

Gerrit Schärmann

List of Publications by Year in descending order

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219
papers

17,360
citations

34105

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15266

126
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237
all docs

237
docs citations

237
times ranked

19044
citing authors

#	ARTICLE	IF	CITATIONS
1	COSMO: a new approach to dielectric screening in solvents with explicit expressions for the screening energy and its gradient. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1993, , 799-805.	0.9	8,014
2	External Validation and Prediction Employing the Predictive Squared Correlation Coefficient " Test Set Activity Mean vs Training Set Activity Mean. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 2140-2145.	5.4	461
3	MIXTURE TOXICITY AND ITS MODELING BY QUANTITATIVE STRUCTURE"ACTIVITY RELATIONSHIPS. <i>Environmental Toxicology and Chemistry</i> , 2003, 22, 1900.	4.3	326
4	A new risk assessment approach for the prioritization of 500 classical and emerging organic microcontaminants as potential river basin specific pollutants under the European Water Framework Directive. <i>Science of the Total Environment</i> , 2011, 409, 2064-2077.	8.0	259
5	Persistent organic pollutants in agricultural soils of central Germany. <i>Science of the Total Environment</i> , 2001, 277, 187-198.	8.0	217
6	Prediction of the pKa of Carboxylic Acids Using the ab Initio Continuum-Solvation Model PCM-UAHF. <i>Journal of Physical Chemistry A</i> , 1998, 102, 6706-6712.	2.5	204
7	Structural AlertsA New Classification Model to Discriminate Excess Toxicity from Narcotic Effect Levels of Organic Compounds in the Acute Daphnid Assay. <i>Chemical Research in Toxicology</i> , 2005, 18, 536-555.	3.3	174
8	The SOLUTIONS project: Challenges and responses for present and future emerging pollutants in land and water resources management. <i>Science of the Total Environment</i> , 2015, 503-504, 22-31.	8.0	163
9	From the exposome to mechanistic understanding of chemical-induced adverse effects. <i>Environment International</i> , 2017, 99, 97-106.	10.0	146
10	A European perspective on alternatives to animal testing for environmental hazard identification and risk assessment. <i>Regulatory Toxicology and Pharmacology</i> , 2013, 67, 506-530.	2.7	139
11	Group contribution methods to estimate water solubility of organic chemicals. <i>Chemosphere</i> , 1995, 30, 2061-2077.	8.2	132
12	Pesticides from wastewater treatment plant effluents affect invertebrate communities. <i>Science of the Total Environment</i> , 2017, 599-600, 387-399.	8.0	131
13	High Extraction Efficiency for POPs in Real Contaminated Soil Samples Using Accelerated Solvent Extraction. <i>Analytical Chemistry</i> , 2000, 72, 1294-1300.	6.5	125
14	Biomonitoring of airborne inorganic and organic pollutants by means of pine tree barks. I. Temporal and spatial variations. <i>Science of the Total Environment</i> , 1999, 232, 49-58.	8.0	120
15	Pesticides are the dominant stressors for vulnerable insects in lowland streams. <i>Water Research</i> , 2021, 201, 117262.	11.3	118
16	Calibrating the Uptake Kinetics of Semipermeable Membrane Devices in Water:Â Impact of Hydrodynamics. <i>Environmental Science & Technology</i> , 2002, 36, 290-296.	10.0	117
17	Prediction of Michael-Type Acceptor Reactivity toward Glutathione. <i>Chemical Research in Toxicology</i> , 2010, 23, 1576-1585.	3.3	115
18	ACUTE TO CHRONIC RATIOS IN AQUATIC TOXICITY"VARIATION ACROSS TROPHIC LEVELS AND RELATIONSHIP WITH CHEMICAL STRUCTURE. <i>Environmental Toxicology and Chemistry</i> , 2006, 25, 2937.	4.3	110

