.4	20
309	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
310	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
311	In silico-aided prediction of biological properties of chemicals: oestrogen receptor-mediated effects. Chemical Society Reviews, 2008, 37, 441-450.	38.1	33
312	Comparison of genistein metabolism in rats and humans using liver microsomes and hepatocytes. Food and Chemical Toxicology, 2008, 46, 939-948.	3.6	40
313	Levels of PCDD/F and dioxin-like PCB in Baltic fish of different age and gender. Chemosphere, 2008, 71, 369-378.	8.2	57
314	A comparison of DEMETRA individual QSARs with an index for evaluation of uncertainty. Chemosphere, 2008, 71, 1845-1852.	8.2	4
315	The proposal of architecture for chemical splitting to optimize QSAR models for aquatic toxicity. Chemosphere, 2008, 72, 772-780.	8.2	31
316	Estrogenicity profile and estrogenic compounds determined in river sediments by chemical analysis, ELISA and yeast assays. Chemosphere, 2008, 73, 1078-1089.	8.2	77
317	A new hybrid system of QSAR models for predicting bioconcentration factors (BCF). Chemosphere, 2008, 73, 1701-1707.	8.2	92
318	Definition and Detection of Outliers in Chemical Space. Journal of Chemical Information and Modeling, 2008, 48, 1592-1601.	5.4	18
319	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
320	Regulatory Perspectives in the Use and Validation of QSAR. A Case Study: DEMETRA Model forDaphniaToxicity. Environmental Science & Technology, 2008, 42, 491-496.	10.0	21
321	Regulatory Assessment of Chemicals within OECD Member Countries, EU and in Russia. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2008, 26, 40-88.	2.9	11
322	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
323	QSAR trout toxicity models on aromatic pesticides. Journal of Environmental Science and Health - Part B Pesticides, Food Contaminants, and Agricultural Wastes, 2008, 43, 633-637.	1.5	5
324	Toxicity study of allelochemical-like pesticides by a combination of 3D-QSAR, docking, Local Binding Energy (LBE) and GRID approaches. SAR and QSAR in Environmental Research, 2007, 18, 675-692.	2.2	15

#	Article	IF	Citations
325	E-MODELLING: FOUNDATIONS AND CASES FOR APPLYING AI TO LIFE SCIENCES. International Journal on Artificial Intelligence Tools, 2007, 16, 243-268.	1.0	7
326	SMILES in QSPR/QSAR Modeling: Results and Perspectives. Current Drug Discovery Technologies, 2007, 4, 77-116.	1.2	50
327	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
328	The specificity of the QSAR models for regulatory purposes: the example of the DEMETRA projectâ€. SAR and QSAR in Environmental Research, 2007, 18, 209-220.	2.2	4
329	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
330	QSARs for regulatory purposes: the case for pesticide authorization. , 2007, , 1-57.		5
331	Databases for pesticide ecotoxicity. , 2007, , 59-81.		2
332	Characterization of chemical structures. , 2007, , 83-109.		0
333	Hybrid systems. , 2007, , 149-183.		3
334	Validation of the models. , 2007, , 185-199.		9
335	The quality criteria of the DEMETRA models for regulatory purposes. , 2007, , 283-301.		3
336	Results of DEMETRA models. , 2007, , 201-281.		6
337	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
338	SMILES as an alternative to the graph in QSAR modelling of bee toxicity. Computational Biology and Chemistry, 2007, 31, 57-60.	2.3	52
339	Optimisation of correlation weights of SMILES invariants for modelling oral quail toxicity. European Journal of Medicinal Chemistry, 2007, 42, 606-613.	5.5	26
340	Predicting toxicity through computers: a changing world. Chemistry Central Journal, 2007, 1, 32.	2.6	27
