Grace Patlewicz

List of Publications by Year
in descending order

134 papers	9,217 citations	44069 48 h-index	42399 92 g-index
142 all docs	142 docs citations	142 times ranked	4822 citing authors

#	Article	IF	Citations
1	Comparing the performance and coverage of selected in silico (liver) metabolism tools relative to reported studies in the literature to inform analogue selection in read-across: A case study. Computational Toxicology, 2022, 21, 100208.	3.3	7
2	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.	3.3	29
3	Assembly and Curation of Lists of Per- and Polyfluoroalkyl Substances (PFAS) to Support Environmental Science Research. Frontiers in Environmental Science, 2022, 10, .	3.3	25
4	Evaluation of Variability Across Rat Acute Oral Systemic Toxicity Studies. Toxicological Sciences, 2022, 188, 34-47.	3.1	22
5	Editorial: Advances and Refinements in the Development and Application of Threshold of Toxicological Concern. Frontiers in Toxicology, 2022, 4, 882321.	3.1	1
6	Systematic Evidence Map for Over One Hundred and Fifty Per- and Polyfluoroalkyl Substances (PFAS). Environmental Health Perspectives, 2022, 130, 56001.	6.0	36
7	Principles and procedures for assessment of acute toxicity incorporating in silico methods. Computational Toxicology, 2022, 24, 100237.	3.3	5
8	NAM-supported read-across: From case studies to regulatory guidance in safety assessment. ALTEX: Alternatives To Animal Experimentation, 2021, 38, 140-150.	1.5	19
9	Generalized Read-Across prediction using genra-py. Bioinformatics, 2021, 37, 3380-3381.	4.1	12
10	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	6.0	63
11	An evaluation of existing QSAR models and structural alerts and development of new ensemble models for genotoxicity using a newly compiled experimental dataset. Computational Toxicology, 2021, 18, 100167.	3.3	12
12	Bioactivity profiling of per- and polyfluoroalkyl substances (PFAS) identifies potential toxicity pathways related to molecular structure. Toxicology, 2021, 457, 152789.	4.2	57
13	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
14	Integrating publicly available information to screen potential candidates for chemical prioritization under the Toxic Substances Control Act: A proof of concept case study using genotoxicity and carcinogenicity. Computational Toxicology, 2021, 20, 100185.	3.3	4
15	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
16	A New OECD Definition for Per- and Polyfluoroalkyl Substances. Environmental Science & Technology, 2021, 55, 15575-15578.	10.0	134
17	Implementing in vitro bioactivity data to modernize priority setting of chemical inventories. ALTEX: Alternatives To Animal Experimentation, 2021, , .	1.5	6
18	An evaluation of the performance of selected (Q)SARs/expert systems for predicting acute oral toxicity. Computational Toxicology, 2020, 16, 100135.	3.3	9

#	Article	IF	Citations
19	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
20	Derivation of New Threshold of Toxicological Concern Values for Exposure via Inhalation for Environmentally-Relevant Chemicals. Frontiers in Toxicology, 2020, 2, 580347.	3.1	12
21	Navigating the Minefield of Computational Toxicology and Informatics: Looking Back and Charting a New Horizon. Frontiers in Toxicology, 2020, 2, 2.	3.1	5
22	Identification of novel activators of the metal responsive transcription factor (MTF-1) using a gene expression biomarker in a microarray compendium. Metallomics, 2020, 12, 1400-1415.	2.4	13
23	Internationalization of read-across as a validated new approach method (NAM) for regulatory toxicology. ALTEX: Alternatives To Animal Experimentation, 2020, 37, 579-606.	1.5	48
24	Transitioning the generalised read-across approach (GenRA) to quantitative predictions: A case study using acute oral toxicity data. Computational Toxicology, 2019, 12, 100097.	3.3	14