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19	Kinetic Glutathione Chemoassay To Quantify Thiol Reactivity of Organic Electrophiles—Application to α,β -Unsaturated Ketones, Acrylates, and Propiolates. <i>Chemical Research in Toxicology</i> , 2009, 22, 742-750.	3.3	100
20	Structure-Based Classification of Antibacterial Activity. <i>Journal of Chemical Information and Computer Sciences</i> , 2002, 42, 869-878.	2.8	97
21	New hydrolysis products of the beta-lactam antibiotic amoxicillin, their pH-dependent formation and search in municipal wastewater. <i>Water Research</i> , 2016, 88, 880-888.	11.3	97
22	Membrane-Enclosed Sorptive Coating. An Integrative Passive Sampler for Monitoring Organic Contaminants in Water. <i>Analytical Chemistry</i> , 2001, 73, 5191-5200.	6.5	96
23	Multivariate Discrimination between Modes of Toxic Action of Phenols. <i>QSAR and Combinatorial Science</i> , 2002, 21, 12.	1.2	93
24	Maternal phthalate exposure promotes allergic airway inflammation over 2 generations through epigenetic modifications. <i>Journal of Allergy and Clinical Immunology</i> , 2018, 141, 741-753.	2.9	92
25	Chemical Safety Assessment Using Read-Across: Assessing the Use of Novel Testing Methods to Strengthen the Evidence Base for Decision Making. <i>Environmental Health Perspectives</i> , 2015, 123, 1232-1240.	6.0	89
26	Correlation of aerobic biodegradability of sulfonated azo dyes with the chemical structure. <i>Chemosphere</i> , 2001, 45, 1-9.	8.2	88
27	QSAR analysis of the acute fish toxicity of organic phosphorothionates using theoretically derived molecular descriptors. <i>Environmental Toxicology and Chemistry</i> , 1990, 9, 417-428.	4.3	86
28	Accelerated Solvent Extraction of Semivolatile Organic Compounds from Biomonitoring Samples of Pine Needles and Mosses. <i>Analytical Chemistry</i> , 1998, 70, 4827-4835.	6.5	86
29	Quantitative Structure–Activity Analysis of the Algae Toxicity of Nitroaromatic Compounds. <i>Chemical Research in Toxicology</i> , 2000, 13, 441-450.	3.3	86
30	Fate of POPs (DDX, HCHs, PCBs) in upper soil layers of pine forests. <i>Science of the Total Environment</i> , 2002, 286, 143-154.	8.0	81
31	Aqueous Solubility–Molecular Size Relationships: A Mechanistic Case Study Using C10- to C19-Alkanes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 2760-2765.	2.5	78
32	Calibration of the Chemcatcher® passive sampler for monitoring selected polar and semi-polar pesticides in surface water. <i>Environmental Pollution</i> , 2008, 155, 52-60.	7.5	75
33	Evaluation of regional heavy metal deposition by multivariate analysis of element contents in pine tree barks. <i>Water, Air, and Soil Pollution</i> , 1995, 84, 367-383.	2.4	74
34	Quantitative Read-Across for Predicting the Acute Fish Toxicity of Organic Compounds. <i>Environmental Science & Technology</i> , 2011, 45, 4616-4622.	10.0	74
35	Occurrence and Toxicity of 331 Organic Pollutants in Large Rivers of North Germany over a Decade (1994 to 2004). <i>Environmental Science & Technology</i> , 2011, 45, 6167-6174.	10.0	73
36	ALGAL TOXICITY OF NITROBENZENES: COMBINED EFFECT ANALYSIS AS A PHARMACOLOGICAL PROBE FOR SIMILAR MODES OF INTERACTION. <i>Environmental Toxicology and Chemistry</i> , 2005, 24, 324.	4.3	71

