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List of Publications by Year in descending order

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papers

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docs citations

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times ranked

9719
citing authors

#	ARTICLE	IF	CITATIONS
1	Evaluation of Per- and Polyfluoroalkyl Substances (PFAS) <i>In Vitro</i> Toxicity Testing for Developmental Neurotoxicity. <i>Chemical Research in Toxicology</i> , 2023, 36, 402-419.	3.5	15
2	A New CSRML Structure-Based Fingerprint Method for Profiling and Categorizing Per- and Polyfluoroalkyl Substances (PFAS). <i>Chemical Research in Toxicology</i> , 2023, 36, 508-534.	3.5	8
3	Identification of Branched and Linear Forms of PFOA and Potential Precursors: A User-Friendly SMILES Structure-based Approach. <i>Frontiers in Environmental Science</i> , 2022, 10, 1-865488.	3.3	30
4	Wikipedia on the CompTox Chemicals Dashboard: Connecting Resources to Enrich Public Chemical Data. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 4888-4905.	5.7	5
5	The Tox21 10K Compound Library: Collaborative Chemistry Advancing Toxicology. <i>Chemical Research in Toxicology</i> , 2021, 34, 189-216.	3.5	163
6	Expanded high-throughput screening and chemotype-enrichment analysis of the phase II: e1k ToxCast library for human sodium-iodide symporter (NIS) inhibition. <i>Archives of Toxicology</i> , 2021, 95, 1723-1737.	4.3	15
7	Bioactivity profiling of per- and polyfluoroalkyl substances (PFAS) identifies potential toxicity pathways related to molecular structure. <i>Toxicology</i> , 2021, 457, 152789.	4.3	64
8	Predicting compound amenability with liquid chromatography-mass spectrometry to improve non-targeted analysis. <i>Analytical and Bioanalytical Chemistry</i> , 2021, 413, 7495-7508.	3.9	16
9	A New OECD Definition for Per- and Polyfluoroalkyl Substances. <i>Environmental Science & Technology</i> , 2021, 55, 15575-15578.	10.5	178
10	Utility of In Vitro Bioactivity as a Lower Bound Estimate of In Vivo Adverse Effect Levels and in Risk-Based Prioritization. <i>Toxicological Sciences</i> , 2020, 173, 202-225.	3.1	151
11	Bioactivity screening of environmental chemicals using imaging-based high-throughput phenotypic profiling. <i>Toxicology and Applied Pharmacology</i> , 2020, 389, 114876.	2.9	86
12	Concentrationâ€“response evaluation of ToxCast compounds for multivariate activity patterns of neural network function. <i>Archives of Toxicology</i> , 2020, 94, 469-484.	4.3	33
13	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. <i>Environmental Health Perspectives</i> , 2020, 128, 27002.	8.2	131
14	EPAâ€™s DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research. <i>Computational Toxicology</i> , 2019, 12, 100096.	3.4	135
15	Comparing and contrasting the coverage of publicly available structural alerts for protein binding. <i>Computational Toxicology</i> , 2019, 12, 100100.	3.4	3
16	The Next Generation Blueprint of Computational Toxicology at the U.S. Environmental Protection Agency. <i>Toxicological Sciences</i> , 2019, 169, 317-332.	3.1	249
17	High-throughput screening and chemotype-enrichment analysis of ToxCast phase II chemicals evaluated for human sodium-iodide symporter (NIS) inhibition. <i>Environment International</i> , 2019, 126, 377-386.	10.1	45
18	Using prepared mixtures of ToxCast chemicals to evaluate non-targeted analysis (NTA) method performance. <i>Analytical and Bioanalytical Chemistry</i> , 2019, 411, 835-851.	3.9	59