25	Evaluating potential refinements to existing Threshold of Toxicological Concern (TTC) values for environmentally-relevant compounds. Regulatory Toxicology and Pharmacology, 2019, 109, 104505.	2.7	34
26	Quantitative prediction of repeat dose toxicity values using GenRA. Regulatory Toxicology and Pharmacology, 2019, 109, 104480.	2.7	8
27	Comparing and contrasting the coverage of publicly available structural alerts for protein binding. Computational Toxicology, 2019, 12, 100100.	3.3	3
28	Predicting estrogen receptor activation by a group of substituted phenols: An integrated approach to testing and assessment case study. Regulatory Toxicology and Pharmacology, 2019, 106, 278-291.	2.7	17
29	Exploring current read-across applications and needs among selected U.S. Federal Agencies. Regulatory Toxicology and Pharmacology, 2019, 106, 197-209.	2.7	23
30	The Next Generation Blueprint of Computational Toxicology at the U.S. Environmental Protection Agency. Toxicological Sciences, 2019, 169, 317-332.	3.1	225
31	A Chemical Category-Based Prioritization Approach for Selecting 75 Per- and Polyfluoroalkyl Substances (PFAS) for Tiered Toxicity and Toxicokinetic Testing. Environmental Health Perspectives, 2019, 127, 14501.	6.0	75
32	Integrating data gap filling techniques: A case study predicting TEFs for neurotoxicity TEQs to facilitate the hazard assessment of polychlorinated biphenyls. Regulatory Toxicology and Pharmacology, 2019, 101, 12-23.	2.7	11
33	Generalized Read-Across (GenRA): A workflow implemented into the EPA CompTox Chemicals Dashboard. ALTEX: Alternatives To Animal Experimentation, 2019, 36, 462-465.	1.5	33
34	An evaluation of selected (Q)SARs/expert systems for predicting skin sensitisation potential. SAR and QSAR in Environmental Research, 2018, 29, 439-468.	2.2	18
35	Navigating through the minefield of read-across frameworks: A commentary perspective. Computational Toxicology, 2018, 6, 39-54.	3.3	44
36	In silico toxicology protocols. Regulatory Toxicology and Pharmacology, 2018, 96, 1-17.	2.7	159

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37	Alternative approaches for acute inhalation toxicity testing to address global regulatory and non-regulatory data requirements: An international workshop report. Toxicology in Vitro, 2018, 48, 53-70.	2.4	62
38	Nonâ€animal assessment of skin sensitization hazard: Is an integrated testing strategy needed, and if so what should be integrated?. Journal of Applied Toxicology, 2018, 38, 41-50.	2.8	37
39	Pathway-based predictive approaches for non-animal assessment of acute inhalation toxicity. Toxicology in Vitro, 2018, 52, 131-145.	2.4	66
40	Extending the Generalised Read-Across approach (GenRA): A systematic analysis of the impact of physicochemical property information on read-across performance. Computational Toxicology, 2018, 8, 34-50.	3.3	13
41	A mechanistic framework for integrating chemical structure and high-throughput screening results to improve toxicity predictions. Computational Toxicology, 2018, 8, 1-12.	3.3	12
42	Predictive models for acute oral systemic toxicity: A workshop to bridge the gap from research to regulation. Computational Toxicology, 2018, 8, 21-24.	3.3	62
43	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
44	What determines skin sensitization potency: Myths, maybes and realities. The 500 molecular weight cutâ€off: An updated analysis. Journal of Applied Toxicology, 2017, 37, 105-116.	2.8	30
45	Retrospective mining of toxicology data to discover multispecies and chemical class effects: Anemia as a case study. Regulatory Toxicology and Pharmacology, 2017, 86, 74-92.	2.7	15
46	Application of IATA â€“ A case study in evaluating the global and local performance of a Bayesian network model for skin sensitization. SAR and QSAR in Environmental Research, 2017, 28, 297-310.	2.2	6