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37	Predicting Michael-acceptor reactivity and toxicity through quantum chemical transition-state calculations. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 8400.	2.8	69
38	Chemical Domain of QSAR Models from Atom-Centered Fragments. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 2660-2669.	5.4	67
39	Effect-directed fractionation and identification of cytochrome P450A1-inducing halogenated aromatic hydrocarbons in a contaminated sediment. <i>Environmental Toxicology and Chemistry</i> , 2002, 21, 2654-2662.	4.3	66
40	Prediction of the Sorption of Organic Compounds into Soil Organic Matter from Molecular Structure. <i>Environmental Science & Technology</i> , 2006, 40, 7005-7011.	10.0	66
41	FIXED-EFFECT-LEVEL TOXICITY EQUIVALENTS—A SUITABLE PARAMETER FOR ASSESSING ETHOXYRESORUFIN-O-DEETHYLASE INDUCTION POTENCY IN COMPLEX ENVIRONMENTAL SAMPLES. <i>Environmental Toxicology and Chemistry</i> , 2000, 19, 2493.	4.3	63
42	Stepwise Discrimination between Four Modes of Toxic Action of Phenols in the <i>Tetrahymena pyriformis</i> Assay. <i>Chemical Research in Toxicology</i> , 2003, 16, 974-987.	3.3	62
43	Model and Mechanism: N-Hydroxylation of Primary Aromatic Amines by Cytochrome...P450. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 744-748.	13.8	62
44	Modeling Photoinduced Algal Toxicity of Polycyclic Aromatic Hydrocarbons. <i>Environmental Science & Technology</i> , 2005, 39, 4141-4149.	10.0	60
45	Anaerobic Microbial Transformation of Halogenated Aromatics and Fate Prediction Using Electron Density Modeling. <i>Environmental Science & Technology</i> , 2015, 49, 6018-6028.	10.0	60
46	Thiol Reactivity and Its Impact on the Ciliate Toxicity of α,β -Unsaturated Aldehydes, Ketones, and Esters. <i>Chemical Research in Toxicology</i> , 2010, 23, 1905-1912.	3.3	58
47	IDENTIFICATION OF TOXIC PRODUCTS OF ANTHRACENE PHOTOMODIFICATION IN SIMULATED SUNLIGHT. <i>Environmental Toxicology and Chemistry</i> , 2003, 22, 2228.	4.3	57
48	Epoxide and Thiirane Toxicity In vitro with the Ciliates <i>Tetrahymena pyriformis</i> : Structural Alerts Indicating Excess Toxicity. <i>Environmental Science & Technology</i> , 2011, 45, 5812-5819.	10.0	57
49	Modelling pKa of Carboxylic Acids and Chlorinated Phenols. <i>QSAR and Combinatorial Science</i> , 1996, 15, 121-132.	1.2	55
50	Polychlorinated naphthalenes in sediments from the industrial region of Bitterfeld. <i>Environmental Pollution</i> , 2003, 121, 81-85.	7.5	55
51	Prediction of the Temperature Dependency of Henry's Law Constant from Chemical Structure. <i>Environmental Science & Technology</i> , 2005, 39, 6705-6711.	10.0	53
52	Local Electrophilicity Predicts the Toxicity-Relevant Reactivity of Michael Acceptors. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 1605-1610.	4.6	53
53	Title is missing!. <i>Hydrobiologia</i> , 2001, 8, 161-178.	0.9	52
54	QUANTITATIVE STRUCTURE-PROPERTY RELATIONSHIPS FOR PREDICTING HENRY'S LAW CONSTANT FROM MOLECULAR STRUCTURE. <i>Environmental Toxicology and Chemistry</i> , 2003, 22, 1755.	4.3	52

