John F Wambaugh

List of Publications by Year
in descending order

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88 papers	6,846 citations	61984 43 h-index	62596 80 g-index
96 all docs	96 docs citations	96 times ranked	5011 citing authors

#	Article	IF	Citations
1	The CompTox Chemistry Dashboard: a community data resource for environmental chemistry. Journal of Cheminformatics, 2017, 9, 61.	6.1	674
2	ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology. Chemical Research in Toxicology, 2016, 29, 1225-1251.	3.3	456
3	Integration of Dosimetry, Exposure, and High-Throughput Screening Data in Chemical Toxicity Assessment. Toxicological Sciences, 2012, 125, 157-174.	3.1	336
4	httk: R Package for High-Throughput Toxicokinetics. Journal of Statistical Software, 2017, 79, 1-26.	3.7	256
5	The Next Generation Blueprint of Computational Toxicology at the U.S. Environmental Protection Agency. Toxicological Sciences, 2019, 169, 317-332.	3.1	225
6	Superconducting Fluxon Pumps and Lenses. Physical Review Letters, 1999, 83, 5106-5109.	7.8	222
7	Incorporating Human Dosimetry and Exposure into High-ThroughputIn VitroToxicity Screening. Toxicological Sciences, 2010, 117, 348-358.	3.1	222
8	Toxicity testing in the 21st century: progress in the past decade and future perspectives. Archives of Toxicology, 2020, 94, 1-58.	4.2	209
9	Incorporating High-Throughput Exposure Predictions With Dosimetry-AdjustedIn VitroBioactivity to Inform Chemical Toxicity Testing. Toxicological Sciences, 2015, 148, 121-136.	3.1	190
10	High Throughput Heuristics for Prioritizing Human Exposure to Environmental Chemicals. Environmental Science & Technology, 2014, 48, 12760-12767.	10.0	185
11	Editor's Highlight: Analysis of the Effects of Cell Stress and Cytotoxicity onIn VitroAssay Activity Across a Diverse Chemical and Assay Space. Toxicological Sciences, 2016, 152, 323-339.	3.1	171
12	In vitro to in vivo extrapolation for high throughput prioritization and decision making. Toxicology in Vitro, 2018, 47, 213-227.	2.4	162
13	Integrating tools for non-targeted analysis research and chemical safety evaluations at the US EPA. Journal of Exposure Science and Environmental Epidemiology, 2018, 28, 411-426.	3.9	148
14	From the exposome to mechanistic understanding of chemical-induced adverse effects. Environment International, 2017, 99, 97-106.	10.0	146
15	Linking high resolution mass spectrometry data with exposure and toxicity forecasts to advance high-throughput environmental monitoring. Environment International, 2016, 88, 269-280.	10.0	143
16	High-Throughput Models for Exposure-Based Chemical Prioritization in the ExpoCast Project. Environmental Science & Technology, 2013, 47, 130711145716006.	10.0	132
17	An Intuitive Approach for Predicting Potential Human Health Risk with the Tox21 10k Library. Environmental Science & Technology, 2017, 51, 10786-10796.	10.0	120
18	Toxicokinetic Triage for Environmental Chemicals. Toxicological Sciences, 2015, 147, 55-67.	3.1	117

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19	In Vitro and Modelling Approaches to Risk Assessment from the U.S. Environmental Protection Agency ToxCast Programme. Basic and Clinical Pharmacology and Toxicology, 2014, 115, 69-76.	2.5	114
20	Exploring consumer exposure pathways and patterns of use for chemicals in the environment. Toxicology Reports, 2015, 2, 228-237.	3.3	113
21	Relative Impact of Incorporating Pharmacokinetics on Predicting In Vivo Hazard and Mode of Action from High-Throughput In Vitro Toxicity Assays. Toxicological Sciences, 2013, 132, 327-346.	3.1	104
22	Evaluating In Vitro-In Vivo Extrapolation of Toxicokinetics. Toxicological Sciences, 2018, 163, 152-169.	3.1	98
23	Modeling Single and Repeated Dose Pharmacokinetics of PFOA in Mice. Toxicological Sciences, 2009, 107, 331-341.	3.1	89
24	Suspect Screening Analysis of Chemicals in Consumer Products. Environmental Science & Technology, 2018, 52, 3125-3135.	10.0	88
25	GRADE Guidelines 30: the GRADE approach to assessing the certaintyÂof modeled evidenceâ€"An overview in the context of healthÂdecision-making. Journal of Clinical Epidemiology, 2021, 129, 138-150.	5.0	81
26	Identifying populations sensitive to environmental chemicals by simulating toxicokinetic variability. Environment International, 2017, 106, 105-118.	10.0	80
27	Development of a consumer product ingredient database for chemical exposure screening and prioritization. Food and Chemical Toxicology, 2014, 65, 269-279.	3.6	79
28	Consensus Modeling of Median Chemical Intake for the U.S. Population Based on Predictions of Exposure Pathways. Environmental Science & Technology, 2019, 53, 719-732.	10.0	78
29	Computational Exposure Science: An Emerging Discipline to Support 21st-Century Risk Assessment. Environmental Health Perspectives, 2016, 124, 697-702.	6.0	74
30	Incorporating Population Variability and Susceptible Subpopulations into Dosimetry for High-Throughput Toxicity Testing. Toxicological Sciences, 2014, 142, 210-224.	3.1	71
31	High-throughput screening of chemicals as functional substitutes using structure-based classification models. Green Chemistry, 2017, 19, 1063-1074.	9.0	66
32	Comparative pharmacokinetics of perfluorononanoic acid in rat and mouse. Toxicology, 2011, 281, 48-55.	4.2	65
33	Simulating Microdosimetry in a Virtual Hepatic Lobule. PLoS Computational Biology, 2010, 6, e1000756.	3.2	56
34	Utilizing Threshold of Toxicological Concern (TTC) with high throughput exposure predictions (HTE) as a risk-based prioritization approach for thousands of chemicals. Computational Toxicology, 2018, 7, 58-67.	3.3	53
35	New Approach Methods to Evaluate Health Risks of Air Pollutants: Critical Design Considerations for In Vitro Exposure Testing. International Journal of Environmental Research and Public Health, 2020, 17, 2124.	2.6	51
36	A Method for Identifying Prevalent Chemical Combinations in the U.S. Population. Environmental Health Perspectives, 2017, 125, 087017.	6.0	50