47	A systematic evaluation of analogs and automated read-across prediction of estrogenicity: A case study using hindered phenols. Computational Toxicology, 2017, 4, 22-30.	3.3	15
48	Navigating through the minefield of read-across tools: A review of in silico tools for grouping. Computational Toxicology, 2017, 3, 1-18.	3.3	80
49	Predicting Organ Toxicity Using in Vitro Bioactivity Data and Chemical Structure. Chemical Research in Toxicology, 2017, 30, 2046-2059.	3.3	49
50	Is skin penetration a determining factor in skin sensitization potential and potency? Refuting the notion of a LogKow threshold for skin sensitization. Journal of Applied Toxicology, 2017, 37, 117-127.	2.8	24
51	The CompTox Chemistry Dashboard: a community data resource for environmental chemistry. Journal of Cheminformatics, 2017, 9, 61.	6.1	674
52	ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology. Chemical Research in Toxicology, 2016, 29, 1225-1251.	3.3	456
53	Validation of Computational Methods. Advances in Experimental Medicine and Biology, 2016, 856, 165-187.	1.6	13
54	Chemical applicability domain of the Local Lymph Node Assay (LLNA) for skin sensitization potency. Part 1. Underlying physical organic chemistry principles and the extent to which they are represented in the LLNA validation dataset. Regulatory Toxicology and Pharmacology, 2016, 80, 247-254.	2.7	17

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55	Systematically evaluating read-across prediction and performance using a local validity approach characterized by chemical structure and bioactivity information. Regulatory Toxicology and Pharmacology, 2016, 79, 12-24.	2.7	70
56	Guidance on assessing the methodological and reporting quality of toxicologically relevant studies: A scoping review. Environment International, 2016, 92-93, 630-646.	10.0	58
57	Current and Future Perspectives on the Development, Evaluation, and Application of in Silico Approaches for Predicting Toxicity. Chemical Research in Toxicology, 2016, 29, 438-451.	3.3	72
58	Integrated Approaches to Testing and Assessment. Advances in Experimental Medicine and Biology, 2016, 856, 317-342.	1.6	15
59	Toward Good Read-Across Practice (GRAP) guidance. ALTEX: Alternatives To Animal Experimentation, 2016, 33, 149-166.	1.5	134
60	An exposure:activity profiling method for interpreting high-throughput screening data for estrogenic activityâ€"Proof of concept. Regulatory Toxicology and Pharmacology, 2015, 71, 398-408.	2.7	45
61	Building scientific confidence in the development and evaluation of read-across. Regulatory Toxicology and Pharmacology, 2015, 72, 117-133.	2.7	56
62	Proposing a scientific confidence framework to help support the application of adverse outcome pathways for regulatory purposes. Regulatory Toxicology and Pharmacology, 2015, 71, 463-477.	2.7	87
63	A feasibility study: Can information collected to classify for mutagenicity be informative in predicting carcinogenicity?. Regulatory Toxicology and Pharmacology, 2015, 72, 17-25.	2.7	18
64	The adverse outcome pathway for rodent liver tumor promotion by sustained activation of the aryl hydrocarbon receptor. Regulatory Toxicology and Pharmacology, 2015, 73, 172-190.	2.7	42
65	Integrated testing and assessment approaches for skin sensitization: a commentary. Journal of Applied Toxicology, 2014, 34, 436-440.	2.8	10
66	The challenge of using read-across within the EU REACH regulatory framework; how much uncertainty is too much? Dipropylene glycol methyl ether acetate, an exemplary case study. Regulatory Toxicology and Pharmacology, 2014, 68, 212-221.	2.7	47
67	Towards AOP application â€“ Implementation of an integrated approach to testing and assessment (IATA) into a pipeline tool for skin sensitization. Regulatory Toxicology and Pharmacology, 2014, 69, 529-545.	2.7	89