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55	Prediction of liquid viscosity for organic compounds by a quantitative structure-property relationship. <i>Journal of Physical Organic Chemistry</i> , 2000, 13, 80-86.	1.9	51
56	Use of semipermeable membrane devices (SPMDs). <i>Environmental Science and Pollution Research</i> , 2001, 8, 27-34.	5.3	51
57	Octanol/Water Partition Coefficient of Selected Herbicides: Determination Using Shake-Flask Method and Reversed-Phase High-Performance Liquid Chromatography. <i>Journal of Chemical & Engineering Data</i> , 2004, 49, 1639-1642.	1.9	51
58	Description of the Electronic Structure of Organic Chemicals Using Semiempirical and Ab Initio Methods for Development of Toxicological QSARs. <i>Journal of Chemical Information and Modeling</i> , 2005, 45, 106-114.	5.4	51
59	Pesticide impact on aquatic invertebrates identified with Chemcatcher® passive samplers and the SPEARpesticides index. <i>Science of the Total Environment</i> , 2015, 537, 69-80.	8.0	51
60	Distribution of polychlorinated biphenyls, phthalic acid esters, polycyclic aromatic hydrocarbons and organochlorine substances in the Moscow River, Russia. <i>Environmental Pollution</i> , 2016, 210, 409-418.	7.5	51
61	Anthropogenic impacts on natural nitrogen isotope variations in <i>Pinus sylvestris</i> stands in an industrially polluted area. <i>Environmental Pollution</i> , 1997, 97, 175-181.	7.5	50
62	Contribution of waste water treatment plants to pesticide toxicity in agriculture catchments. <i>Ecotoxicology and Environmental Safety</i> , 2017, 145, 135-141.	6.0	49
63	Metabolic Mechanism of Aryl Phosphorus Flame Retardants by Cytochromes P450: A Combined Experimental and Computational Study on Triphenyl Phosphate. <i>Environmental Science & Technology</i> , 2018, 52, 14411-14421.	10.0	49
64	Advances in bioconcentration prediction. <i>Chemosphere</i> , 1988, 17, 1551-1574.	8.2	48
65	Rapid semi-continuous calibration and field test of membrane-enclosed silicone collector as passive water sampler. <i>Journal of Chromatography A</i> , 2006, 1124, 187-195.	3.7	47
66	Model Selection Based on Structural Similarity Method Description and Application to Water Solubility Prediction. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 636-641.	5.4	46
67	Identification of river basin specific pollutants and derivation of environmental quality standards: A case study in the Slovak Republic. <i>TrAC - Trends in Analytical Chemistry</i> , 2012, 41, 133-145.	11.4	46
68	Quantitative and qualitative models for carcinogenicity prediction for non-congeneric chemicals using CP ANN method for regulatory uses. <i>Molecular Diversity</i> , 2010, 14, 581-594.	3.9	45
69	Multivariate mode-of-action analysis of acute toxicity of phenols. <i>Aquatic Toxicology</i> , 1997, 38, 277-296.	4.0	43
70	Prediction of the Intrinsic Hydrogen Bond Acceptor Strength of Organic Compounds by Local Molecular Parameters. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 956-962.	5.4	43
71	Structure-activity relationships for chloro- and nitrophenol toxicity in the pollen tube growth test. <i>Environmental Toxicology and Chemistry</i> , 1996, 15, 1702-1708.	4.3	42
72	A comparative survey of chemistry-driven in silico methods to identify hazardous substances under REACH. <i>Regulatory Toxicology and Pharmacology</i> , 2013, 66, 301-314.	2.7	42

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73	Quantitative Structure-Property Relationships for the Polarizability, Solvatochromic Parameters and Lipophilicity. QSAR and Combinatorial Science, 1990, 9, 326-333.	1.2	41
74	Immission patterns of airborne pollutants in Argentina and Germany II. Biomonitoring of organochlorine compounds and polycyclic aromatics. Chemosphere, 1997, 34, 2505-2518.	8.2	41
75	Prediction of the Intrinsic Hydrogen Bond Acceptor Strength of Chemical Substances from Molecular Structure. Journal of Physical Chemistry A, 2009, 113, 10104-10112.	2.5	41
76	STRUCTURE-ACTIVITY RELATIONSHIPS FOR CHLORO- AND NITROPHENOL TOXICITY IN THE POLLEN TUBE GROWTH TEST. Environmental Toxicology and Chemistry, 1996, 15, 1702.	4.3	40
77	Modeling the H bond donor strength of -OH , -NH , and -CH sites by local molecular parameters. Journal of Computational Chemistry, 2009, 30, 1454-1464.	3.3	39
78	Computational Evidence for $\hat{\text{I}}\pm$ -Nitrosamino Radical as Initial Metabolite for Both the P450 Dealkylation and Denitrosation of Carcinogenic Nitrosamines. Journal of Physical Chemistry B, 2012, 116, 903-912.	2.6	39
79	Gas chromatographic determination of perfluorocarboxylic acids in aqueous samples – A tutorial review. Analytica Chimica Acta, 2017, 949, 8-22.	5.4	38
80	Perspectives for integrating human and environmental risk assessment and synergies with socio-economic analysis. Science of the Total Environment, 2013, 456-457, 307-316.	8.0	37
81	Quantum chemical analysis of the energy of proton transfer from phenol and chlorophenols to H ₂ O in the gas phase and in aqueous solution. Journal of Chemical Physics, 1998, 109, 9523-9528.	3.0	36
82	Ecotoxicological Hazard and Risk Assessment of Heavy Metal Contents in Agricultural Soils of Central Germany. Ecotoxicology and Environmental Safety, 1999, 42, 191-201.	6.0	36
83	Application of Neural Networks to Modeling and Estimating Temperature-Dependent Liquid Viscosity of Organic Compounds. Journal of Chemical Information and Computer Sciences, 2001, 41, 776-790.	2.8	35
84	Read-Across Prediction of the Acute Toxicity of Organic Compounds toward the Water Flea <i>Daphnia magna</i> . Molecular Informatics, 2013, 32, 108-120.	2.5	35
85	Cytotoxicity of metals toward rainbow trout R1 cell line. Environmental Toxicology and Water Quality, 1994, 9, 273-279.	0.5	34
86	A novel in vitro system for the determination of bioconcentration factors and the internal dose in zebrafish (<i>Danio rerio</i>) eggs. Chemosphere, 2009, 77, 928-933.	8.2	34
87	Acute and Chronic Toxicity toward the Bacteria <i>Vibrio fischeri</i> of Organic Narcotics and Epoxides: Structural Alerts for Epoxide Excess Toxicity. Chemical Research in Toxicology, 2010, 23, 1936-1946.	3.3	34
88	Diffusion Coefficients of Substituted Benzenes at High Dilution in Water. Journal of Chemical & Engineering Data, 1996, 41, 33-36.	1.9	33
89	Water solubility and octanol/water-partitioning of hydrophobic chlorinated organic substances determined by using SPME/GC. Fresenius' Journal of Analytical Chemistry, 1998, 360, 52-57.	1.5	33
90	Comparative application of solid-phase microextraction fibre assemblies and semi-permeable membrane devices as passive air samplers for semi-volatile chlorinated organic compounds. A case study on the landfill 'Grube Antonie' in Bitterfeld, Germany. Environmental Pollution, 2006, 144, 414-422.	7.5	33