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19	EPA's non-targeted analysis collaborative trial (ENTACT): genesis, design, and initial findings. <i>Analytical and Bioanalytical Chemistry</i> , 2019, 411, 853-866.	3.9	123
20	Suspect Screening Analysis of Chemicals in Consumer Products. <i>Environmental Science & Technology</i> , 2018, 52, 3125-3135.	10.5	93
21	Integrating tools for non-targeted analysis research and chemical safety evaluations at the US EPA. <i>Journal of Exposure Science and Environmental Epidemiology</i> , 2018, 28, 411-426.	4.1	160
22	Screening the ToxCast phase II libraries for alterations in network function using cortical neurons grown on multi-well microelectrode array (mwMEA) plates. <i>Archives of Toxicology</i> , 2018, 92, 487-500.	4.3	52
23	Rapid experimental measurements of physicochemical properties to inform models and testing. <i>Science of the Total Environment</i> , 2018, 636, 901-909.	8.2	18
24	A mechanistic framework for integrating chemical structure and high-throughput screening results to improve toxicity predictions. <i>Computational Toxicology</i> , 2018, 8, 1-12.	3.4	12
25	The CompTox Chemistry Dashboard: a community data resource for environmental chemistry. <i>Journal of Cheminformatics</i> , 2017, 9, 61.	6.4	743
26	Comment on "On the Utility of ToxCast and ToxPi as Methods for Identifying New Obesogens". <i>Environmental Health Perspectives</i> , 2017, 125, A8-A11.	8.2	6
27	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. <i>Environmental Health Perspectives</i> , 2016, 124, 1023-1033.	8.2	278
28	Using ToxCast Data to Reconstruct Dynamic Cell State Trajectories and Estimate Toxicological Points of Departure. <i>Environmental Health Perspectives</i> , 2016, 124, 910-919.	8.2	67
29	ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology. <i>Chemical Research in Toxicology</i> , 2016, 29, 1225-1251.	3.5	482
30	Editor's Highlight: Analysis of the Effects of Cell Stress and Cytotoxicity on <i>In Vitro</i> Assay Activity Across a Diverse Chemical and Assay Space. <i>Toxicological Sciences</i> , 2016, 152, 323-339.	3.1	183
31	Linking high resolution mass spectrometry data with exposure and toxicity forecasts to advance high-throughput environmental monitoring. <i>Environment International</i> , 2016, 88, 269-280.	10.1	154
32	Integrated Model of Chemical Perturbations of a Biological Pathway Using 18 <i>In Vitro</i> High-Throughput Screening Assays for the Estrogen Receptor. <i>Toxicological Sciences</i> , 2015, 148, 137-154.	3.1	258
33	New Publicly Available Chemical Query Language, CSRML, To Support Chemotype Representations for Application to Data Mining and Modeling. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 510-528.	5.7	191
34	Profiling of the Tox21 Chemical Collection for Mitochondrial Function to Identify Compounds that Acutely Decrease Mitochondrial Membrane Potential. <i>Environmental Health Perspectives</i> , 2015, 123, 49-56.	8.2	159
35	Phenotypic screening of the ToxCast chemical library to classify toxic and therapeutic mechanisms. <i>Nature Biotechnology</i> , 2014, 32, 583-591.	20.8	180
36	QSAR Modeling: Where Have You Been? Where Are You Going To?. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 4977-5010.	6.6	1,475

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37	EADB: An Estrogenic Activity Database for Assessing Potential Endocrine Activity. <i>Toxicological Sciences</i> , 2013, 135, 277-291.	3.1	72
38	Profiling 976 ToxCast Chemicals across 331 Enzymatic and Receptor Signaling Assays. <i>Chemical Research in Toxicology</i> , 2013, 26, 878-895.	3.5	170
39	Real-Time Growth Kinetics Measuring Hormone Mimicry for ToxCast Chemicals in T-47D Human Ductal Carcinoma Cells. <i>Chemical Research in Toxicology</i> , 2013, 26, 1097-1107.	3.5	43
40	Perspectives on validation of high-throughput assays supporting 21st century toxicity testing. <i>ALTEX: Alternatives To Animal Experimentation</i> , 2013, 30, 51-66.	1.3	123
41	Aggregating Data for Computational Toxicology Applications: The U.S. Environmental Protection Agency (EPA) Aggregated Computational Toxicology Resource (ACToR) System. <i>International Journal of Molecular Sciences</i> , 2012, 13, 1805-1831.	4.2	104
42	Integration of Dosimetry, Exposure, and High-Throughput Screening Data in Chemical Toxicity Assessment. <i>Toxicological Sciences</i> , 2012, 125, 157-174.	3.1	344
43	Update on EPA's ToxCast Program: Providing High Throughput Decision Support Tools for Chemical Risk Management. <i>Chemical Research in Toxicology</i> , 2012, 25, 1287-1302.	3.5	418
44	Genetic toxicology in the 21st century: Reflections and future directions. <i>Environmental and Molecular Mutagenesis</i> , 2011, 52, 339-354.	2.0	87
45	Activity profiles of 309 ToxCast chemicals evaluated across 292 biochemical targets. <i>Toxicology</i> , 2011, 282, 1-15.	4.3	126
46	Use of <i>in vitro</i> HTS-Derived Concentration-Response Data as Biological Descriptors Improves the Accuracy of QSAR Models of <i>in vivo</i> Toxicity. <i>Environmental Health Perspectives</i> , 2011, 119, 364-370.	8.2	106
47	<i>In vitro</i> Screening of Environmental Chemicals for Targeted Testing Prioritization: The ToxCast Project. <i>Environmental Health Perspectives</i> , 2010, 118, 485-492.	8.2	530
48	Endocrine Profiling and Prioritization of Environmental Chemicals Using ToxCast Data. <i>Environmental Health Perspectives</i> , 2010, 118, 1714-1720.	8.2	292
49	Impact of Environmental Chemicals on Key Transcription Regulators and Correlation to Toxicity End Points within EPA's ToxCast Program. <i>Chemical Research in Toxicology</i> , 2010, 23, 578-590.	3.5	193
50	Advancing Exposure Characterization for Chemical Evaluation and Risk Assessment. <i>Journal of Toxicology and Environmental Health - Part B: Critical Reviews</i> , 2010, 13, 299-313.	6.9	91
51	The Toxicity Data Landscape for Environmental Chemicals. <i>Environmental Health Perspectives</i> , 2009, 117, 685-695.	8.2	430
52	A Novel Two-Step Hierarchical Quantitative Structure-Activity Relationship Modeling Work Flow for Predicting Acute Toxicity of Chemicals in Rodents. <i>Environmental Health Perspectives</i> , 2009, 117, 1257-1264.	8.2	59
53	DSSTox chemical-index files for exposure-related experiments in ArrayExpress and Gene Expression Omnibus: enabling toxico-chemogenomics data linkages. <i>Bioinformatics</i> , 2009, 25, 692-694.	4.2	22
54	Toward a Public Toxicogenomics Capability for Supporting Predictive Toxicology: Survey of Current Resources and Chemical Indexing of Experiments in GEO and ArrayExpress. <i>Toxicological Sciences</i> , 2009, 109, 358-371.	3.1	23

