Gerrit SchÃ¼Ã¼rmann

List of Publications by Year
in descending order

219 papers	17,360 citations	34100 52 h-index	15265 126 g-index
237 all docs	237 docs citations	237 times ranked	19044 citing authors

#	Article	IF	Citations
1	The Ecoâ€Exposome Concept: Supporting an Integrated Assessment of Mixtures of Environmental Chemicals. Environmental Toxicology and Chemistry, 2022, 41, 30-45.	4.3	25
2	Calibration and field application of the Atlantic HLB Disk containing ChemcatcherÂ® passive sampler â€“ Quantitative monitoring of herbicides, other pesticides, and transformation products in German streams. Journal of Hazardous Materials, 2021, 410, 124538.	12.4	18
3	Pesticides are the dominant stressors for vulnerable insects in lowland streams. Water Research, 2021, 201, 117262.	11.3	118
4	Amino Reactivity of Glutardialdehyde andÂMonoaldehydesâ”€Chemoassay Profile vs Skin Sensitization Potency. Chemical Research in Toxicology, 2021, 34, 2353-2365.	3.3	4
5	Outer-sphere electron transfer does not underpin B₁₂-dependent olefinic reductive dehalogenation in anaerobes. Physical Chemistry Chemical Physics, 2021, 23, 27520-27524.	2.8	3
6	Polyethersulfone as suitable passive sampler for waterborne hydrophobic organic compounds â€“ Laboratory calibration and field test in the Sosiani river, Kenya. Science of the Total Environment, 2020, 699, 134056.	8.0	8
7	Dehalococcoides-Mediated B₁₂-Dependent Reductive Dehalogenation of Aromatics Does Not Proceed through Outer-Sphere Electron Transfer. Environmental Science & Technology, 2020, 54, 15751-15758.	10.0	6
8	In Silico Finding of Key Interaction Mediated Î±3Î²4 and Î±7 Nicotinic Acetylcholine Receptor Ligand Selectivity of Quinuclidine-Triazole Chemotype. International Journal of Molecular Sciences, 2020, 21, 6189.	4.1	5
9	Development of Novel Analogs of the Monocarboxylate Transporter Ligand FACH and Biological Validation of One Potential Radiotracer for Positron Emission Tomography (PET) Imaging. Molecules, 2020, 25, 2309.	3.8	4
10	A machine learning approach to discriminate MR1 binders: The importance of the phenol and carbonyl fragments. Journal of Molecular Structure, 2020, 1217, 128459.	3.6	3
11	ERGO: Breaking Down the Wall between Human Health and Environmental Testing of Endocrine Disrupters. International Journal of Molecular Sciences, 2020, 21, 2954.	4.1	31
12	Computational material flow analysis for thousands of chemicals of emerging concern in European waters. Journal of Hazardous Materials, 2020, 397, 122655.	12.4	31
13	Compartmentâ€Specific Screening Tools for Persistence: Potential Role and Application in the Regulatory Context. Integrated Environmental Assessment and Management, 2019, 15, 470-481.	2.9	4
14	Exposure and ecotoxicological risk assessment of mixtures of top prescribed pharmaceuticals in Swedish freshwaters. Chemosphere, 2019, 220, 344-352.	8.2	33
15	Strengthen the European collaborative environmental research to meet European policy goals for achieving a sustainable, non-toxic environment. Environmental Sciences Europe, 2019, 31, .	5.5	7
16	Interaction Mode and Regioselectivity in Vitamin B₁₂-Dependent Dehalogenation of Aryl Halides by Dehalococcoides mccartyi Strain CBDB1. Environmental Science & Technology, 2018, 52, 1834-1843.	10.0	10
17	PBT assessment under REACH: Screening for low aquatic bioaccumulation with QSAR classifications based on physicochemical properties to replace BCF in vivo testing on fish. Science of the Total Environment, 2018, 616-617, 97-106.	8.0	26
18	Maternal phthalate exposure promotes allergic airway inflammation over 2 generations through epigenetic modifications. Journal of Allergy and Clinical Immunology, 2018, 141, 741-753.	2.9	92

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19	Metabolic Mechanism of Aryl Phosphorus Flame Retardants by Cytochromes P450: A Combined Experimental and Computational Study on Triphenyl Phosphate. Environmental Science & Technology, 2018, 52, 14411-14421.	10.0	49