341	In vivo exposure of carp to graded concentrations of bisphenol A. General and Comparative Endocrinology, 2007, 153, 15-24.	1.8	111
342	Structural features of diverse ligands influencing binding affinities to Estrogen Î± and Estrogen Î² receptors. Part I: molecular descriptors calculated from minimal energy conformation of isolated ligands. Molecular Diversity, 2007, 11, 153-169.	3.9	9

#	Article	IF	Citations
343	Structural features of diverse ligands influencing binding affinities to estrogen Î± and estrogen Î² receptors. Part II. Molecular descriptors calculated from conformation of the ligands in the complex resulting from previous docking study. Molecular Diversity, 2007, 11, 171-181.	3.9	15
344	Grid Computing for the Estimation of Toxicity: Acute Toxicity on Fathead Minnow (Pimephales) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 70		14
345	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
346	Top-Priority Fragment QSAR Approach in Predicting Pesticide Aquatic Toxicity. Chemical Research in Toxicology, 2006, 19, 1533-1539.	3.3	21
347	Preliminary Analysis of Toxicity of Benzoxazinones and Their Metabolites forFolsomia candida. Journal of Agricultural and Food Chemistry, 2006, 54, 1099-1104.	5.2	12
348	QSAR Models forDaphnia magnaToxicity Prediction of Benzoxazinone Allelochemicals and Their Transformation Products. Journal of Agricultural and Food Chemistry, 2006, 54, 1111-1115.	5.2	17
349	Virtual Screening for Aryl Hydrocarbon Receptor Binding Prediction. Journal of Medicinal Chemistry, 2006, 49, 5702-5709.	6.4	27
350	Data-driven modeling and prediction of acute toxicity of pesticide residues. SIGKDD Explorations: Newsletter of the Special Interest Group (SIG) on Knowledge Discovery & Data Mining, 2006, 8, 71-79.	4.0	2
351	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
352	Harmonised pesticide risk trend indicator for food (HAPERITIF): the methodological approach. Pest Management Science, 2006, 62, 1168-1176.	3.4	13
353	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
354	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
355	Correlation weighting of valence shells in QSAR analysis of toxicity. Bioorganic and Medicinal Chemistry, 2006, 14, 3923-3928.	3.0	24
356	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
357	Ecotoxicity prediction by adaptive fuzzy partitioning: comparing descriptors computed on 2D and 3D structures. SAR and QSAR in Environmental Research, 2006, 17, 225-251.	2.2	13
358	Environmental Agent Susceptibility Assessment Using Existing and Novel Biomarkers as Rapid Noninvasive Testing Methods. Annals of the New York Academy of Sciences, 2005, 1040, 381-386.	3.8	5
359	Description of the Electronic Structure of Organic Chemicals Using Semiempirical and ab initio Methods for Development of Toxicological QSARs.. ChemInform, 2005, 36, no.	0.0	0
360	3D-QSAR and Molecular Mechanics Study for the Differences in the Azole Activity Against Yeastlike and Filamentous Fungi and Their Relation to P450DM Inhibition. Part 1. 3-Substituted-4(3H)-quinazolinones.. ChemInform, 2005, 36, no.	0.0	0

#	Article	IF	Citations
361	3D-QSAR and Molecular Mechanics Study for the Differences in the Azole Activity against Yeastlike and Filamentous Fungi and Their Relation to P450DM Inhibition. 1. 3-Substituted-4(3H)-quinazolinones. Journal of Chemical Information and Modeling, 2005, 45, 634-644.	5.4	15
362	QSAR Model for Predicting Pesticide Aquatic Toxicity. Journal of Chemical Information and Modeling, 2005, 45, 1767-1774.	5.4	44
