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List of Publications by Year
in descending order

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86 papers	11,372 citations	36271 51 h-index	51562 86 g-index
89 all docs	89 docs citations	89 times ranked	7844 citing authors

#	Article	IF	Citations
1	QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010.	2.9	1,401
2	The ToxCast Program for Prioritizing Toxicity Testing of Environmental Chemicals. Toxicological Sciences, 2007, 95, 5-12.	1.4	851
3	The CompTox Chemistry Dashboard: a community data resource for environmental chemistry. Journal of Cheminformatics, 2017, 9, 61.	2.8	674
4	In Vitro Screening of Environmental Chemicals for Targeted Testing Prioritization: The ToxCast Project. Environmental Health Perspectives, 2010, 118, 485-492.	2.8	519
5	ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology. Chemical Research in Toxicology, 2016, 29, 1225-1251.	1.7	456
6	The Toxicity Data Landscape for Environmental Chemicals. Environmental Health Perspectives, 2009, 117, 685-695.	2.8	418
7	Update on EPAâ€™s ToxCast Program: Providing High Throughput Decision Support Tools for Chemical Risk Management. Chemical Research in Toxicology, 2012, 25, 1287-1302.	1.7	410
8	Integration of Dosimetry, Exposure, and High-Throughput Screening Data in Chemical Toxicity Assessment. Toxicological Sciences, 2012, 125, 157-174.	1.4	336
9	Endocrine Profiling and Prioritization of Environmental Chemicals Using ToxCast Data. Environmental Health Perspectives, 2010, 118, 1714-1720.	2.8	274
10	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	2.8	264
11	Integrated Model of Chemical Perturbations of a Biological Pathway Using 18In VitroHigh-Throughput Screening Assays for the Estrogen Receptor. Toxicological Sciences, 2015, 148, 137-154.	1.4	251
12	The Next Generation Blueprint of Computational Toxicology at the U.S. Environmental Protection Agency. Toxicological Sciences, 2019, 169, 317-332.	1.4	225
13	ACToR â€" Aggregated Computational Toxicology Resource. Toxicology and Applied Pharmacology, 2008, 233, 7-13.	1.3	195
14	Impact of Environmental Chemicals on Key Transcription Regulators and Correlation to Toxicity End Points within EPAâ€™s ToxCast Program. Chemical Research in Toxicology, 2010, 23, 578-590.	1.7	190
15	New Publicly Available Chemical Query Language, CSRML, To Support Chemotype Representations for Application to Data Mining and Modeling. Journal of Chemical Information and Modeling, 2015, 55, 510-528.	2.5	183
16	Phenotypic screening of the ToxCast chemical library to classify toxic and therapeutic mechanisms. Nature Biotechnology, 2014, 32, 583-591.	9.4	175
17	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.	1.4	171
18	Profiling 976 ToxCast Chemicals across 331 Enzymatic and Receptor Signaling Assays. Chemical Research in Toxicology, 2013, 26, 878-895.	1.7	162

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19	Profiling of the Tox21 Chemical Collection for Mitochondrial Function to Identify Compounds that Acutely Decrease Mitochondrial Membrane Potential. Environmental Health Perspectives, 2015, 123, 49-56.	2.8	154
20	Computational Toxicologyâ€"A State of the Science Mini Review. Toxicological Sciences, 2008, 103, 14-27.	1.4	152
21	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.	1.8	148
22	The Tox21 10K Compound Library: Collaborative Chemistry Advancing Toxicology. Chemical Research in Toxicology, 2021, 34, 189-216.	1.7	145
23	Linking high resolution mass spectrometry data with exposure and toxicity forecasts to advance high-throughput environmental monitoring. Environment International, 2016, 88, 269-280.	4.8	143