20	Computational Insight into the Activation Mechanism of Carcinogenic Nâ€™-Nitrosonornicotine (NNN) Catalyzed by Cytochrome P450. Environmental Science & Technology, 2018, 52, 11838-11847.	10.0	7
21	Glutathione Adduct Patterns of Michael-Acceptor Carbonyls. Environmental Science & Technology, 2017, 51, 4018-4026.	10.0	13
22	Anaerobic Dehalogenation of Chloroanilines by Dehalococcoides mccartyi Strain CBDB1 and Dehalobacter Strain 14DCB1 via Different Pathways as Related to Molecular Electronic Structure. Environmental Science & Technology, 2017, 51, 3714-3724.	10.0	21
23	The benzene metabolite 1,4-benzoquinone reduces regulatory T-cell function: AÂpotential mechanism for tobacco smokeâ€“associated atopic dermatitis. Journal of Allergy and Clinical Immunology, 2017, 140, 603-605.	2.9	2
24	An Integrated Data-Driven Strategy for Safe-by-Design Nanoparticles: The FP7 MODERN Project. Advances in Experimental Medicine and Biology, 2017, 947, 257-301.	1.6	6
25	Pesticides from wastewater treatment plant effluents affect invertebrate communities. Science of the Total Environment, 2017, 599-600, 387-399.	8.0	131
26	Passive sampling for spatial and temporal monitoring of organic pollutants in surface water of a rural-urban river in Kenya. Science of the Total Environment, 2017, 601-602, 453-460.	8.0	17
27	Adsorption of perfluorocarboxylic acids at the silica surface. Chemical Communications, 2017, 53, 589-592.	4.1	24
28	From the exposome to mechanistic understanding of chemical-induced adverse effects. Environment International, 2017, 99, 97-106.	10.0	146
29	Contribution of waste water treatment plants to pesticide toxicity in agriculture catchments. Ecotoxicology and Environmental Safety, 2017, 145, 135-141.	6.0	49
30	Gas chromatographic determination of perfluorocarboxylic acids in aqueous samples â€“ A tutorial review. Analytica Chimica Acta, 2017, 949, 8-22.	5.4	38
31	Perfluoroalkyl acids in aqueous samples from Germany and Kenya. Environmental Science and Pollution Research, 2017, 24, 11031-11043.	5.3	19
32	Nontargeted detection and identification of (aromatic) amines in environmental samples based on diagnostic derivatization and LC-high resolution mass spectrometry. Chemosphere, 2017, 166, 300-310.	8.2	22
33	Inhalation TTC values: A new integrative grouping approach considering structural, toxicological and mechanistic features. Regulatory Toxicology and Pharmacology, 2016, 78, 8-23.	2.7	21
34	Chemoavailability of Organic Electrophiles: Impact of Hydrophobicity and Reactivity on Their Aquatic Excess Toxicity. Chemical Research in Toxicology, 2016, 29, 952-962.	3.3	31
35	Varying Chirality Across Nicotinic Acetylcholine Receptor Subtypes: Selective Binding of Quinuclidine Triazole Compounds. ACS Medicinal Chemistry Letters, 2016, 7, 890-895.	2.8	10
36	Distribution of polychlorinated biphenyls, phthalic acid esters, polycyclic aromatic hydrocarbons and organochlorine substances in the Moscow River, Russia. Environmental Pollution, 2016, 210, 409-418.	7.5	51

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37	Development and application of screening tools for biodegradation in waterâ€“sediment systems and soil. Science of the Total Environment, 2016, 544, 1020-1030.	8.0	12
38	New hydrolysis products of the beta-lactam antibiotic amoxicillin, their pH-dependent formation and search in municipal wastewater. Water Research, 2016, 88, 880-888.	11.3	97
39	Variation in predicted internal concentrations in relation to PBPK model complexity for rainbow trout. Science of the Total Environment, 2016, 550, 586-597.	8.0	13
40	Inhalation threshold of toxicological concern (TTC) â€" Structural alerts discriminate high from low repeated-dose inhalation toxicity. Environment International, 2016, 88, 123-132.	10.0	20