363	An Automated Group Contribution Method in Predicting Aquatic Toxicity:â€‰ The Diatomic Fragment Approach. Chemical Research in Toxicology, 2005, 18, 740-746.	3.3	20
364	Thermodynamic Descriptors Derived from Density Functional Theory Calculations in Prediction of Aquatic Toxicity. Journal of Chemical Information and Modeling, 2005, 45, 379-385.	5.4	6
365	Identification of the Structural Requirements of the Receptor-Binding Affinity of Diphenolic Azoles to Estrogen Receptors Î± and Î² by Three-Dimensional Quantitative Structureâ”Activity Relationship and Structureâ”Activity Relationship Analysis. Journal of Medicinal Chemistry, 2005, 48, 7628-7636.	6.4	21
366	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
367	GCâ€“MS analysis of dichlobenil and its metabolites in groundwater. Talanta, 2005, 68, 146-154.	5.5	43
368	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
369	Modelling Aquatic Toxicity with Advanced Computational Techniques: Procedures to Standardize Data and Compare Models. Lecture Notes in Computer Science, 2004, , 235-248.	1.3	4
370	A Protocol to Select High Quality Datasets of Ecotoxicity Values for Pesticides. Journal of Environmental Science and Health - Part B Pesticides, Food Contaminants, and Agricultural Wastes, 2004, 39, 641-652.	1.5	19
371	MULTICLASS CLASSIFIER FROM A COMBINATION OF LOCAL EXPERTS: TOWARD DISTRIBUTED COMPUTATION FOR REAL-PROBLEM CLASSIFIERS. International Journal of Pattern Recognition and Artificial Intelligence, 2004, 18, 801-817.	1.2	12
372	Classification of Potential Endocrine Disrupters on the Basis of Molecular Structure Using a Nonlinear Modeling Method.. ChemInform, 2004, 35, no.	0.0	0
373	Predictive Models for Aquatic Toxicity of Aldehydes Designed for Various Model Chemistries.. ChemInform, 2004, 35, no.	0.0	0
374	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
375	QSAR modelling of aldehyde toxicity against a protozoan, Tetrahymena pyriformis by optimization of correlation weights of nearest neighboring codes. Computational and Theoretical Chemistry, 2004, 679, 225-228.	1.5	19
376	QSAR in Ecotoxicity:â€‰ An Overview of Modern Classification Techniques. Journal of Chemical Information and Computer Sciences, 2004, 44, 105-112.	2.8	39
377	Combining Unsupervised and Supervised Artificial Neural Networks to PredictAquatic Toxicity. Journal of Chemical Information and Computer Sciences, 2004, 44, 1897-1902.	2.8	35
378	Predictive Models for Aquatic Toxicity of Aldehydes Designed for Various Model Chemistries. Journal of Chemical Information and Computer Sciences, 2004, 44, 976-984.	2.8	16

#	Article	IF	Citations
379	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
380	Organic Contaminants in Leachates from Industrial Waste Landfills. Handbook of Environmental Chemistry, 2004, , 71-97.	0.4	1
381	ANVAS: artificial neural variables adaptation system for descriptor selection. Journal of Computer-Aided Molecular Design, 2003, 17, 335-346.	2.9	7
382	Database mining with adaptive fuzzy partition: Application to the prediction of pesticide toxicity on rats. Environmental Toxicology and Chemistry, 2003, 22, 983-991.	4.3	14
383	Tuning Neutral and Fuzzy-Neutral Networks for Toxicity Modeling.. ChemInform, 2003, 34, no.	0.0	0
384	Emerging organic contaminants in leachates from industrial waste landfills and industrial effluent. TrAC - Trends in Analytical Chemistry, 2003, 22, 757-765.	11.4	29
385	Predicting Toxicity against the fathead Minnow by Adaptive Fuzzy Partition. QSAR and Combinatorial Science, 2003, 22, 210-219.	1.4	21
386	Tuning Neural and Fuzzy-Neural Networks for Toxicity Modeling. Journal of Chemical Information and Computer Sciences, 2003, 43, 513-518.	2.8	28
