

Ralph KÃ¼hne

List of Publications by Year in descending order

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Version: 2024-02-01

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	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
2	Exposure and ecotoxicological risk assessment of mixtures of top prescribed pharmaceuticals in Swedish freshwaters. <i>Chemosphere</i> , 2019, 220, 344-352.	8.2	33
3	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
4	Applicability of the fish embryo acute toxicity (FET) test (OECD 236) in the regulatory context of Registration, Evaluation, Authorisation, and Restriction of Chemicals (REACH). <i>Environmental Toxicology and Chemistry</i> , 2018, 37, 657-670.	4.3	97
5	Model-predicted occurrence of multiple pharmaceuticals in Swedish surface waters and their flushing to the Baltic Sea. <i>Environmental Pollution</i> , 2017, 223, 595-604.	7.5	22
6	An Integrated Data-Driven Strategy for Safe-by-Design Nanoparticles: The FP7 MODERN Project. <i>Advances in Experimental Medicine and Biology</i> , 2017, 947, 257-301.	1.6	6
7	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
8	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
9	Micropollutants in European rivers: A mode of action survey to support the development of effect-based tools for water monitoring. <i>Environmental Toxicology and Chemistry</i> , 2016, 35, 1887-1899.	4.3	161
10	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
11	Evaluation of route-to-route extrapolation factors based on assessment of repeated dose toxicity studies compiled in the database RepDose [®] . <i>Toxicology Letters</i> , 2016, 261, 32-40.	0.8	13
12	Variation in predicted internal concentrations in relation to PBPK model complexity for rainbow trout. <i>Science of the Total Environment</i> , 2016, 550, 586-597.	8.0	13
13	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
14	A Branch-and-Bound Approach for Tautomer Enumeration. <i>Molecular Informatics</i> , 2015, 34, 263-275.	2.5	2
15	Fish Embryo Toxicity Test: Identification of Compounds with Weak Toxicity and Analysis of Behavioral Effects To Improve Prediction of Acute Toxicity for Neurotoxic Compounds. <i>Environmental Science & Technology</i> , 2015, 49, 7002-7011.	10.0	99
16	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
17	Integrated testing strategy (ITS) for bioaccumulation assessment under REACH. <i>Environment International</i> , 2014, 69, 40-50.	10.0	14
18	Organic chemicals jeopardize the health of freshwater ecosystems on the continental scale. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 9549-9554.	7.1	604

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19	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
20	Read-Across Prediction of the Acute Toxicity of Organic Compounds toward the Water Flea <i>Daphnia magna</i> . <i>Molecular Informatics</i> , 2013, 32, 108-120.	2.5	35
21	The OSIRIS Weight of Evidence approach: ITS mutagenicity and ITS carcinogenicity. <i>Regulatory Toxicology and Pharmacology</i> , 2013, 67, 170-181.	2.7	14
22	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
23	Quantitative Read-Across for Predicting the Acute Fish Toxicity of Organic Compounds. <i>Environmental Science & Technology</i> , 2011, 45, 4616-4622.	10.0	74
24	Effects of Pesticides Monitored with Three Sampling Methods in 24 Sites on Macroinvertebrates and Microorganisms. <i>Environmental Science & Technology</i> , 2011, 45, 1665-1672.	10.0	163
25	Prediction of the Dissociation Constant pK_a of Organic Acids from Local Molecular Parameters of Their Electronic Ground State. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 2336-2344.	5.4	15
26	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
27	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
28	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
29	Predicting rate constants of OH radical reactions with organic substances: advances for oxygenated organics through a molecular orbital HF/6-31G** approach. <i>Theoretical Chemistry Accounts</i> , 2010, 127, 355-367.	1.4	6
30	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
31	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
32	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
33	Comparative Analysis of QSAR Models for Predicting pK_a 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
34	Modeling the H bond donor strength of \ddot{X}_2OH , \ddot{X}_2NH , and \ddot{X}_2CH sites by local molecular parameters. <i>Journal of Computational Chemistry</i> , 2009, 30, 1454-1464.	3.3	39
35	Estimation of Soil Organic Carbon Normalized Sorption Coefficient (K_{oc}) Using Least Squares-Support Vector Machine. <i>QSAR and Combinatorial Science</i> , 2009, 28, 561-567.	1.4	27
36	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