41	A Branchâ€andâ€Bound Approach for Tautomer Enumeration. Molecular Informatics, 2015, 34, 263-275.	2.5	2
42	Chemical Safety Assessment Using Read-Across: Assessing the Use of Novel Testing Methods to Strengthen the Evidence Base for Decision Making. Environmental Health Perspectives, 2015, 123, 1232-1240.	6.0	89
43	Computational Biotransformation Profile of Paracetamol Catalyzed by Cytochrome P450. Chemical Research in Toxicology, 2015, 28, 585-596.	3.3	15
44	New systematically modified vesamicol analogs and their affinity and selectivity for the vesicular acetylcholine transporter â€" A critical examination of the lead structure. European Journal of Medicinal Chemistry, 2015, 100, 50-67.	5.5	12
45	Anaerobic Microbial Transformation of Halogenated Aromatics and Fate Prediction Using Electron Density Modeling. Environmental Science & Technology, 2015, 49, 6018-6028.	10.0	60
46	Calibration of ChemcatcherÂ® passive sampler for selected highly hydrophobic organic substances under fresh and sea water conditions. Environmental Science: Water Research and Technology, 2015, 1, 218-226.	2.4	9
47	White paper on the promotion of an integrated risk assessment concept in European regulatory frameworks for chemicals. Science of the Total Environment, 2015, 521-522, 211-218.	8.0	21
48	Pesticide impact on aquatic invertebrates identified with ChemcatcherÂ® passive samplers and the SPEARpesticides index. Science of the Total Environment, 2015, 537, 69-80.	8.0	51
49	Modeling and predicting pKa values of mono-hydroxylated polychlorinated biphenyls (HO-PCBs) and polybrominated diphenyl ethers (HO-PBDEs) by local molecular descriptors. Chemosphere, 2015, 138, 829-836.	8.2	14
50	The SOLUTIONS project: Challenges and responses for present and future emerging pollutants in land and water resources management. Science of the Total Environment, 2015, 503-504, 22-31.	8.0	163
51	Comparison of heavy metal content in two sludge drying reed beds of different age. Ecological Engineering, 2015, 74, 48-55.	3.6	17
52	Linear solvation energy relationships as classifier in non-target analysis â€" An approach for isocratic liquid chromatography. Journal of Chromatography A, 2014, 1324, 96-103.	3.7	8
53	Optimizing the aquatic toxicity assessment under REACH through an integrated testing strategy (ITS). Environmental Research, 2014, 135, 156-164.	7.5	11
54	Sorption of chlorimuron-ethyl on montmorillonite clays: effects of exchangeable cations, pH, and ionic strength. Environmental Science and Pollution Research, 2014, 21, 11587-11597.	5.3	6

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55	Integrated testing strategy (ITS) for bioaccumulation assessment under REACH. Environment International, 2014, 69, 40-50.	10.0	14
56	Individual and combined effects of mycotoxins from typical indoor moulds. Toxicology in Vitro, 2013, 27, 1970-1978.	2.4	14
57	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
58	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
59	Model and Mechanism: Nâ€Hydroxylation of Primary Aromatic Amines by Cytochromeâ€...P450. Angewandte Chemie - International Edition, 2013, 52, 744-748.	13.8	62
60	Readâ€Across Prediction of the Acute Toxicity of Organic Compounds toward the Water Flea Daphnia magna. Molecular Informatics, 2013, 32, 108-120.	2.5	35
61	Model Suite for Predicting the Aquatic Toxicity of Î±,Î²â€Unsaturated Esters Triggered by Their Chemoavailability. Molecular Informatics, 2013, 32, 98-107.	2.5	5
62	The OSIRIS Weight of Evidence approach: ITS mutagenicity and ITS carcinogenicity. Regulatory Toxicology and Pharmacology, 2013, 67, 170-181.	2.7	14
63	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
64	TTC: A new concept for inhalation exposure. Toxicology Letters, 2013, 221, S230.	0.8	1