387	Modeling Toxicity by Using Supervised Kohonen Neural Networks. Journal of Chemical Information and Computer Sciences, 2003, 43, 485-492.	2.8	46
388	Polychlorinated Dibenzo-p-Dioxins and Dibenzofurans in the Air of Seveso, Italy, 26 Years after the Explosion. Environmental Science & Technology, 2003, 37, 1503-1508.	10.0	15
389	Organic tracers identification as a convenient strategy in industrial landfills monitoring. Chemosphere, 2003, 51, 677-683.	8.2	11
390	Predicting logP of pesticides using different software. Chemosphere, 2003, 53, 1155-1164.	8.2	94
391	Database mining with adaptive fuzzy partition: application to the prediction of pesticide toxicity on rats. Environmental Toxicology and Chemistry, 2003, 22, 983-91.	4.3	3
392	Development of an Enzyme-Linked Immunosorbent Assay (ELISA) for the Herbicide Propanil. International Journal of Environmental Analytical Chemistry, 2002, 82, 865-878.	3.3	5
393	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
394	The Importance of Scaling in Data Mining for Toxicity Prediction. Journal of Chemical Information and Computer Sciences, 2002, 42, 1250-1255.	2.8	41
395	Polychlorinated dibenzo-p-dioxins and dibenzofurans in River Po sediments. Chemosphere, 2002, 49, 749-754.	8.2	24
396	Chemical Analysis, Distributed Modelling and Risk Indices. Three Fundamental Pillars in Risk Assessment. Scientific World Journal, The, 2002, 2, 1611-1625.	2.1	9

#	Article	IF	Citations
397	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
398	The Importance of Scaling in Data Mining for Toxicity Prediction.. ChemInform, 2002, 33, 222-222.	0.0	0
399	Combining Classifiers of Pesticides Toxicity through a Neuro-fuzzy Approach. Lecture Notes in Computer Science, 2002, , 293-303.	1.3	13
400	Interpretation of Quantitative Structureâ˜'Property and â˜'Activity Relationships. Journal of Chemical Information and Computer Sciences, 2001, 41, 679-685.	2.8	110
401	A POLARIZATION FLUORESCENCE IMMUNOASSAY FOR THE HERBICIDE PROPANIL. Analytical Letters, 2001, 34, 2285-2301.	1.8	31
402	Predicting toxicity: a mechanism of action model of chemical mutagenicity. Mutation Research - Fundamental and Molecular Mechanisms of Mutagenesis, 2001, 479, 141-171.	1.0	6
403	Factors Influencing Predictive Models for Toxicology. SAR and QSAR in Environmental Research, 2001, 12, 593-603.	2.2	32
404	Mixing a Symbolic and a Subsymbolic Expert to Improve Carcinogenicity Prediction of Aromatic Compounds. Lecture Notes in Computer Science, 2001, , 126-135.	1.3	7
405	Pharmaceuticals as Environmental Contaminants: Modelling Distribution and Fate. , 2001, , 91-102.		5
406	Fractionation and toxicity evaluation of waste waters. Journal of Chromatography A, 2000, 889, 149-154.	3.7	26
407	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
408	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
409	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
410	Increased concentrations of nitrophenols in leaves from a damaged forestal site. Chemosphere, 1999, 38, 1495-1503.	8.2	54
411	Deuterated internal standards for gas chromatographic-mass spectrometric analysis of polar organophosphorus pesticides in water samples. Journal of Chromatography A, 1998, 822, 91-99.	3.7	17
412	Hybrid toxicology expert system: architecture and implementation of a multi-domain hybrid expert system for toxicology. Chemometrics and Intelligent Laboratory Systems, 1998, 43, 135-145.	3.5	8
413	Industrial pollutants in ground waters from Northern Milan. Chemosphere, 1998, 36, 2007-2017.	8.2	9
414	A case study of indoor pollution by Chinese cooking. Toxicological and Environmental Chemistry, 1998, 65, 217-224.	1.2	13