24	Utility of In Vitro Bioactivity as a Lower Bound Estimate of In Vivo Adverse Effect Levels and in Risk-Based Prioritization. Toxicological Sciences, 2020, 173, 202-225.	1.4	138
25	Distributed structure-searchable toxicity (DSSTox) public database network: a proposal. Mutation Research - Fundamental and Molecular Mechanisms of Mutagenesis, 2002, 499, 27-52.	0.4	137
26	A New OECD Definition for Per- and Polyfluoroalkyl Substances. Environmental Science & Technology, 2021, 55, 15575-15578.	4.6	134
27	EPAâ€™s DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research. Computational Toxicology, 2019, 12, 100096.	1.8	127
28	Activity profiles of 309 ToxCastâ„¢ chemicals evaluated across 292 biochemical targets. Toxicology, 2011, 282, 1-15.	2.0	124
29	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	2.8	120
30	Perspectives on validation of high-throughput assays supporting 21st century toxicity testing. ALTEX: Alternatives To Animal Experimentation, 2013, 30, 51-66.	0.9	118
31	EPAâ€™s non-targeted analysis collaborative trial (ENTACT): genesis, design, and initial findings. Analytical and Bioanalytical Chemistry, 2019, 411, 853-866.	1.9	116
32	Evaluation of high-throughput genotoxicity assays used in profiling the US EPA ToxCastâ„¢ chemicals. Regulatory Toxicology and Pharmacology, 2009, 55, 188-199.	1.3	105
33	The Expanding Role of Predictive Toxicology: An Update on the (Q)SAR Models for Mutagens and Carcinogens. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2007, 25, 53-97.	2.9	103
34	Use of in Vitro HTS-Derived Concentrationâ€"Response Data as Biological Descriptors Improves the Accuracy of QSAR Models of in Vivo Toxicity. Environmental Health Perspectives, 2011, 119, 364-370.	2.8	103
35	Aggregating Data for Computational Toxicology Applications: The U.S. Environmental Protection Agency (EPA) Aggregated Computational Toxicology Resource (ACToR) System. International Journal of Molecular Sciences, 2012, 13, 1805-1831.	1.8	103
36	The Development and Validation of Expert Systems for Predicting Toxicity. ATLA Alternatives To Laboratory Animals, 1997, 25, 223-251.	0.7	96

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37	Suspect Screening Analysis of Chemicals in Consumer Products. Environmental Science & Technology, 2018, 52, 3125-3135.	4.6	88
38	Advancing Exposure Characterization for Chemical Evaluation and Risk Assessment. Journal of Toxicology and Environmental Health - Part B: Critical Reviews, 2010, 13, 299-313.	2.9	87
39	Genetic toxicology in the 21st century: Reflections and future directions. Environmental and Molecular Mutagenesis, 2011, 52, 339-354.	0.9	84
40	Use of Cell Viability Assay Data Improves the Prediction Accuracy of Conventional Quantitative Structureâ€“Activity Relationship Models of Animal Carcinogenicity. Environmental Health Perspectives, 2008, 116, 506-513.	2.8	82
41	Structure-based methods for predicting mutagenicity and carcinogenicity: are we there yet?. Mutation Research - Fundamental and Molecular Mechanisms of Mutagenesis, 1998, 400, 493-507.	0.4	77
42	Identification and Characterization of Novel Stable Deoxyguanosine and Deoxyadenosine Adducts of Benzo[a]pyrene-7,8-quinone from Reactions at Physiological pH. Chemical Research in Toxicology, 2004, 17, 827-838.	1.7	71
43	Bioactivity screening of environmental chemicals using imaging-based high-throughput phenotypic profiling. Toxicology and Applied Pharmacology, 2020, 389, 114876.	1.3	71
44	Quantitative comparison of molecular electrostatic potentials for structure-activity studies. Journal of Computational Chemistry, 1991, 12, 959-969.	1.5	70
45	Toxicity Data Informatics: Supporting a New Paradigm for Toxicity Prediction. Toxicology Mechanisms and Methods, 2008, 18, 103-118.	1.3	68