65	The OSIRIS Weight of Evidence approach: ITS for skin sensitisation. Regulatory Toxicology and Pharmacology, 2013, 67, 146-156.	2.7	30
66	The OSIRIS Weight of Evidence approach: ITS for the endpoints repeated-dose toxicity (RepDose ITS). Regulatory Toxicology and Pharmacology, 2013, 67, 157-169.	2.7	19
67	Prediction of gas chromatographic retention indices as classifier in non-target analysis of environmental samples. Journal of Chromatography A, 2013, 1285, 139-147.	3.7	17
68	Computational Evidence for Î±-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
69	Linear solvation energy relationships as classifiers in non-target analysis â€“ A gas chromatographic approach. Journal of Chromatography A, 2012, 1264, 95-103.	3.7	9
70	Chemoassay Screening of DNA-Reactive Mutagenicity with 4-(4-Nitrobenzyl)pyridineâ€‰â€“â€‰Application to Epoxides, Oxetanes, and Sulfur Heterocycles. Chemical Research in Toxicology, 2012, 25, 2092-2102.	3.3	23
71	Identification of river basin specific pollutants and derivation of environmental quality standards: A case study in the Slovak Republic. TrAC - Trends in Analytical Chemistry, 2012, 41, 133-145.	11.4	46
72	Structural Alerts for the Excess Toxicity of Acrylates, Methacrylates, and Propiolates Derived from Their Short-Term and Long-Term Bacterial Toxicity. Chemical Research in Toxicology, 2012, 25, 170-180.	3.3	27

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73	Quantitative Read-Across for Predicting the Acute Fish Toxicity of Organic Compounds. Environmental Science & Technology, 2011, 45, 4616-4622.	10.0	74
74	Prediction of the Dissociation Constant pK_a of Organic Acids from Local Molecular Parameters of Their Electronic Ground State. Journal of Chemical Information and Modeling, 2011, 51, 2336-2344.	5.4	15
75	Epoxide and Thiirane Toxicity In vitro with the Ciliates Tetrahymena pyriformis: Structural Alerts Indicating Excess Toxicity. Environmental Science & Technology, 2011, 45, 5812-5819.	10.0	57
76	Occurrence and Toxicity of 331 Organic Pollutants in Large Rivers of North Germany over a Decade (1994 to 2004). Environmental Science & Technology, 2011, 45, 6167-6174.	10.0	73
77	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. Science of the Total Environment, 2011, 409, 2064-2077.	8.0	259
78	Determination of lindane leachability in soilâ€“biosolid systems and its bioavailability in wheat plants. Chemosphere, 2011, 84, 397-402.	8.2	17
79	Linear Solvation Energy Relationships as classifiers in non-target analysisâ€”A capillary liquid chromatography approach. Journal of Chromatography A, 2011, 1218, 8192-8196.	3.7	31
80	Predicting Michael-acceptor reactivity and toxicity through quantum chemical transition-state calculations. Organic and Biomolecular Chemistry, 2011, 9, 8400.	2.8	69
81	Prediction models for the Abraham hydrogen bond donor strength: comparison of semiâ€empirical,ab initio, and DFT methods. Journal of Physical Organic Chemistry, 2011, 24, 1072-1080.	1.9	30
82	1-Methyl-4-(4-nitrobenzoyl)pyridinium perchlorate. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o2542-o2543.	0.2	0
83	Predicting rate constants of OH radical reactions with organic substances: advances for oxygenated organics through a molecular orbital HF/6-31G** approach. Theoretical Chemistry Accounts, 2010, 127, 355-367.	1.4	6
84	Application of preparative capillary gas chromatography (pcGC), automated structure generation and mutagenicity prediction to improve effect-directed analysis of genotoxicants in a contaminated groundwater. Environmental Science and Pollution Research, 2010, 17, 885-897.	5.3	31
85	Quantitative and qualitative models for carcinogenicity prediction for non-congeneric chemicals using CP ANN method for regulatory uses. Molecular Diversity, 2010, 14, 581-594.	3.9	45
86	Tautomer Identification and Tautomer Structure Generation Based on the InChI Code. Journal of Chemical Information and Modeling, 2010, 50, 1223-1232.	5.4	23