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55	Evaluation of high-throughput genotoxicity assays used in profiling the US EPA ToxCast [®] chemicals. <i>Regulatory Toxicology and Pharmacology</i> , 2009, 55, 188-199.	2.8	107
56	ACToR [®] Aggregated Computational Toxicology Resource. <i>Toxicology and Applied Pharmacology</i> , 2008, 233, 7-13.	2.9	202
57	Computational Toxicology [®] A State of the Science Mini Review. <i>Toxicological Sciences</i> , 2008, 103, 14-27.	3.1	156
58	Toxicity Data Informatics: Supporting a New Paradigm for Toxicity Prediction. <i>Toxicology Mechanisms and Methods</i> , 2008, 18, 103-118.	2.7	70
59	Use of Cell Viability Assay Data Improves the Prediction Accuracy of Conventional Quantitative Structure-Activity Relationship Models of Animal Carcinogenicity. <i>Environmental Health Perspectives</i> , 2008, 116, 506-513.	8.2	82
60	The Expanding Role of Predictive Toxicology: An Update on the (Q)SAR Models for Mutagens and Carcinogens. <i>Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews</i> , 2007, 25, 53-97.	3.0	103
61	The ToxCast Program for Prioritizing Toxicity Testing of Environmental Chemicals. <i>Toxicological Sciences</i> , 2007, 95, 5-12.	3.1	880
62	Future of Toxicology Predictive Toxicology: An Expanded View of Chemical Toxicity. <i>Chemical Research in Toxicology</i> , 2006, 19, 1257-1262.	3.5	67
63	The Art of Data Mining the Minefields of Toxicity Databases to Link Chemistry to Biology. <i>Current Computer-Aided Drug Design</i> , 2006, 2, 135-150.	1.2	34
64	Bromochloro-haloacetic acids: Effects on mouse embryos in vitro and QSAR considerations. <i>Reproductive Toxicology</i> , 2006, 21, 260-266.	3.1	24
65	Chemical Effects in Biological Systems [®] Data Dictionary (CEBS-DD): A Compendium of Terms for the Capture and Integration of Biological Study Design Description, Conventional Phenotypes, and Omics Data. <i>Toxicological Sciences</i> , 2005, 88, 585-601.	3.1	43
66	Challenges in constructing statistically based structure-activity relationship models for developmental toxicity. <i>Birth Defects Research Part A: Clinical and Molecular Teratology</i> , 2004, 70, 902-911.	1.6	16
67	Identification and Characterization of Novel Stable Deoxyguanosine and Deoxyadenosine Adducts of Benzo[a]pyrene-7,8-quinone from Reactions at Physiological pH. <i>Chemical Research in Toxicology</i> , 2004, 17, 827-838.	3.5	72
68	Interaction of organophosphate pesticides and related compounds with the androgen receptor. <i>Environmental Health Perspectives</i> , 2003, 111, 545-552.	8.2	50
69	Public Sources of Mutagenicity and Carcinogenicity Data. , 2003, , .		7
70	Distributed structure-searchable toxicity (DSSTox) public database network: a proposal. <i>Mutation Research - Fundamental and Molecular Mechanisms of Mutagenesis</i> , 2002, 499, 27-52.	1.0	140
71	An Evaluation of the Mutagenicity, Metabolism, and DNA Adduct Formation of 5-Nitrobenzo[b]naphtho[2,1-d]thiophene. <i>Chemical Research in Toxicology</i> , 2001, 14, 661-671.	3.5	16
72	The optimal fragmentation principle [®] Reply. <i>Drug Discovery Today</i> , 2001, 6, 235-237.	6.6	2