68	TIMES-SS â€“ Recent refinements resulting from an industrial skin sensitisation consortium. SAR and QSAR in Environmental Research, 2014, 25, 367-391.	2.2	30
69	A Mechanistic Approach to Modeling Respiratory Sensitization. Chemical Research in Toxicology, 2014, 27, 219-239.	3.3	33
70	Applying Adverse Outcome Pathways (AOPs) to support Integrated Approaches to Testing and Assessment (IATA). Regulatory Toxicology and Pharmacology, 2014, 70, 629-640.	2.7	291
71	Developing scientific confidence in HTS-derived prediction models: Lessons learned from an endocrine case study. Regulatory Toxicology and Pharmacology, 2014, 69, 443-450.	2.7	27
72	Read-across approaches - misconceptions, promises and challenges ahead. ALTEX: Alternatives To Animal Experimentation, 2014, 31, 387-396.	1.5	90

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73	Use of category approaches, read-across and (Q)SAR: General considerations. Regulatory Toxicology and Pharmacology, 2013, 67, 1-12.	2.7	105
74	Use and validation of HT/HC assays to support 21st century toxicity evaluations. Regulatory Toxicology and Pharmacology, 2013, 65, 259-268.	2.7	35
75	Evidence-based toxicology for the 21st century: Opportunities and challenges. ALTEX: Alternatives To Animal Experimentation, 2013, 30, 74-104.	1.5	42
76	Investigating the Relationship between in Vitroâ€“in Vivo Genotoxicity: Derivation of Mechanistic QSAR Models for in Vivo Liver Genotoxicity and in Vivo Bone Marrow Micronucleus Formation Which Encompass Metabolism. Chemical Research in Toxicology, 2012, 25, 277-296.	3.3	23
77	A roadmap for the development of alternative (non-animal) methods for systemic toxicity testing. ALTEX: Alternatives To Animal Experimentation, 2012, 29, 3-91.	1.5	190
78	Chemistry-Based Risk Assessment for Skin Sensitization: Quantitative Mechanistic Modeling for the SNAr Domain. Chemical Research in Toxicology, 2011, 24, 1003-1011.	3.3	34
79	Non-testing approaches under REACH â€“ help or hindrance? Perspectives from a practitioner within industry. SAR and QSAR in Environmental Research, 2011, 22, 67-88.	2.2	16
80	Network Topological Indices from Chem-Bioinformatics to Legal Sciences and back. Current Bioinformatics, 2011, 6, 53-70.	1.5	14
81	Markov Entropy Centrality: Chemical, Biological, Crime, and Legislative Networks. , 2011, , 199-258.		5
82	Can mutagenicity information be useful in an Integrated Testing Strategy (ITS) for skin sensitization?. SAR and QSAR in Environmental Research, 2010, 21, 619-656.	2.2	8
83	Predicting Drugs and Proteins in Parasite Infections with Topological Indices of Complex Networks: Theoretical Backgrounds, Applications and Legal Issues. Current Pharmaceutical Design, 2010, 16, 2737-2764.	1.9	54
84	Use of Genotoxicity Information in the Development of Integrated Testing Strategies (ITS) for Skin Sensitization. Chemical Research in Toxicology, 2010, 23, 1519-1540.	3.3	22
85	Chemistry Based Nonanimal Predictive Modeling for Skin Sensitization. Emerging Topics in Ecotoxicology, 2009, , 61-83.	1.5	7
86	A Minireview of Available Skin Sensitization (Q)SARs/Expert Systems. QSAR and Combinatorial Science, 2008, 27, 60-76.	1.4	44
87	A Review of (Q)SAR Models for Skin and Eye Irritation and Corrosion. QSAR and Combinatorial Science, 2008, 27, 49-59.	1.4	32
88	Chemical reactivity indices and mechanismâ€based readâ€across for nonâ€animal based assessment of skin sensitisation potential. Journal of Applied Toxicology, 2008, 28, 443-454.	2.8	67
89	A Comparison of Reactivity Schemes for the Prediction Skin Sensitization Potential. Chemical Research in Toxicology, 2008, 21, 521-541.	3.3	36