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37	Comparison of modeling approaches to prioritize chemicals based on estimates of exposure and exposure potential. Science of the Total Environment, 2013, 458-460, 555-567.	8.0	49
38	Characterization and prediction of chemical functions and weight fractions in consumer products. Toxicology Reports, 2016, 3, 723-732.	3.3	49
39	Using Nuclear Receptor Activity to Stratify Hepatocarcinogens. PLoS ONE, 2011, 6, e14584.	2.5	48
40	Virtual Tissues in Toxicology. Journal of Toxicology and Environmental Health - Part B: Critical Reviews, 2010, 13, 314-328.	6.5	47
41	New approach methodologies for exposure science. Current Opinion in Toxicology, 2019, 15, 76-92.	5.0	46
42	Advancing internal exposure and physiologically-based toxicokinetic modeling for 21st-century risk assessments. Journal of Exposure Science and Environmental Epidemiology, 2019, 29, 11-20.	3.9	45
43	Dosimetric Anchoring of In Vivo and In Vitro Studies for Perfluorooctanoate and Perfluorooctanesulfonate. Toxicological Sciences, 2013, 136, 308-327.	3.1	44
44	Advancements in Life Cycle Human Exposure and Toxicity Characterization. Environmental Health Perspectives, 2018, 126, 125001.	6.0	44
45	A Liver-Centric Multiscale Modeling Framework for Xenobiotics. PLoS ONE, 2016, 11, e0162428.	2.5	44
46	High-throughput PBTK models for in vitro to in vivo extrapolation. Expert Opinion on Drug Metabolism and Toxicology, 2021, 17, 903-921.	3.3	42
47	High-throughput dietary exposure predictions for chemical migrants from food contact substances for use in chemical prioritization. Environment International, 2017, 108, 185-194.	10.0	40
48	Assessing Toxicokinetic Uncertainty and Variability in Risk Prioritization. Toxicological Sciences, 2019, 172, 235-251.	3.1	40
49	Using the concordance of in vitro and in vivo data to evaluate extrapolation assumptions. PLoS ONE, 2019, 14, e0217564.	2.5	37
50	IVIVE: Facilitating the Use of In Vitro Toxicity Data in Risk Assessment and Decision Making. Toxics, 2022, 10, 232.	3.7	35
51	PBPK model reporting template for chemical risk assessment applications. Regulatory Toxicology and Pharmacology, 2020, 115, 104691.	2.7	33
52	Database of pharmacokinetic time-series data and parameters for 144 environmental chemicals. Scientific Data, 2020, 7, 122.	5.3	33
53	Incorporating exposure information into the toxicological prioritization index decision support framework. Science of the Total Environment, 2012, 435-436, 316-325.	8.0	32
54	Evaluation and calibration of high-throughput predictions of chemical distribution to tissues. Journal of Pharmacokinetics and Pharmacodynamics, 2017, 44, 549-565.	1.8	32