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73	Theoretical Study of the SNV Reaction of Trichloroethylene (TCE) and CH ₃ S- as a Model for Glutathione Conjugation of TCE. <i>Chemical Research in Toxicology</i> , 1999, 12, 308-316.	3.5	10
74	Application of artificial intelligence and computer-based methods to predicting chemical toxicity. <i>Knowledge Engineering Review</i> , 1999, 14, 307-317.	2.7	17
75	Structure-based methods for predicting mutagenicity and carcinogenicity: are we there yet?. <i>Mutation Research - Fundamental and Molecular Mechanisms of Mutagenesis</i> , 1998, 400, 493-507.	1.0	77
76	Quantitative Structure-Based Modeling Applied to Characterization and Prediction of Chemical Toxicity. <i>Methods</i> , 1998, 14, 264-276.	3.9	48
77	Theoretical Evaluation of Two Plausible Routes for Bioactivation of S-(1,1-Difluoro-2,2-dihaloethyl)-l-cysteine Conjugates: Thiirane vs Thionoacyl Fluoride Pathway. <i>Chemical Research in Toxicology</i> , 1997, 10, 103-110.	3.5	16
78	The Development and Validation of Expert Systems for Predicting Toxicity. <i>ATLA Alternatives To Laboratory Animals</i> , 1997, 25, 223-251.	1.4	96
79	Conformational Aspects of Glutathione Conjugates of Chlorinated Alkenes: A Computational Study. <i>Chemical Research in Toxicology</i> , 1996, 9, 667-675.	3.5	2
80	QSARS of mutagens and carcinogens: Two case studies illustrating problems in the construction of models for noncongeneric chemicals. <i>Mutation Research - Genetic Toxicology Testing and Biomonitoring of Environmental Or Occupational Exposure</i> , 1996, 371, 29-46.	1.2	46
81	Quantitative structure-activity relationships for the developmental toxicity of haloacetic acids in mammalian whole embryo culture. <i>Teratology</i> , 1996, 53, 352-360.	1.5	67
82	Synthesis and Characterization of Adducts of Alachlor and 2-Chloro-N-(2,6-diethylphenyl)acetamide with 2'-Deoxyguanosine, Thymidine, and Their 3'-Monophosphates. <i>Chemical Research in Toxicology</i> , 1995, 8, 209-217.	3.5	15
83	Role of computational chemistry in support of hazard identification (ID): mechanism-based SARs. <i>Toxicology Letters</i> , 1995, 79, 115-122.	1.3	6
84	Structure-activity study of paracetamol analogs: inhibition of replicative DNA synthesis in V79 Chinese hamster cells. <i>Chemical Research in Toxicology</i> , 1991, 4, 151-156.	3.5	27
85	Quantitative comparison of molecular electrostatic potentials for structure-activity studies. <i>Journal of Computational Chemistry</i> , 1991, 12, 959-969.	3.5	70
86	A CASE-SAR analysis of polycyclic aromatic hydrocarbon carcinogenicity. <i>Mutation Research - Genetic Toxicology Testing and Biomonitoring of Environmental Or Occupational Exposure</i> , 1990, 242, 285-303.	1.2	33
87	Modified molecular charge similarity indices for choosing molecular analogues. <i>International Journal of Quantum Chemistry</i> , 1987, 31, 309-323.	2.1	18
88	Photodissociation of the energy selected nitrobenzene ion. <i>Journal of Chemical Physics</i> , 1986, 84, 1424-1431.	3.1	16