90	FS04.3â€¨Hair dyes, prediction of sensitization potential with QSAR. Contact Dermatitis, 2008, 50, 137-137.	1.4	0

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91	P38â€¨Quantitative structure activity relationships for fragrance aldehydes. Contact Dermatitis, 2008, 50, 192-192.	1.4	0
92	Toxmatchâ€”A chemical classification and activity prediction tool based on similarity measures. Regulatory Toxicology and Pharmacology, 2008, 52, 77-84.	2.7	32
93	An evaluation of the implementation of the Cramer classification scheme in the Toxtree software. SAR and QSAR in Environmental Research, 2008, 19, 495-524.	2.2	359
94	A feasibility study developing an integrated testing strategy assessing skin irritation potential of chemicals. Toxicology Letters, 2008, 180, 9-20.	0.8	38
95	Skin, drug and chemical reactions. Drug Discovery Today Disease Mechanisms, 2008, 5, e211-e220.	0.8	7
96	Toxmatchâ€“a new software tool to aid in the development and evaluation of chemically similar groups. SAR and QSAR in Environmental Research, 2008, 19, 397-412.	2.2	64
97	Current Topics on Software Use in Medicinal Chemistry: Intellectual Property, Taxes, and Regulatory Issues. Current Topics in Medicinal Chemistry, 2008, 8, 1666-1675.	2.1	60
98	Evaluation of SARs for the prediction of skin irritation/corrosion potentialâ€“structural inclusion rules in the BfR decision support systemâ€. SAR and QSAR in Environmental Research, 2007, 18, 331-342.	2.2	23
99	An evaluation of selected global (Q)SARs/expert systems for the prediction of skin sensitisation potential. SAR and QSAR in Environmental Research, 2007, 18, 515-541.	2.2	77
100	Global (Q)SARs for skin sensitisationâ€“assessment against OECD principlesâ€“. SAR and QSAR in Environmental Research, 2007, 18, 343-365.	2.2	39
101	The role of the European Chemicals Bureau in promoting the regulatory use of (Q)SAR methods. SAR and QSAR in Environmental Research, 2007, 18, 111-125.	2.2	130
102	Electrophilic Chemistry Related to Skin Sensitization. Reaction Mechanistic Applicability Domain Classification for a Published Data Set of 106 Chemicals Tested in the Mouse Local Lymph Node Assay. Chemical Research in Toxicology, 2007, 20, 44-60.	3.3	142
103	Skin Sensitisation and Epidermal Disposition: The Relevance of Epidermal Disposition for Sensitisation Hazard Identification and Risk Assessment. ATLA Alternatives To Laboratory Animals, 2007, 35, 137-154.	1.0	69
104	TIMES-SSâ€”A promising tool for the assessment of skin sensitization hazard. A characterization with respect to the OECD validation principles for (Q)SARs and an external evaluation for predictivity. Regulatory Toxicology and Pharmacology, 2007, 48, 225-239.	2.7	91
105	TIMES-SSâ€”A Mechanistic Evaluation of an External Validation Study Using Reaction Chemistry Principles. Chemical Research in Toxicology, 2007, 20, 1321-1330.	3.3	56
106	Mechanistic Applicability Domain Classification of a Local Lymph Node Assay Dataset for Skin Sensitization. Chemical Research in Toxicology, 2007, 20, 1019-1030.	3.3	1,334
107	Predicting Toxicological and Ecotoxicological Endpoints. , 2007, , 427-465.		9
108	Mechanistic Applicability Domains for Non-Animal Based Prediction of Toxicological Endpoints. QSAR Analysis of the Schiff Base Applicability Domain for Skin Sensitization. Chemical Research in Toxicology, 2006, 19, 1228-1233.	3.3	141

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109	Validation of counter propagation neural network models for predictive toxicology according to the OECD principles: a case study. SAR and QSAR in Environmental Research, 2006, 17, 265-284.	2.2	50
110	Non-enzymatic glutathione reactivity and in vitro toxicity: A non-animal approach to skin sensitization. Toxicology in Vitro, 2006, 20, 239-247.	2.4	91
111	Computational Methods to Predict Drug Safety. Current Computer-Aided Drug Design, 2006, 2, 151-168.	1.2	1