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55	Challenges in working towards an internal threshold of toxicological concern (iTTC) for use in the safety assessment of cosmetics: Discussions from the Cosmetics Europe iTTC Working Group workshop. Regulatory Toxicology and Pharmacology, 2019, 103, 63-72.	2.7	30
56	Empirical models for anatomical and physiological changes in a human mother and fetus during pregnancy and gestation. PLoS ONE, 2019, 14, e0215906.	2.5	30
57	Chemical Characterization of Recycled Consumer Products Using Suspect Screening Analysis. Environmental Science & Technology, 2021, 55, 11375-11387.	10.0	30
58	Ratchet-induced segregation and transport of nonspherical grains. Physical Review E, 2002, 65, 031308.	2.1	28
59	High-throughput toxicogenomic screening of chemicals in the environment using metabolically competent hepatic cell cultures. Npj Systems Biology and Applications, 2021, 7, 7.	3.0	28
60	Simulating Quantitative Cellular Responses Using Asynchronous Threshold Boolean Network Ensembles. BMC Systems Biology, 2011, 5, 109.	3.0	27
61	Designing QSARs for Parameters of High-Throughput Toxicokinetic Models Using Open-Source Descriptors. Environmental Science & Technology, 2021, 55, 6505-6517.	10.0	27
62	Defining toxicological tipping points in neuronal network development. Toxicology and Applied Pharmacology, 2018, 354, 81-93.	2.8	26
63	Using chemical structure information to develop predictive models for in vitro toxicokinetic parameters to inform high-throughput risk-assessment. Computational Toxicology, 2020, 16, 100136.	3.3	22
64	High-throughput in-silico prediction of ionization equilibria for pharmacokinetic modeling. Science of the Total Environment, 2018, 615, 150-160.	8.0	19
65	Force networks and elasticity in granular silos. European Physical Journal E, 2010, 32, 135-145.	1.6	17
66	Rapid experimental measurements of physicochemical properties to inform models and testing. Science of the Total Environment, 2018, 636, 901-909.	8.0	17
67	Identifiability of PBPK models with applications to dimethylarsinic acid exposure. Journal of Pharmacokinetics and Pharmacodynamics, 2015, 42, 591-609.	1.8	16
68	Comparing models for perfluorooctanoic acid pharmacokinetics using Bayesian analysis. Journal of Pharmacokinetics and Pharmacodynamics, 2008, 35, 683-712.	1.8	14
69	Estimating uncertainty in the context of new approach methodologies for potential use in chemical safety evaluation. Current Opinion in Toxicology, 2019, 15, 40-47.	5.0	14
70	Development and evaluation of a high throughput inhalation model for organic chemicals. Journal of Exposure Science and Environmental Epidemiology, 2020, 30, 866-877.	3.9	13
71	Predicting compound amenability with liquid chromatography-mass spectrometry to improve non-targeted analysis. Analytical and Bioanalytical Chemistry, 2021, 413, 7495-7508.	3.7	12
72	High-throughput screening tools facilitate calculation of a combined exposure-bioactivity index for chemicals with endocrine activity. Environment International, 2020, 137, 105470.	10.0	10

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73	Systems Toxicology from Genes to Organs. Methods in Molecular Biology, 2013, 930, 375-397.	0.9	10
74	Opportunities and challenges related to saturation of toxicokinetic processes: Implications for risk assessment. Regulatory Toxicology and Pharmacology, 2021, 127, 105070.	2.7	10
75	Simple models for granular force networks. Physica D: Nonlinear Phenomena, 2010, 239, 1818-1826.	2.8	9
76	Pharmacokinetic profile of Perfluorobutane Sulfonate and activation of hepatic nuclear receptor target genes in mice. Toxicology, 2020, 441, 152522.	4.2	9
77	Repeat-dose toxicity prediction with Generalized Read-Across (GenRA) using targeted transcriptomic data: A proof-of-concept case study. Computational Toxicology, 2021, 19, 100171.	3.3	8
78	Response to perturbations for granular flow in a hopper. Physical Review E, 2007, 76, 051303.	2.1	7
79	Shear and loading in channels: Oscillatory shearing and edge currents of superconducting vortices. Physical Review B, 2003, 67, .	3.2	6
80	Development of a quantitative morphological assessment of toxicantâ€treated zebrafish larvae using brightfield imaging and highâ€content analysis. Journal of Applied Toxicology, 2016, 36, 1214-1222.	2.8	5
81	Quantitative in vitro to in vivo extrapolation for developmental toxicity potency of valproic acid analogues. Birth Defects Research, 2022, 114, 1037-1055.	1.5	4
82	Modeling In Vitro Cell-Based Assays Experiments. Developments in Environmental Modelling, 2012, 25, 51-71.	0.3	3
83	Comment on: Dong et al. (2017) â€œIssues raised by the reference doses for perfluorooctonate sulfonate and perfluorooctanoic acid.â€. Environment International, 2018, 121, 1372-1374.	10.0	3
84	Incorporating human exposure information in a weight of evidence approach to inform design of repeated dose animal studies. Regulatory Toxicology and Pharmacology, 2021, 127, 105073.	2.7	2
85	Response to "Accurate Risk-Based Chemical Screening * Relies on Robust Exposure Estimates". Toxicological Sciences, 2012, 128, 297-299.	3.1	0
86	P68â€”Parsimonious development of a physiologically based pharmacokinetic model for PFOA. Reproductive Toxicology, 2012, 33, 624.	2.9	0
87	Free access platforms for integrating environmental chemical exposure and hazard information. Toxicology Letters, 2018, 295, S29.	0.8	0
88	Dosimetric Anchoring of Toxicological Studies. Molecular and Integrative Toxicology, 2015, , 337-361.	0.5	0