87	Prediction of Michael-Type Acceptor Reactivity toward Glutathione. Chemical Research in Toxicology, 2010, 23, 1576-1585.	3.3	115
88	Acute and Chronic Toxicity toward the Bacteria Vibrio fischeri of Organic Narcotics and Epoxides: Structural Alerts for Epoxide Excess Toxicity. Chemical Research in Toxicology, 2010, 23, 1936-1946.	3.3	34
89	Comparative Analysis of QSAR Models for Predicting pKa of Organic Oxygen Acids and Nitrogen Bases from Molecular Structure. Journal of Chemical Information and Modeling, 2010, 50, 1949-1960.	5.4	28
90	Local Electrophilicity Predicts the Toxicity-Relevant Reactivity of Michael Acceptors. Journal of Physical Chemistry Letters, 2010, 1, 1605-1610.	4.6	53

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91	Thiol Reactivity and Its Impact on the Ciliate Toxicity of Î±,Î²-Unsaturated Aldehydes, Ketones, and Esters. Chemical Research in Toxicology, 2010, 23, 1905-1912.	3.3	58
92	Modeling the H bond donor strength of ï£¿OH, ï£¿NH, and ï£¿CH sites by local molecular parameters. Journal of Computational Chemistry, 2009, 30, 1454-1464.	3.3	39
93	Estimation of Soil Organic Carbon Normalized Sorption Coefficient (K_{oc}) Using Least Squaresâ€Support Vector Machine. QSAR and Combinatorial Science, 2009, 28, 561-567.	1.4	27
94	A novel in vitro system for the determination of bioconcentration factors and the internal dose in zebrafish (Danio rerio) eggs. Chemosphere, 2009, 77, 928-933.	8.2	34
95	Prediction of the Intrinsic Hydrogen Bond Acceptor Strength of Organic Compounds by Local Molecular Parameters. Journal of Chemical Information and Modeling, 2009, 49, 956-962.	5.4	43
96	Applicability domain of TTC (Threshold of Toxicological Concern) schemesâ€"A conceptual approach. Toxicology Letters, 2009, 189, S11.	0.8	0
97	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
98	Kinetic Glutathione Chemoassay To Quantify Thiol Reactivity of Organic Electrophilesâ€"Application to Î±,Î²-Unsaturated Ketones, Acrylates, and Propiolates. Chemical Research in Toxicology, 2009, 22, 742-750.	3.3	100
99	Chemical Domain of QSAR Models from Atom-Centered Fragments. Journal of Chemical Information and Modeling, 2009, 49, 2660-2669.	5.4	67
100	External Validation and Prediction Employing the Predictive Squared Correlation Coefficient â€" Test Set Activity Mean vs Training Set Activity Mean. Journal of Chemical Information and Modeling, 2008, 48, 2140-2145.	5.4	461
101	First CoMFA Characterization of Vesamicol Analogs as Ligands for the Vesicular Acetylcholine Transporter. Journal of Medicinal Chemistry, 2008, 51, 2128-2136.	6.4	10
102	Determination of Temperature-Dependent Henryâ€™s Law Constant of Four Oxygenated Solutes in Water Using Headspace Solid-Phase Microextraction Technique. Journal of Chemical & Engineering Data, 2008, 53, 2873-2877.	1.9	8
103	Calibration of the ChemcatcherÂ® passive sampler for monitoring selected polar and semi-polar pesticides in surface water. Environmental Pollution, 2008, 155, 52-60.	7.5	75
104	Indirect Photolysis of Organic Compounds: Prediction of OH Reaction Rate Constants through Molecular Orbital Calculations. Journal of Physical Chemistry A, 2008, 112, 11391-11399.	2.5	15
105	Chapter 10 Membrane-enclosed sorptive coating for the monitoring of organic compounds in water. Comprehensive Analytical Chemistry, 2007, 48, 231-249.	1.3	3
106	Comment on â€œDiscriminating toxicant classes by mode of action: 3. Substructure indicatorsâ€•(M.) Tj ETQq0 0 0 rgBT /Overlock 10 T 2007, 18, 621-624.	2.2	3
107	Estimation of Compartmental Half-lives of Organic Compounds â€“ Structural Similarityversus EPI-Suite. QSAR and Combinatorial Science, 2007, 26, 542-549.	1.4	33
108	Silicone rod extraction of pharmaceuticals from water. Analytical and Bioanalytical Chemistry, 2007, 387, 1417-1421.	3.7	28