112	The local lymph node assay and skin sensitization: a cut-down screen to reduce animal requirements?. Contact Dermatitis, 2006, 54, 181-185.	1.4	41
113	Structure?activity relationships for skin sensitization: recent improvements to Derek for Windows. Contact Dermatitis, 2006, 55, 342-347.	1.4	48
114	A Stepwise Approach for Defining the Applicability Domain of SAR and QSAR Models. Journal of Chemical Information and Modeling, 2005, 45, 839-849.	5.4	243
115	A Stepwise Approach for Defining the Applicability Domain of SAR and QSAR Models.. ChemInform, 2005, 36, no.	0.0	0
116	Skin Sensitization: Modeling Based on Skin Metabolism Simulation and Formation of Protein Conjugates. International Journal of Toxicology, 2005, 24, 189-204.	1.2	79
117	Skin Sensitization:â€‰ Reaction Mechanistic Applicability Domains for Structureâ^'Activity Relationships. Chemical Research in Toxicology, 2005, 18, 1420-1426.	3.3	165
118	A chemical dataset for evaluation of alternative approaches to skinâ€sensitization testing. Contact Dermatitis, 2004, 50, 274-288.	1.4	129
119	Further evaluation of quantitative structure-activity relationship models for the prediction of the skin sensitization potency of selected fragrance allergens. Contact Dermatitis, 2004, 50, 91-97.	1.4	62
120	Creating molecular diversity from antioxidants in Brazilian propolis. Combination of TOPS-MODE QSAR and virtual structure generation. Molecular Diversity, 2004, 8, 21-33.	3.9	40
121	From Knowledge Generation to Knowledge Archive. A General Strategy Using TOPS-MODE with DEREK to Formulate New Alerts for Skin Sensitization.. ChemInform, 2004, 35, no.	0.0	0
122	From Knowledge Generation to Knowledge Archive. A General Strategy Using TOPS-MODE with DEREK To Formulate New Alerts for Skin Sensitization. Journal of Chemical Information and Computer Sciences, 2004, 44, 688-698.	2.8	47
123	QUANTITATIVE STRUCTUREâ€"ACTIVITY RELATIONSHIPS FOR PREDICTING SKIN AND RESPIRATORY SENSITIZATION. Environmental Toxicology and Chemistry, 2003, 22, 1855.	4.3	29
124	QUANTITATIVE STRUCTUREâ€"ACTIVITY RELATIONSHIPS FOR PREDICTING SKIN AND EYE IRRITATION. Environmental Toxicology and Chemistry, 2003, 22, 1862.	4.3	20
125	QUANTITATIVE STRUCTUREâ€"ACTIVITY RELATIONSHIPS FOR PREDICTING PERCUTANEOUS ABSORPTION RATES. Environmental Toxicology and Chemistry, 2003, 22, 1870.	4.3	33
126	QUANTITATIVE STRUCTUREâ€"ACTIVITY RELATIONSHIPS FOR PREDICTING MUTAGENICITY AND CARCINOGENICITY. Environmental Toxicology and Chemistry, 2003, 22, 1885.	4.3	50

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127	QSARs for the skin sensitization potential of aldehydes and related compounds. QSAR and Combinatorial Science, 2003, 22, 196-203.	1.4	53
128	Computer-Aided Knowledge Generation for Understanding Skin Sensitization Mechanisms: The TOPS-MODE Approach. Chemical Research in Toxicology, 2003, 16, 1226-1235.	3.3	81
129	Investigation of the skin sensitizing activity of linalool. Contact Dermatitis, 2002, 47, 161-164.	1.4	32
130	Structure-activity relationships for selected fragrance allergens. Contact Dermatitis, 2002, 47, 219-226.	1.4	68
131	Mechanism based structure-activity relationships for skin sensitisation--the carbonyl group domain. SAR and QSAR in Environmental Research, 2002, 13, 145-152.	2.2	24
132	Skinâ€sensitization structureâ€activity relationships for aldehydes. Contact Dermatitis, 2001, 44, 331-336.	1.4	98
133	A QSAR model for the eye irritation of cationic surfactants. Toxicology in Vitro, 2000, 14, 79-84.	2.4	36
134	Development of the InTelligence And Machine LEarning (TAME) Toolkit for Introductory Data Science, Chemical-Biological Analyses, Predictive Modeling, and Database Mining for Environmental Health Research. Frontiers in Toxicology, 0, 4, .	3.1	4