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91	Estimation of Compartmental Half-lives of Organic Compounds – Structural Similarity versus EPI-Suite. <i>QSAR and Combinatorial Science</i> , 2007, 26, 542-549.	1.4	33
92	Exposure and ecotoxicological risk assessment of mixtures of top prescribed pharmaceuticals in Swedish freshwaters. <i>Chemosphere</i> , 2019, 220, 344-352.	8.2	33
93	Development of Both Linear and Nonlinear Methods To Predict the Liquid Viscosity at 20 °C of Organic Compounds. <i>Journal of Chemical Information and Computer Sciences</i> , 1997, 37, 1122-1128.	2.8	31
94	Application of preparative capillary gas chromatography (pcGC), automated structure generation and mutagenicity prediction to improve effect-directed analysis of genotoxicants in a contaminated groundwater. <i>Environmental Science and Pollution Research</i> , 2010, 17, 885-897.	5.3	31
95	Linear Solvation Energy Relationships as classifiers in non-target analysis – A capillary liquid chromatography approach. <i>Journal of Chromatography A</i> , 2011, 1218, 8192-8196.	3.7	31
96	Chemoavailability of Organic Electrophiles: Impact of Hydrophobicity and Reactivity on Their Aquatic Excess Toxicity. <i>Chemical Research in Toxicology</i> , 2016, 29, 952-962.	3.3	31
97	ERGO: Breaking Down the Wall between Human Health and Environmental Testing of Endocrine Disruptors. <i>International Journal of Molecular Sciences</i> , 2020, 21, 2954.	4.1	31
98	Computational material flow analysis for thousands of chemicals of emerging concern in European waters. <i>Journal of Hazardous Materials</i> , 2020, 397, 122655.	12.4	31
99	Dialysis of Persistent Organic Pollutants and Polycyclic Aromatic Hydrocarbons from Semipermeable Membranes. A Procedure Using an Accelerated Solvent Extraction Device. <i>Analytical Chemistry</i> , 2004, 76, 5503-5509.	6.5	30
100	Prediction models for the Abraham hydrogen bond donor strength: comparison of semi-empirical, <i>ab initio</i> , and DFT methods. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 1072-1080.	1.9	30
101	The OSIRIS Weight of Evidence approach: ITS for skin sensitisation. <i>Regulatory Toxicology and Pharmacology</i> , 2013, 67, 146-156.	2.7	30
102	¹⁵ N/ ¹⁴ N Analysis of Amino Acids with GC-C-IRMS - Methodical Investigations and Ecotoxicological Applications. <i>Isotopes in Environmental and Health Studies</i> , 1995, 31, 367-375.	1.0	29
103	Predictive QSPR models for estimating soil sorption coefficients: potential and limitations based on dominating processes. <i>Science of the Total Environment</i> , 1991, 109-110, 343-354.	8.0	28
104	Modeling Discrimination between Antibacterial and Non-Antibacterial Activity based on 3D Molecular Descriptors. <i>QSAR and Combinatorial Science</i> , 2003, 22, 113-128.	1.4	28
105	Silicone rod extraction of pharmaceuticals from water. <i>Analytical and Bioanalytical Chemistry</i> , 2007, 387, 1417-1421.	3.7	28
106	Comparative Analysis of QSAR Models for Predicting pKa of Organic Oxygen Acids and Nitrogen Bases from Molecular Structure. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 1949-1960.	5.4	28
107	Airborne trichloroacetic acid and its deposition in the catchment area of the Caspian Sea. <i>Environmental Pollution</i> , 1999, 104, 359-364.	7.5	27
108	Estimation of Soil Organic Carbon Normalized Sorption Coefficient (<i>K_{oc}</i>) Using Least Squares – Support Vector Machine. <i>QSAR and Combinatorial Science</i> , 2009, 28, 561-567.	1.4	27