#	Article	IF	Citations
415	An interlaboratory analysis on labile pesticides. Toxicological and Environmental Chemistry, 1998, 65, 173-184.	1.2	1
416	Metabolites of Alachlor in Water:Â Identification by Mass Spectrometry and Chemical Synthesis. Environmental Science & Technology, 1997, 31, 3637-3646.	10.0	30
417	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
418	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
419	Analysis of organic micropollutants in sediment samples of the Venice Lagoon, Italy. Water, Air, and Soil Pollution, 1997, 99, 237-244.	2.4	19
420	Computational predictive programs (expert systems) in toxicology. Toxicology, 1997, 119, 213-225.	4.2	97
421	Analysis of Organic Micropollutants in Sediment Samples of the Venice Lagoon, Italy. , 1997, , 237-244.		1
422	Alachlor and its metabolites in surface water. Chemosphere, 1996, 32, 229-237.	8.2	22
423	Sterols in sediment samples from Venice Lagoon, Italy. Chemosphere, 1996, 33, 2383-2393.	8.2	68
424	Solid-phase extraction coupled with electrochemical detection for the determination of the herbicide bromofenoxim in water samples at low-and sub-Âµg lâ€“1levels. Analyst, The, 1996, 121, 1839-1843.	3.5	6
425	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
426	Detection and Quanification of Trihalomethanes in Drinking Water from Alexandria, Egypt. Bulletin of Environmental Contamination and Toxicology, 1996, 56, 397-404.	2.7	10
427	Identification of organic contaminants in leachates from industrial waste landfills. TrAC - Trends in Analytical Chemistry, 1996, 15, 305-310.	11.4	25
428	Analysis of chlorinated 1,3-butadienes by solid-phase microextraction and gas chromatography-mass spectrometry. Journal of Chromatography A, 1996, 737, 85-91.	3.7	21
429	Synthesis and use of deuterated fenamiphos and its metabolites as internal standards for mass spectrometric analysis in water. Journal of Chromatography A, 1996, 754, 207-219.	3.7	6
430	Determination and Stability of Phenmediphan, Ethofumesate and Fenamiphos in Ground Water Samples Using Automated Solid Phase Extraction Cartridges Followed by Liquid Chromatography High Flow Pneumatically Assisted Electrospray Mass Spectrometry. International Journal of Environmental Analytical Chemistry, 1996, 65, 69-82.	3.3	11
431	Pollution of ground and drinking water with volatile organic compounds: Solidâ€phase microextraction and GC/MS analysis. Toxicological and Environmental Chemistry, 1996, 55, 73-81.	1.2	4
432	Batch square-wave voltammetric and flow-injection amperometric determination of trace amounts of bromofenoxim. Analytica Chimica Acta, 1995, 310, 153-160.	5.4	9

#	Article	IF	Citations
433	Selective sulfur oxygenation in phosphoroamidate, thionophosphate, and thiophosphate agrochemicals by perfluoro-cis-2,3-dialkyloxaziridine. Tetrahedron, 1995, 51, 7981-7992.	1.9	15
434	A NICI-GC-MS Method to Analyze Endosulfan in Biological Samples. International Journal of Environmental Analytical Chemistry, 1995, 58, 67-72.	3.3	4
435	Impurities Released from Extractive Phases Used in the Analysis of Pesticides. International Journal of Environmental Analytical Chemistry, 1995, 58, 23-30.	3.3	4
436	Analysis of bromofenoxim by supercritical fluid chromatography and comparison with an HPLC method. Toxicological and Environmental Chemistry, 1995, 47, 119-128.	1.2	4
437	GC Analysis of Some Organochlorine Pesticides using a Brominated Internal Standard. International Journal of Environmental Analytical Chemistry, 1995, 58, 55-66.	3.3	2