46	EADB: An Estrogenic Activity Database for Assessing Potential Endocrine Activity. Toxicological Sciences, 2013, 135, 277-291.	1.4	68
47	Quantitative structure-activity relationships for the developmental toxicity of haloacetic acids in mammalian whole embryo culture. , 1996, 53, 352-360.		66
48	Using ToxCastâ„¢ Data to Reconstruct Dynamic Cell State Trajectories and Estimate Toxicological Points of Departure. Environmental Health Perspectives, 2016, 124, 910-919.	2.8	65
49	Future of ToxicologyPredictive Toxicology:Â An Expanded View of â€œChemical Toxicityâ€• Chemical Research in Toxicology, 2006, 19, 1257-1262.	1.7	63
50	A Novel Two-Step Hierarchical Quantitative Structureâ€“Activity Relationship Modeling Work Flow for Predicting Acute Toxicity of Chemicals in Rodents. Environmental Health Perspectives, 2009, 117, 1257-1264.	2.8	59
51	Bioactivity profiling of per- and polyfluoroalkyl substances (PFAS) identifies potential toxicity pathways related to molecular structure. Toxicology, 2021, 457, 152789.	2.0	57
52	Using prepared mixtures of ToxCast chemicals to evaluate non-targeted analysis (NTA) method performance. Analytical and Bioanalytical Chemistry, 2019, 411, 835-851.	1.9	54
53	Interaction of organophosphate pesticides and related compounds with the androgen receptor.. Environmental Health Perspectives, 2003, 111, 545-552.	2.8	50
54	Quantitative Structure-Based Modeling Applied to Characterization and Prediction of Chemical Toxicity. Methods, 1998, 14, 264-276.	1.9	48

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55	QSARS of mutagens and carcinogens: Two case studies illustrating problems in the construction of models for noncongeneric chemicals. Mutation Research - Genetic Toxicology Testing and Biomonitoring of Environmental Or Occupational Exposure, 1996, 371, 29-46.	1.2	46
56	Screening the ToxCast phase II libraries for alterations in network function using cortical neurons grown on multi-well microelectrode array (mwMEA) plates. Archives of Toxicology, 2018, 92, 487-500.	1.9	46
57	High-throughput screening and chemotype-enrichment analysis of ToxCast phase II chemicals evaluated for human sodium-iodide symporter (NIS) inhibition. Environment International, 2019, 126, 377-386.	4.8	45
58	Chemical Effects in Biological Systemsâ€"Data Dictionary (CEBS-DD): A Compendium of Terms for the Capture and Integration of Biological Study Design Description, Conventional Phenotypes, and â€˜Omics Data. Toxicological Sciences, 2005, 88, 585-601.	1.4	43
59	Real-Time Growth Kinetics Measuring Hormone Mimicry for ToxCast Chemicals in T-47D Human Ductal Carcinoma Cells. Chemical Research in Toxicology, 2013, 26, 1097-1107.	1.7	41
60	The Art of Data Mining the Minefields of Toxicity Databases to Link Chemistry to Biology. Current Computer-Aided Drug Design, 2006, 2, 135-150.	0.8	34
61	A CASE-SAR analysis of polycyclic aromatic hydrocarbon carcinogenicity. Mutation Research - Genetic Toxicology Testing and Biomonitoring of Environmental Or Occupational Exposure, 1990, 242, 285-303.	1.2	33
62	Identification of Branched and Linear Forms of PFOA and Potential Precursors: A User-Friendly SMILES Structure-based Approach. Frontiers in Environmental Science, 2022, 10, 1-865488.	1.5	29
63	Concentrationâ€"response evaluation of ToxCast compounds for multivariate activity patterns of neural network function. Archives of Toxicology, 2020, 94, 469-484.	1.9	28
64	Structure-activity study of paracetamol analogs: inhibition of replicative DNA synthesis in V79 Chinese hamster cells. Chemical Research in Toxicology, 1991, 4, 151-156.	1.7	27