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109	Structural Alerts for the Excess Toxicity of Acrylates, Methacrylates, and Propiolates Derived from Their Short-Term and Long-Term Bacterial Toxicity. <i>Chemical Research in Toxicology</i> , 2012, 25, 170-180.	3.3	27
110	Evaluation of various molecular parameters as predictors of bioconcentration in fish. <i>Ecotoxicology and Environmental Safety</i> , 1988, 15, 324-335.	6.0	26
111	Prediction of Physicochemical Properties of Organic Compounds from 2D Molecular Structure – Fragment Methods vs. LFER Models. <i>Chimia</i> , 2006, 60, 691-698.	0.6	26
112	PBT assessment under REACH: Screening for low aquatic bioaccumulation with QSAR classifications based on physicochemical properties to replace BCF in vivo testing on fish. <i>Science of the Total Environment</i> , 2018, 616-617, 97-106.	8.0	26
113	One-step cleanup for PAH residue analysis in plant matrices using size-exclusion chromatography. <i>Analytical and Bioanalytical Chemistry</i> , 2003, 376, 53-60.	3.7	25
114	Multilinear Regression and Comparative Molecular Field Analysis (CoMFA) of Azo Dye–Fiber Affinities. 2. Inclusion of Solution-Phase Molecular Orbital Descriptors. <i>Journal of Chemical Information and Computer Sciences</i> , 2003, 43, 1502-1512.	2.8	25
115	The Eco-Exposome Concept: Supporting an Integrated Assessment of Mixtures of Environmental Chemicals. <i>Environmental Toxicology and Chemistry</i> , 2022, 41, 30-45.	4.3	25
116	Gas-phase and solution-phase proton transfer to H ₂ O analyzed by high-level ab initio quantum chemistry including complete basis set and Gaussian theory schemes. <i>Chemical Physics Letters</i> , 1999, 302, 471-479.	2.6	24
117	Establishing Causality between Pollution and Effects at Different Levels of Biological Organization: The VALIMAR Project. <i>Human and Ecological Risk Assessment (HERA)</i> , 2003, 9, 171-194.	3.4	24
118	Adsorption of perfluorocarboxylic acids at the silica surface. <i>Chemical Communications</i> , 2017, 53, 589-592.	4.1	24
119	Application of different RP-HPLC methods for the determination of the octanol/water partition coefficient of selected tetrachlorobenzyltoluenes. <i>Chemosphere</i> , 2001, 45, 721-728.	8.2	23
120	Tautomer Identification and Tautomer Structure Generation Based on the InChI Code. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 1223-1232.	5.4	23
121	Chemoassay Screening of DNA-Reactive Mutagenicity with 4-(4-Nitrobenzyl)pyridine – Application to Epoxides, Oxetanes, and Sulfur Heterocycles. <i>Chemical Research in Toxicology</i> , 2012, 25, 2092-2102.	3.3	23
122	Prediction of aqueous solubility and the octanol-water partition coefficient for lipophilic organic compounds using molecular descriptors and physicochemical properties. <i>Chemosphere</i> , 1990, 21, 877-888.	8.2	22
123	Nontargeted detection and identification of (aromatic) amines in environmental samples based on diagnostic derivatization and LC-high resolution mass spectrometry. <i>Chemosphere</i> , 2017, 166, 300-310.	8.2	22
124	Backpropagation neural networks – recognition vs. prediction capability. <i>Environmental Toxicology and Chemistry</i> , 1994, 13, 743-747.	4.3	21
125	Estimation of vapour pressures for hydrocarbons and halogenated hydrocarbons from chemical structure by a neural network. <i>Chemosphere</i> , 1997, 34, 671-686.	8.2	21
126	Urease inhibition: a tool for toxicity identification in sediment elutriates. <i>Chemosphere</i> , 2000, 40, 829-834.	8.2	21