438	A Library Report on the Analysis of Pesticides Subject to Investigation for the European Communities Commission. International Journal of Environmental Analytical Chemistry, 1995, 58, 31-42.	3.3	5
439	Fate of 1-O-octadecyl-2-O-methyl-rac-glycero-3-phosphocholine (ET18-OME) in malignant cells, normal cells, and isolated and perfused rat liver. Drug Metabolism and Disposition, 1995, 23, 113-8.	3.3	6
440	A simple method for determination of Nâ€nitrosamine traces in trifluralin samples by gas chromatographyâ€mass spectrometry. Toxicological and Environmental Chemistry, 1994, 45, 199-204.	1.2	4
441	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
442	Synthesis and use of pentadeuteroethyl ethofumesate as an internal standard for the determination of ethofumesate and its metabolites in water by gas chromatography-mass spectrometry. Journal of Chromatography A, 1994, 688, 243-250.	3.7	7
443	Diurnal, weekly and seasonal air concentrations of PCDD and PCDF in an industrial area. Fresenius' Journal of Analytical Chemistry, 1994, 348, 141-143.	1.5	3
444	Mass Spectrometric Studies of Flavonoids. Natural Product Research, 1994, 4, 247-254.	0.4	3
445	A GC-MS method for the analysis of fecal and plant sterols in sediment samples. Chemosphere, 1994, 29, 1393-1405.	8.2	27
446	Urinary excretion of platelet activating factor in patients with immune-mediated glomerulonephritis. Kidney International, 1993, 43, 426-429.	5.2	22
447	Preliminary survey on 2,3,7,8-TCDD in cellulose-containing consumer products on the italian market. Chemosphere, 1993, 27, 1561-1564.	8.2	2
448	GCâ€MS analysis of nâ€phosphonomethylglycine (glyphosate) samples through derivatization with a perfluoroanhydride and trifluoroethanol: Identification of byâ€products. Toxicological and Environmental Chemistry, 1993, 38, 225-232.	1.2	7
449	PCDD, PCDF, PCB, PAH, cadmium and lead in roadside soil: relationship between road distance and concentration. Chemosphere, 1992, 24, 1077-1083.	8.2	38
450	Characterization of organic and inorganic pollutants in the Adige river (Italy). Chemosphere, 1992, 25, 1665-1674.	8.2	10

#	Article	IF	Citations
451	Incineration of agro-industrial wastes and macro- and micropollutants emission. Chemosphere, 1992, 24, 1545-1551.	8.2	9
452	Quantification of 4,4â€²-diaminodiphenylmethane by gas chromatography negative ion chemical lonization mass spectrometry. Microchemical Journal, 1992, 46, 352-359.	4.5	3
453	Metabolic profile of atrazine and N-nitrosoatrazine in rat urine. Bulletin of Environmental Contamination and Toxicology, 1992, 48, 701-8.	2.7	11
454	Mass spectrometric identification of urinary and plasma metabolites of 2-(6â€™-carboxyhexyl)-3-n-hexylcyclohexylamine, a new antiaggregating agent. European Journal of Drug Metabolism and Pharmacokinetics, 1992, 17, 93-101.	1.6	1
455	Analysis by fast atom bombardment mass spectrometry of phospholipids from tubuli, glomeruli, and urine of normal rats and rats with acute renal failure. Biochemical Medicine and Metabolic Biology, 1992, 48, 219-226.	0.7	1
456	Specific gas chromatographyâ€”mass spectrometry analytical method for the determination of cyhexatin in animal feed. Journal of Chromatography A, 1992, 605, 129-133.	3.7	2
457	Increased urinary excretion of platelet activating factor in mice with lupus nephritis. Life Sciences, 1991, 48, 1429-1437.	4.3	17
458	Synthesis and destruction of PCDD and PCDF inside a municipal solid waste incinerator. Chemosphere, 1991, 23, 715-722.	8.2	22
459	â€œDe novoâ€•synthesis of PCDD, PCDF, PCB, PCN and PAH in a pilot incinerator. Chemosphere, 1991, 22, 1045-1052.	8.2	45