65	Chemical structure indexing of toxicity data on the internet: moving toward a flat world. Current Opinion in Drug Discovery & Development, 2006, 9, 314-25.	1.9	27
66	A novel approach: chemical relational databases, and the role of the ISSCAN database on assessing chemical carcinogenicity. Annali Dell'Istituto Superiore Di Sanita, 2008, 44, 48-56.	0.2	26
67	Bromochloro-haloacetic acids: Effects on mouse embryos in vitro and QSAR considerations. Reproductive Toxicology, 2006, 21, 260-266.	1.3	24
68	Toward a Public Toxicogenomics Capability for Supporting Predictive Toxicology: Survey of Current Resources and Chemical Indexing of Experiments in GEO and ArrayExpress. Toxicological Sciences, 2009, 109, 358-371.	1.4	23
69	DSSTox chemical-index files for exposure-related experiments in ArrayExpress and Gene Expression Omnibus: enabling toxico-chemogenomics data linkages. Bioinformatics, 2009, 25, 692-694.	1.8	22
70	Modified molecular charge similarity indices for choosing molecular analogues. International Journal of Quantum Chemistry, 1987, 31, 309-323.	1.0	18
71	Application of artificial intelligence and computer-based methods to predicting chemical toxicity. Knowledge Engineering Review, 1999, 14, 307-317.	2.1	17
72	Rapid experimental measurements of physicochemical properties to inform models and testing. Science of the Total Environment, 2018, 636, 901-909.	3.9	17

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73	Photodissociation of the energy selected nitrobenzene ion. Journal of Chemical Physics, 1986, 84, 1424-1431.	1.2	16
74	Theoretical Evaluation of Two Plausible Routes for Bioactivation of S-(1,1-Difluoro-2,2-dihaloethyl)-l-cysteine Conjugates:â€‰ Thiirane vs Thionoacyl Fluoride Pathway. Chemical Research in Toxicology, 1997, 10, 103-110.	1.7	16
75	An Evaluation of the Mutagenicity, Metabolism, and DNA Adduct Formation of 5-Nitrobenzo[b]naphtho[2,1-d]thiophene. Chemical Research in Toxicology, 2001, 14, 661-671.	1.7	16
76	Synthesis and Characterization of Adducts of Alachlor and 2-Chloro-N-(2,6-diethylphenyl)acetamide with 2'-Deoxyguanosine, Thymidine, and Their 3'-Monophosphates. Chemical Research in Toxicology, 1995, 8, 209-217.	1.7	15
77	Expanded high-throughput screening and chemotype-enrichment analysis of the phase II: e1k ToxCast library for human sodium-iodide symporter (NIS) inhibition. Archives of Toxicology, 2021, 95, 1723-1737.	1.9	15
78	A mechanistic framework for integrating chemical structure and high-throughput screening results to improve toxicity predictions. Computational Toxicology, 2018, 8, 1-12.	1.8	12
79	Predicting compound amenability with liquid chromatography-mass spectrometry to improve non-targeted analysis. Analytical and Bioanalytical Chemistry, 2021, 413, 7495-7508.	1.9	12
80	Theoretical Study of the SNV Reaction of Trichloroethylene (TCE) and CH3S- as a Model for Glutathione Conjugation of TCE. Chemical Research in Toxicology, 1999, 12, 308-316.	1.7	10
81	Public Sources of Mutagenicity and Carcinogenicity Data. , 2003, , .		7
82	Role of computational chemistry in support of hazard identification (ID): mechanism-based SARs. Toxicology Letters, 1995, 79, 115-122.	0.4	6
83	Comment on â€œOn the Utility of ToxCastâ„¢ and ToxPi as Methods for Identifying New Obesogensâ€: Environmental Health Perspectives, 2017, 125, A8-A11.	2.8	6
84	Comparing and contrasting the coverage of publicly available structural alerts for protein binding. Computational Toxicology, 2019, 12, 100100.	1.8	3
85	Conformational Aspects of Glutathione Conjugates of Chlorinated Alkenes:Â A Computational Study. Chemical Research in Toxicology, 1996, 9, 667-675.	1.7	2
86	The optimal fragmentation principleâ€“Reply. Drug Discovery Today, 2001, 6, 235-237.	3.2	2