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127	Comparative Molecular Field Analysis (CoMFA) of Anionic Azo Dye-Fiber Affinities I: Gas-Phase Molecular Orbital Descriptors. <i>Journal of Chemical Information and Computer Sciences</i> , 2002, 42, 788-795.	2.8	21
128	White paper on the promotion of an integrated risk assessment concept in European regulatory frameworks for chemicals. <i>Science of the Total Environment</i> , 2015, 521-522, 211-218.	8.0	21
129	Inhalation TTC values: A new integrative grouping approach considering structural, toxicological and mechanistic features. <i>Regulatory Toxicology and Pharmacology</i> , 2016, 78, 8-23.	2.7	21
130	Anaerobic Dehalogenation of Chloroanilines by <i>Dehalococcoides mccartyi</i> Strain CBDB1 and <i>Dehalobacter</i> Strain 14DCB1 via Different Pathways as Related to Molecular Electronic Structure. <i>Environmental Science & Technology</i> , 2017, 51, 3714-3724.	10.0	21
131	Acute aquatic toxicity of alkyl phenol ethoxylates. <i>Ecotoxicology and Environmental Safety</i> , 1991, 21, 227-233.	6.0	20
132	Simple Algorithms for Determining the Molecular Symmetry. <i>Journal of Chemical Information and Computer Sciences</i> , 1999, 39, 728-737.	2.8	20
133	Impact of Orthogonal Signal Correction (OSC) on the Predictive Ability of CoMFA Models for the Ciliate Toxicity of Nitrobenzenes Dedicated to Professor Werner Klein, Schmallenberg (Germany), on the occasion of his 65th birthday. <i>QSAR and Combinatorial Science</i> , 2002, 21, 3.	1.2	20
134	Structure-Activity Relationships for the Toxicity of Substituted Poly-hydroxylated Benzenes to <i>Tetrahymena pyriformis</i> : Influence of Free Radical Formation. <i>QSAR and Combinatorial Science</i> , 2003, 22, 575-582.	1.4	20
135	Inhalation threshold of toxicological concern (TTC) – Structural alerts discriminate high from low repeated-dose inhalation toxicity. <i>Environment International</i> , 2016, 88, 123-132.	10.0	20
136	Solubility and partitioning studies with polycyclic aromatic hydrocarbons using an optimized SPME procedure. <i>Fresenius' Journal of Analytical Chemistry</i> , 1999, 363, 426-428.	1.5	19
137	The OSIRIS Weight of Evidence approach: ITS for the endpoints repeated-dose toxicity (RepDose ITS). <i>Regulatory Toxicology and Pharmacology</i> , 2013, 67, 157-169.	2.7	19
138	Perfluoroalkyl acids in aqueous samples from Germany and Kenya. <i>Environmental Science and Pollution Research</i> , 2017, 24, 11031-11043.	5.3	19
139	QSAR analysis of the acute toxicity of oxyethylated surfactants. <i>Chemosphere</i> , 1990, 21, 467-478.	8.2	18
140	Quantum chemical approach to estimate physicochemical compound properties: Application to substituted benzenes. <i>Environmental Toxicology and Chemistry</i> , 1995, 14, 2067-2076.	4.3	18
141	Prediction of Henry's law constant of benzene derivatives using quantum chemical continuum-solvation models. <i>Journal of Computational Chemistry</i> , 2000, 21, 17-34.	3.3	18
142	Title is missing!. <i>Hydrobiologia</i> , 2001, 8, 319-336.	0.9	18
143	Ecotoxicological Profiling of Transect River Elbe Sediments. <i>Clean - Soil, Air, Water</i> , 2005, 33, 555-569.	0.6	18
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