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109	Model Selection Based on Structural Similarityâ˜Method Description and Application to Water Solubility Prediction. Journal of Chemical Information and Modeling, 2006, 46, 636-641.	5.4	46
110	Prediction of the Sorption of Organic Compounds into Soil Organic Matter from Molecular Structure. Environmental Science & Technology, 2006, 40, 7005-7011.	10.0	66
111	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 â€œGrube Antonieâ€•in Bitterfeld, Germany. Environmental Pollution, 2006, 144, 414-422.	7.5	33
112	Prediction of Physicochemical Properties of Organic Compounds from 2D Molecular Structure â€“ Fragment Methods vs. LFER Models. Chimia, 2006, 60, 691-698.	0.6	26
113	Rapid semi-continuous calibration and field test of membrane-enclosed silicone collector as passive water sampler. Journal of Chromatography A, 2006, 1124, 187-195.	3.7	47
114	ACUTE TO CHRONIC RATIOS IN AQUATIC TOXICITYâ€”VARIATION ACROSS TROPHIC LEVELS AND RELATIONSHIP WITH CHEMICAL STRUCTURE. Environmental Toxicology and Chemistry, 2006, 25, 2937.	4.3	110
115	Neue Kooperation in den Umweltwissenschaften â€” Assoziation zwischen GDCh und UWSF. Environmental Sciences Europe, 2006, 18, 78-79.	0.1	1
116	Influence of different emission sources on atmospheric organochlorine patterns in Germany. Atmospheric Environment, 2006, 40, 943-957.	4.1	17
117	Indirect determination of low vapour pressures using solid-phase microextractionâ€”application to tetrachlorobenzenes and tetrachlorobenzyltoluenes. Journal of Chromatography A, 2005, 1072, 93-97.	3.7	9
118	Postgraduale Weiterbildung mit dem zertifizierten Abschluss FachÃ¶kotoxikologin/e GDCh/SETAC. Environmental Sciences Europe, 2005, 17, 129-130.	0.1	2
119	Prediction of the Temperature Dependency of Henry's Law Constant from Chemical Structure. Environmental Science & Technology, 2005, 39, 6705-6711.	10.0	53
120	Modeling Photoinduced Algal Toxicity of Polycyclic Aromatic Hydrocarbons. Environmental Science & Technology, 2005, 39, 4141-4149.	10.0	60
121	ALGAL TOXICITY OF NITROBENZENES: COMBINED EFFECT ANALYSIS AS A PHARMACOLOGICAL PROBE FOR SIMILAR MODES OF INTERACTION. Environmental Toxicology and Chemistry, 2005, 24, 324.	4.3	71
122	Ecotoxicological Profiling of Transect River Elbe Sediments. Clean - Soil, Air, Water, 2005, 33, 555-569.	0.6	18
123	Performance of semipermeable membrane devices for sampling of organic contaminants in groundwater. Journal of Environmental Monitoring, 2005, 7, 500.	2.1	16
124	Structural AlertsA New Classification Model to Discriminate Excess Toxicity from Narcotic Effect Levels of Organic Compounds in the Acute Daphnid Assay. Chemical Research in Toxicology, 2005, 18, 536-555.	3.3	174
125	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
126	Octanol/Water Partition Coefficient of Selected Herbicides:â€‰ Determination Using Shake-Flask Method and Reversed-Phase High-Performance Liquid Chromatography. Journal of Chemical & Engineering Data, 2004, 49, 1639-1642.	1.9	51

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127	Dialysis of Persistent Organic Pollutants and Polycyclic Aromatic Hydrocarbons from Semipermeable Membranes. A Procedure Using an Accelerated Solvent Extraction Device. Analytical Chemistry, 2004, 76, 5503-5509.	6.5	30
128	QUANTITATIVE STRUCTUREâ€“PROPERTY RELATIONSHIPS FOR PREDICTING HENRY'S LAW CONSTANT FROM MOLECULAR STRUCTURE. Environmental Toxicology and Chemistry, 2003, 22, 1755.	4.3	52
129	MIXTURE TOXICITY AND ITS MODELING BY QUANTITATIVE STRUCTUREâ€“ACTIVITY RELATIONSHIPS. Environmental Toxicology and Chemistry, 2003, 22, 1900.	4.3	326
130	IDENTIFICATION OF TOXIC PRODUCTS OF ANTHRACENE PHOTOMODIFICATION IN SIMULATED SUNLIGHT. Environmental Toxicology and Chemistry, 2003, 22, 2228.	4.3	57
