Ann M Richard

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	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
2	The Tox21 10K Compound Library: Collaborative Chemistry Advancing Toxicology. Chemical Research in Toxicology, 2021, 34, 189-216.	1.7	145
3	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
4	Bioactivity profiling of per- and polyfluoroalkyl substances (PFAS) identifies potential toxicity pathways related to molecular structure. Toxicology, 2021, 457, 152789.	2.0	57
5	Predicting compound amenability with liquid chromatography-mass spectrometry to improve non-targeted analysis. Analytical and Bioanalytical Chemistry, 2021, 413, 7495-7508.	1.9	12
6	A New OECD Definition for Per- and Polyfluoroalkyl Substances. Environmental Science & Technology, 2021, 55, 15575-15578.	4.6	134
7	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
8	Bioactivity screening of environmental chemicals using imaging-based high-throughput phenotypic profiling. Toxicology and Applied Pharmacology, 2020, 389, 114876.	1.3	71
9	Concentrationâ€“response evaluation of ToxCast compounds for multivariate activity patterns of neural network function. Archives of Toxicology, 2020, 94, 469-484.	1.9	28
10	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	2.8	120
11	EPAâ€™s DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research. Computational Toxicology, 2019, 12, 100096.	1.8	127
12	Comparing and contrasting the coverage of publicly available structural alerts for protein binding. Computational Toxicology, 2019, 12, 100100.	1.8	3
13	The Next Generation Blueprint of Computational Toxicology at the U.S. Environmental Protection Agency. Toxicological Sciences, 2019, 169, 317-332.	1.4	225
14	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
15	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
16	EPAâ€™s non-targeted analysis collaborative trial (ENTACT): genesis, design, and initial findings. Analytical and Bioanalytical Chemistry, 2019, 411, 853-866.	1.9	116
17	Suspect Screening Analysis of Chemicals in Consumer Products. Environmental Science & Technology, 2018, 52, 3125-3135.	4.6	88
18	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

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19	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
20	Rapid experimental measurements of physicochemical properties to inform models and testing. Science of the Total Environment, 2018, 636, 901-909.	3.9	17
21	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
22	The CompTox Chemistry Dashboard: a community data resource for environmental chemistry. Journal of Cheminformatics, 2017, 9, 61.	2.8	674
23	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
24	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	2.8	264
25	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
26	ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology. Chemical Research in Toxicology, 2016, 29, 1225-1251.	1.7	456
27	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
28	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
29	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
30	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
31	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
32	Phenotypic screening of the ToxCast chemical library to classify toxic and therapeutic mechanisms. Nature Biotechnology, 2014, 32, 583-591.	9.4	175
33	QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010.	2.9	1,401
34	EADB: An Estrogenic Activity Database for Assessing Potential Endocrine Activity. Toxicological Sciences, 2013, 135, 277-291.	1.4	68
35	Profiling 976 ToxCast Chemicals across 331 Enzymatic and Receptor Signaling Assays. Chemical Research in Toxicology, 2013, 26, 878-895.	1.7	162
36	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

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37	Perspectives on validation of high-throughput assays supporting 21st century toxicity testing. ALTEX: Alternatives To Animal Experimentation, 2013, 30, 51-66.	0.9	118
38	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
39	Integration of Dosimetry, Exposure, and High-Throughput Screening Data in Chemical Toxicity Assessment. Toxicological Sciences, 2012, 125, 157-174.	1.4	336
40	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
41	Genetic toxicology in the 21st century: Reflections and future directions. Environmental and Molecular Mutagenesis, 2011, 52, 339-354.	0.9	84
42	Activity profiles of 309 ToxCastâ„¢ chemicals evaluated across 292 biochemical targets. Toxicology, 2011, 282, 1-15.	2.0	124
43	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
44	In Vitro Screening of Environmental Chemicals for Targeted Testing Prioritization: The ToxCast Project. Environmental Health Perspectives, 2010, 118, 485-492.	2.8	519
45	Endocrine Profiling and Prioritization of Environmental Chemicals Using ToxCast Data. Environmental Health Perspectives, 2010, 118, 1714-1720.	2.8	274
46	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
47	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
48	The Toxicity Data Landscape for Environmental Chemicals. Environmental Health Perspectives, 2009, 117, 685-695.	2.8	418
49	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
50	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
51	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
52	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
53	ACToR â€" Aggregated Computational Toxicology Resource. Toxicology and Applied Pharmacology, 2008, 233, 7-13.	1.3	195
54	Computational Toxicologyâ€"A State of the Science Mini Review. Toxicological Sciences, 2008, 103, 14-27.	1.4	152

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55	Toxicity Data Informatics: Supporting a New Paradigm for Toxicity Prediction. Toxicology Mechanisms and Methods, 2008, 18, 103-118.	1.3	68
56	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
57	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
58	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
59	The ToxCast Program for Prioritizing Toxicity Testing of Environmental Chemicals. Toxicological Sciences, 2007, 95, 5-12.	1.4	851
60	Future of ToxicologyPredictive Toxicology:Â An Expanded View of â€œChemical Toxicityâ€• Chemical Research in Toxicology, 2006, 19, 1257-1262.	1.7	63
61	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
62	Bromochloro-haloacetic acids: Effects on mouse embryos in vitro and QSAR considerations. Reproductive Toxicology, 2006, 21, 260-266.	1.3	24
63	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
64	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
65	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
66	Interaction of organophosphate pesticides and related compounds with the androgen receptor.. Environmental Health Perspectives, 2003, 111, 545-552.	2.8	50
67	Public Sources of Mutagenicity and Carcinogenicity Data. , 2003, , .		7
68	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
69	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
70	The optimal fragmentation principleâ€“Reply. Drug Discovery Today, 2001, 6, 235-237.	3.2	2
71	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
72	Application of artificial intelligence and computer-based methods to predicting chemical toxicity. Knowledge Engineering Review, 1999, 14, 307-317.	2.1	17

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73	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
74	Quantitative Structure-Based Modeling Applied to Characterization and Prediction of Chemical Toxicity. Methods, 1998, 14, 264-276.	1.9	48
75	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
76	The Development and Validation of Expert Systems for Predicting Toxicity. ATLA Alternatives To Laboratory Animals, 1997, 25, 223-251.	0.7	96
77	Conformational Aspects of Glutathione Conjugates of Chlorinated Alkenes:Â A Computational Study. Chemical Research in Toxicology, 1996, 9, 667-675.	1.7	2
78	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
79	Quantitative structure-activity relationships for the developmental toxicity of haloacetic acids in mammalian whole embryo culture. , 1996, 53, 352-360.		66
80	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
81	Role of computational chemistry in support of hazard identification (ID): mechanism-based SARs. Toxicology Letters, 1995, 79, 115-122.	0.4	6
82	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
83	Quantitative comparison of molecular electrostatic potentials for structure-activity studies. Journal of Computational Chemistry, 1991, 12, 959-969.	1.5	70
84	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
85	Modified molecular charge similarity indices for choosing molecular analogues. International Journal of Quantum Chemistry, 1987, 31, 309-323.	1.0	18
86	Photodissociation of the energy selected nitrobenzene ion. Journal of Chemical Physics, 1986, 84, 1424-1431.	1.2	16