Ralph KÃ¼hne

List of Publications by Year
in descending order

60 papers	3,765 citations	172457 29 h-index	133252 59 g-index
61 all docs	61 docs citations	61 times ranked	4299 citing authors

#	Article	IF	Citations
1	Organic chemicals jeopardize the health of freshwater ecosystems on the continental scale. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 9549-9554.	7.1	604
2	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
3	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
4	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
5	Effects of Pesticides Monitored with Three Sampling Methods in 24 Sites on Macroinvertebrates and Microorganisms. Environmental Science & Technology, 2011, 45, 1665-1672.	10.0	163
6	Micropollutants in European rivers: A mode of action survey to support the development of effectâ€based tools for water monitoring. Environmental Toxicology and Chemistry, 2016, 35, 1887-1899.	4.3	161
7	Group contribution methods to estimate water solubility of organic chemicals. Chemosphere, 1995, 30, 2061-2077.	8.2	132
8	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
9	Fish Embryo Toxicity Test: Identification of Compounds with Weak Toxicity and Analysis of Behavioral Effects To Improve Prediction of Acute Toxicity for Neurotoxic Compounds. Environmental Science & Technology, 2015, 49, 7002-7011.	10.0	99
10	Applicability of the fish embryo acute toxicity (FET) test (OECD 236) in the regulatory context of Registration, Evaluation, Authorisation, and Restriction of Chemicals (REACH). Environmental Toxicology and Chemistry, 2018, 37, 657-670.	4.3	97
11	Multivariate Discrimination between Modes of Toxic Action of Phenols. QSAR and Combinatorial Science, 2002, 21, 12.	1.2	93
12	Quantitative Read-Across for Predicting the Acute Fish Toxicity of Organic Compounds. Environmental Science & Technology, 2011, 45, 4616-4622.	10.0	74
13	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
14	Chemical Domain of QSAR Models from Atom-Centered Fragments. Journal of Chemical Information and Modeling, 2009, 49, 2660-2669.	5.4	67
15	Prediction of the Sorption of Organic Compounds into Soil Organic Matter from Molecular Structure. Environmental Science & Technology, 2006, 40, 7005-7011.	10.0	66
16	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
17	Prediction of the Temperature Dependency of Henry's Law Constant from Chemical Structure. Environmental Science & Technology, 2005, 39, 6705-6711.	10.0	53
18	Contribution of waste water treatment plants to pesticide toxicity in agriculture catchments. Ecotoxicology and Environmental Safety, 2017, 145, 135-141.	6.0	49

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19	Model Selection Based on Structural Similarityâˆ’Method Description and Application to Water Solubility Prediction. Journal of Chemical Information and Modeling, 2006, 46, 636-641.	5.4	46
20	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
21	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
22	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
23	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
24	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
25	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
26	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
27	Estimation of Compartmental Half-lives of Organic Compounds â€" Structural Similarityversus EPI-Suite. QSAR and Combinatorial Science, 2007, 26, 542-549.	1.4	33
28	Exposure and ecotoxicological risk assessment of mixtures of top prescribed pharmaceuticals in Swedish freshwaters. Chemosphere, 2019, 220, 344-352.	8.2	33
29	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
30	Computational material flow analysis for thousands of chemicals of emerging concern in European waters. Journal of Hazardous Materials, 2020, 397, 122655.	12.4	31
31	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
32	Modeling Discrimination between Antibacterial and Non-Antibacterial Activity based on 3D Molecular Descriptors. QSAR and Combinatorial Science, 2003, 22, 113-128.	1.4	28
33	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
34	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
35	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
36	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

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37	Predicting Fate-Related Physicochemical Properties. , 2007, , 375-426.		24
38	Tautomer Identification and Tautomer Structure Generation Based on the InChI Code. Journal of Chemical Information and Modeling, 2010, 50, 1223-1232.	5.4	23
39	Model-predicted occurrence of multiple pharmaceuticals in Swedish surface waters and their flushing to the Baltic Sea. Environmental Pollution, 2017, 223, 595-604.	7.5	22
40	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
41	Estimation of vapour pressures for hydrocarbons and halogenated hydrocarbons from chemical structure by a neural network. Chemosphere, 1997, 34, 671-686.	8.2	21
42	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
43	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
44	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
45	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
46	Influence of different emission sources on atmospheric organochlorine patterns in Germany. Atmospheric Environment, 2006, 40, 943-957.	4.1	17
47	Error propagation in fugacity levelâ€‘II models in the case of uncertain physicochemical compound properties. Environmental Toxicology and Chemistry, 1997, 16, 2067-2069.	4.3	16
48	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
49	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
50	The OSIRIS Weight of Evidence approach: ITS mutagenicity and ITS carcinogenicity. Regulatory Toxicology and Pharmacology, 2013, 67, 170-181.	2.7	14
51	Integrated testing strategy (ITS) for bioaccumulation assessment under REACH. Environment International, 2014, 69, 40-50.	10.0	14
52	Short Communicationâ€"ERROR PROPAGATION IN FUGACITY LEVEL-III MODELS IN THE CASE OF UNCERTAIN PHYSICOCHEMICAL COMPOUND PROPERTIES. Environmental Toxicology and Chemistry, 1997, 16, 2067.	4.3	14
53	Evaluation of route-to-route extrapolation factors based on assessment of repeated dose toxicity studies compiled in the database RepDoseÂ®. Toxicology Letters, 2016, 261, 32-40.	0.8	13
54	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

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55	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
56	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
57	Multimedia level-III partitioning and residence times of xenobiotics in water-rich and water-poor environments. Environmental Toxicology and Chemistry, 2000, 19, 1430-1440.	4.3	4
58	Comment on "Discriminating toxicant classes by mode of action: 3. Substructure indicators"(M.) Tj ETQq0 0 0 rgBT /Overlock 10 T 2007, 18, 621-624.	2.2	3
59	A Branch-and-Bound Approach for Tautomer Enumeration. Molecular Informatics, 2015, 34, 263-275.	2.5	2
60	Applicability domain of TTC (Threshold of Toxicological Concern) schemes—A conceptual approach. Toxicology Letters, 2009, 189, S11.	0.8	0