131	One-step cleanup for PAH residue analysis in plant matrices using size-exclusion chromatography. Analytical and Bioanalytical Chemistry, 2003, 376, 53-60.	3.7	25
132	ToxizitÃtsreduktion durch (Grundwasser-) Sanierung?. Grundwasser, 2003, 8, 32-40.	1.4	0
133	Structure-Activity Relationships for the Toxicity of Substituted Poly-hydroxylated Benzenes toTetrahymena pyriformis: Influence of Free Radical Formation. QSAR and Combinatorial Science, 2003, 22, 575-582.	1.4	20
134	Modeling Discrimination between Antibacterial and Non-Antibacterial Activity based on 3D Molecular Descriptors. QSAR and Combinatorial Science, 2003, 22, 113-128.	1.4	28
135	Multilinear Regression and Comparative Molecular Field Analysis (CoMFA) of Azo Dyeâ^'Fiber Affinities. 2. Inclusion of Solution-Phase Molecular Orbital Descriptors. Journal of Chemical Information and Computer Sciences, 2003, 43, 1502-1512.	2.8	25
136	Stepwise Discrimination between Four Modes of Toxic Action of Phenols in the Tetrahymena pyriformis Assay. Chemical Research in Toxicology, 2003, 16, 974-987.	3.3	62
137	Polychlorinated naphthalenes in sediments from the industrial region of Bitterfeld. Environmental Pollution, 2003, 121, 81-85.	7.5	55
138	Establishing Causality between Pollution and Effects at Different Levels of Biological Organization: The VALIMAR Project. Human and Ecological Risk Assessment (HERA), 2003, 9, 171-194.	3.4	24
139	Calibrating the Uptake Kinetics of Semipermeable Membrane Devices in Water:Â Impact of Hydrodynamics. Environmental Science & Technology, 2002, 36, 290-296.	10.0	117
140	Comparative Molecular Field Analysis (CoMFA) of Anionic Azo Dye-Fiber Affinities I:â€‰ Gas-Phase Molecular Orbital Descriptors. Journal of Chemical Information and Computer Sciences, 2002, 42, 788-795.	2.8	21
141	Structure-Based Classification of Antibacterial Activity. Journal of Chemical Information and Computer Sciences, 2002, 42, 869-878.	2.8	97
142	Aqueous Solubilityâ^'Molecular Size Relationships:â€‰ A Mechanistic Case Study Using C10- to C19-Alkanes. Journal of Physical Chemistry A, 2002, 106, 2760-2765.	2.5	78
143	Effects of trichloroacetic acid on the nitrogen metabolism of Pinus sylvestris â€“ a tracer study. Chemosphere, 2002, 46, 259-266.	8.2	9
144	Fate of POPs (DDX, HCHs, PCBs) in upper soil layers of pine forests. Science of the Total Environment, 2002, 286, 143-154.	8.0	81

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145	Multivariate Discrimination between Modes of Toxic Action of Phenols. QSAR and Combinatorial Science, 2002, 21, 12.	1.2	93
146	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. QSAR and Combinatorial Science, 2002, 21, 3.	1.2	20
147	Effectâ€directed fractionation and identification of cytochrome P4501Aâ€inducing halogenated aromatic hydrocarbons in a contaminated sediment. Environmental Toxicology and Chemistry, 2002, 21, 2654-2662.	4.3	66
148	Application of different RP-HPLC methods for the determination of the octanol/water partition coefficient of selected tetrachlorobenzyltoluenes. Chemosphere, 2001, 45, 721-728.	8.2	23
149	Correlation of aerobic biodegradability of sulfonated azo dyes with the chemical structure. Chemosphere, 2001, 45, 1-9.	8.2	88
150	Persistent organic pollutants in agricultural soils of central Germany. Science of the Total Environment, 2001, 277, 187-198.	8.0	217
151	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
152	Membrane-Enclosed Sorptive Coating. An Integrative Passive Sampler for Monitoring Organic Contaminants in Water. Analytical Chemistry, 2001, 73, 5191-5200.	6.5	96
153	Use of semipermeable membrane devices (SPMDs). Environmental Science and Pollution Research, 2001, 8, 27-34.	5.3	51
154	QSAR Modeling of Antimycobacterial Activity and Activity Against Other Bacteria of 3-Formyl Rifamycin SV Derivatives. QSAR and Combinatorial Science, 2001, 20, 298-318.	1.2	6
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