460	Migration of vinyl chloride into PVC-bottled drinking-water assessed by gas chromatography-mass spectrometry. Food and Chemical Toxicology, 1991, 29, 131-134.	3.6	23
461	Simultaneous determination of isbufylline and its major metabolites in rabbit blood and urine by reversed-phase high-performance liquid chromatography. Biomedical Applications, 1991, 568, 407-418.	1.7	3
462	Dictyostelium cells produce platelet-activating factor in response to cAMP. FEBS Journal, 1991, 196, 609-615.	0.2	21
463	Preparation of 4,4â€²-diaminodiphenylmethane-(2H4) for use as internal standard in the quantification of 4,4â€²-diaminodiphenylmethane. Journal of Labelled Compounds and Radiopharmaceuticals, 1991, 29, 725-728.	1.0	0
464	Mass spectrometric identification of urinary and plasma metabolites of 6-(6'-carboxyhexyl)-7-n-hexyl-1,3-diazaspiro-[4-4]-nonan-2,4-dione, a new cytoprotective agent. Drug Metabolism and Disposition, 1991, 19, 913-6.	3.3	1
465	Syntheses of deuterated leu-enkephalins and their use as internal standards for the quantification of leu-enkephalin by fast atom bombardment mass spectrometry. Journal of Labelled Compounds and Radiopharmaceuticals, 1990, 28, 411-419.	1.0	5
466	Concentrations of PCDD and PCDF in different points of a modern refuse incinerator. Chemosphere, 1990, 21, 507-517.	8.2	27
467	Simultaneous analysis of 50 pesticides in water samples by solid phase extraction and GC-MS. Chemosphere, 1990, 21, 1411-1421.	8.2	66
468	The combustion of municipal solid waste and PCDD and PCDF emissions. On the real scale thermal behavior of PCDD and PCDF in flue gas and fly ash. Chemosphere, 1990, 20, 1907-1914.	8.2	13

#	Article	IF	Citations
469	Characterization of the Major Browning Derivatives of Lysine with 2-Amino-2-Deoxy-D-Glucose. , 1990, , 109-114.		0
470	A Gas Chromatographic Mass Spectrometric Assay for the Determination of Aphidicolin in Plasma of Cancer Patients. Journal of Pharmaceutical Sciences, 1989, 78, 399-401.	3.3	2
471	Molecular species analysis of phospholipids by negative ion fast atom bombardment mass spectrometry: Application of surface precipitation technique. Biomedical & Environmental Mass Spectrometry, 1989, 18, 1051-1056.	1.6	25
472	Measurement of vitamin E in premature infants by reversed-phase high-performance liquid chromatography. Biomedical Applications, 1989, 490, 432-438.	1.7	8
473	Metabolism and pharmacokinetics of p-(3,3-dimethyl-1-triazeno) benzoic acid in M5076 sarcoma-bearing mice. Cancer Chemotherapy and Pharmacology, 1989, 24, 354-358.	2.3	7
474	Development of a mass spectrometric method to quantitate platelet activating factor in mouse urine.. Journal of Lipid Research, 1989, 30, 1977-1981.	4.2	9
475	A fast atom bombardment-mass spectrometric method to quantitate lysophosphatidylserine in rat brain.. Journal of Lipid Research, 1989, 30, 1983-1986.	4.2	8
476	Development of a mass spectrometric method to quantitate platelet activating factor in mouse urine. Journal of Lipid Research, 1989, 30, 1977-81.	4.2	8
477	A fast atom bombardment-mass spectrometric method to quantitate lysophosphatidylserine in rat brain. Journal of Lipid Research, 1989, 30, 1983-6.	4.2	8
478	Identification of microsomal metabolites of spirogermanium. Anticancer Research, 1989, 9, 507-10.	1.1	0
479	Identification of metabolites of tiropramide in human urine. Biomedical & Environmental Mass Spectrometry, 1988, 15, 205-209.	1.6	8
480	Reaction of 2-amino-2-deoxy-d-glucose and lysine: Isolation and characterization of 2,5-bis(tetrahydroxybutyl)pyrazine. Carbohydrate Research, 1988, 184, 67-75.	2.3	17