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37	Applicability domain of TTC (Threshold of Toxicological Concern) schemes – A conceptual approach. Toxicology Letters, 2009, 189, S11.	0.8	0
38	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
39	Chemical Domain of QSAR Models from Atom-Centered Fragments. Journal of Chemical Information and Modeling, 2009, 49, 2660-2669.	5.4	67
40	External Validation and Prediction Employing the Predictive Squared Correlation Coefficient – Test Set Activity Mean vs Training Set Activity Mean. Journal of Chemical Information and Modeling, 2008, 48, 2140-2145.	5.4	461
41	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
42	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
43	Estimation of Compartmental Half-lives of Organic Compounds – Structural Similarity versus EPI-Suite. QSAR and Combinatorial Science, 2007, 26, 542-549.	1.4	33
44	Predicting Fate-Related Physicochemical Properties. , 2007, , 375-426.		24
45	Model Selection Based on Structural Similarity – Method Description and Application to Water Solubility Prediction. Journal of Chemical Information and Modeling, 2006, 46, 636-641.	5.4	46
46	Prediction of the Sorption of Organic Compounds into Soil Organic Matter from Molecular Structure. Environmental Science & Technology, 2006, 40, 7005-7011.	10.0	66
47	Prediction of Physicochemical Properties of Organic Compounds from 2D Molecular Structure – Fragment Methods vs. LFER Models. Chimia, 2006, 60, 691-698.	0.6	26
48	ACUTE TO CHRONIC RATIOS IN AQUATIC TOXICITY – VARIATION ACROSS TROPHIC LEVELS AND RELATIONSHIP WITH CHEMICAL STRUCTURE. Environmental Toxicology and Chemistry, 2006, 25, 2937.	4.3	110
49	Influence of different emission sources on atmospheric organochlorine patterns in Germany. Atmospheric Environment, 2006, 40, 943-957.	4.1	17
50	Prediction of the Temperature Dependency of Henry's Law Constant from Chemical Structure. Environmental Science & Technology, 2005, 39, 6705-6711.	10.0	53
51	Structural Alerts – A 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
52	Modeling Discrimination between Antibacterial and Non-Antibacterial Activity based on 3D Molecular Descriptors. QSAR and Combinatorial Science, 2003, 22, 113-128.	1.4	28
53	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
54	Multivariate Discrimination between Modes of Toxic Action of Phenols. QSAR and Combinatorial Science, 2002, 21, 12.	1.2	93

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55	Multimedia levelâ€” partitioning and residence times of xenobiotics in waterâ€”rich and waterâ€”poor environments. <i>Environmental Toxicology and Chemistry</i> , 2000, 19, 1430-1440.	4.3	4
56	Ecotoxicological Hazard and Risk Assessment of Heavy Metal Contents in Agricultural Soils of Central Germany. <i>Ecotoxicology and Environmental Safety</i> , 1999, 42, 191-201.	6.0	36
57	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
58	Error propagation in fugacity levelâ€” models in the case of uncertain physicochemical compound properties. <i>Environmental Toxicology and Chemistry</i> , 1997, 16, 2067-2069.	4.3	16
59	Short Communicationâ€”ERROR PROPAGATION IN FUGACITY LEVEL-III MODELS IN THE CASE OF UNCERTAIN PHYSICOCHEMICAL COMPOUND PROPERTIES. <i>Environmental Toxicology and Chemistry</i> , 1997, 16, 2067.	4.3	14
60	Group contribution methods to estimate water solubility of organic chemicals. <i>Chemosphere</i> , 1995, 30, 2061-2077.	8.2	132