481	High-performance liquid chromatographic separation and mass spectrometric identification of propafenone, 5-hydroxypropafenone and N-depropylpropafenone. Biomedical Applications, 1988, 424, 211-214.	1.7	12
482	Effect of butylated hydroxyanisole added in vitro or administered to rats on N,N-dibutylnitrosamine and N-butyl-N-(4-hydroxybutyl)nitrosamine metabolism by post-mitochondrial supernatant of liver homogenates. Toxicology, 1988, 48, 71-80.	4.2	7
483	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
484	Mass spectrometric identification of urinary and plasma metabolites of 9-hydroxy-19,20-bis-nor-prostanoic acid (rosaprostol). Prostaglandins, 1988, 35, 665-684.	1.2	1
485	Analysis of atrazine in underground waters at part per trillion levels as an early warning method for contamination and for soil distribution studies. Chemosphere, 1987, 16, 1425-1430.	8.2	25
486	Studies on the tetrachlorodibenzo-p-dioxins (TCDD) and tetrachlorodibenzofurans (TCDF) emitted from an urban incinerator. Chemosphere, 1986, 15, 557-561.	8.2	12

#	Article	IF	Citations
487	High-performance liquid chromatographic assay for the determination of p-(3,3-dimethyl-1-triazeno)benzoic acid in mouse plasma. Biomedical Applications, 1985, 345, 323-331.	1.7	3
488	Horseradish peroxidase/hydrogen peroxide-catalyzed oxidation of VP16-213. Identification of a new metabolite. Chemico-Biological Interactions, 1985, 55, 215-224.	4.0	10
489	A comparison of three methods of soft ionization mass spectrometry of crude phospholipid extracts. Biological Mass Spectrometry, 1985, 12, 643-651.	0.5	16
490	Metabolic studies of a podophyllotoxin derivative (VP16) in the isolated perfused liver. Xenobiotica, 1985, 15, 343-350.	1.1	17
491	Identification and quantitation of 1-arylpiperazines, metabolites resulting from side-chain cleavage of (4-substituted aryl-1-piperazinyl)alkyl heterocyclic derivatives in rat plasma and brain. Journal of Chromatography A, 1984, 283, 211-221.	3.7	16
492	Identification of a nitrosamino aldehyde and a nitrosamino acid resulting from Î²-oxidation of N-nitrosodiethanolamine. Chemico-Biological Interactions, 1984, 51, 103-113.	4.0	11
493	Physicochemical and Analytical Characteristics ofAmiodarone. Journal of Pharmaceutical Sciences, 1984, 73, 829-831.	3.3	36
494	Kinetics of 3-tert-butyl-4-hydroxyanisole (BHA) in man. Food and Chemical Toxicology, 1984, 22, 901-904.	3.6	14
495	Identification of an acidic metabolite ofN-nitrosodiethanolamine isolated from rat urine. Biomedical Mass Spectrometry, 1983, 10, 334-337.	1.9	24
496	Metabolism of the anticancer agent 1-(4-acetylphenyl)-3,3-dimethyltriazene. Biomedical Mass Spectrometry, 1983, 10, 485-488.	1.9	10
497	Quantitative analysis of minaprine and some of its metabolites with application to kinetic studies in rats. Journal of Chromatography A, 1983, 259, 141-149.	3.7	11
498	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
499	Toxicological evaluation of urban waste incinerator emissions. Chemosphere, 1983, 12, 559-564.	8.2	18
500	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
501	Clustering and classification techniques to assess aquatic toxicity. , 0, , .		1
502	Applications of Flexible Molecular Descriptors in the QSPRâ€“QSAR Study of Heterocyclic Drugs. , 0, , 1-38.		5
503	Environmental and Ecological Toxicology: Computational Risk Assessment. , 0, , 625-650.		0
504	Open Computing Grid for Molecular Sciences. , 0, , 1-21.		0

#	Article	IF	Citations
505	Quantitative structureâ€“activity relationship models for bee toxicity. Toxicological and Environmental Chemistry, 0, , 1-12.	1.2	2
506	Integrating rules and neural nets for carcinogenicity prediction. , 0, , .		0