Mark T D Cronin

List of Publications by Year
in descending order

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214 papers	22,757 citations	36203 51 h-index	8370 147 g-index

238 all docs	238 docs citations	238 times ranked	26410 citing authors

#	Article	IF	Citations
1	Free radicals and antioxidants in normal physiological functions and human disease. International Journal of Biochemistry and Cell Biology, 2007, 39, 44-84.	1.2	10,891
2	QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010.	2.9	1,401
3	Methods for reliability and uncertainty assessment and for applicability evaluations of classification- and regression-based QSARs.. Environmental Health Perspectives, 2003, 111, 1361-1375.	2.8	1,108
4	Alternative (non-animal) methods for cosmetics testing: current status and future prospectsâ€"2010. Archives of Toxicology, 2011, 85, 367-485.	1.9	488
5	Pitfalls in QSAR. Computational and Theoretical Chemistry, 2003, 622, 39-51.	1.5	300
6	Use of QSARs in international decision-making frameworks to predict health effects of chemical substances.. Environmental Health Perspectives, 2003, 111, 1391-1401.	2.8	238
7	Quantitative structureâ€"activity relationships (QSARs) in toxicology: a historical perspective. Computational and Theoretical Chemistry, 2003, 622, 1-22.	1.5	205
8	Use of QSARs in international decision-making frameworks to predict ecologic effects and environmental fate of chemical substances.. Environmental Health Perspectives, 2003, 111, 1376-1390.	2.8	192
9	Measurement and Estimation of Electrophilic Reactivity for Predictive Toxicology. Chemical Reviews, 2011, 111, 2562-2596.	23.0	178
10	Quantitative structureâ€"activity relationships (QSARs) for the prediction of skin permeation of exogenous chemicals. Chemosphere, 2002, 48, 603-613.	4.2	168
11	Statement on advancing the assessment of chemical mixtures and their risks for human health and the environment. Environment International, 2020, 134, 105267.	4.8	165
12	The Role of Omics in the Application of Adverse Outcome Pathways for Chemical Risk Assessment. Toxicological Sciences, 2017, 158, 252-262.	1.4	161
13	In silico toxicology protocols. Regulatory Toxicology and Pharmacology, 2018, 96, 1-17.	1.3	159
14	Comparative assessment of methods to develop QSARs for the prediction of the toxicity of phenols to Tetrahymena pyriformis. Chemosphere, 2002, 49, 1201-1221.	4.2	152
15	A European perspective on alternatives to animal testing for environmental hazard identification and risk assessment. Regulatory Toxicology and Pharmacology, 2013, 67, 506-530.	1.3	139
16	Toward Good Read-Across Practice (GRAP) guidance. ALTEX: Alternatives To Animal Experimentation, 2016, 33, 149-166.	0.9	134
17	Structure-toxicity relationships for phenols to Tetrahymena pyriformis. Chemosphere, 1996, 32, 1453-1468.	4.2	129
18	QSAR in Toxicology. 1. Prediction of Aquatic Toxicity. QSAR and Combinatorial Science, 1995, 14, 1-7.	1.4	123

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19	Prediction of Michael-Type Acceptor Reactivity toward Glutathione. Chemical Research in Toxicology, 2010, 23, 1576-1585.	1.7	115
20	Thresholds of Toxicological Concern for cosmetics-related substances: New database, thresholds, and enrichment of chemical space. Food and Chemical Toxicology, 2017, 109, 170-193.	1.8	108
21	Development of Quantitative Structureâ^'Activity Relationships for the Toxicity of Aromatic Compounds toTetrahymena pyriformis:Â Comparative Assessment of the Methodologies. Chemical Research in Toxicology, 2001, 14, 1284-1295.	1.7	105
22	A Review of In Silico Tools as Alternatives to Animal Testing: Principles, Resources and Applications. ATLA Alternatives To Laboratory Animals, 2020, 48, 146-172.	0.7	100
23	Structure-Based Classification of Antibacterial Activity. Journal of Chemical Information and Computer Sciences, 2002, 42, 869-878.	2.8	97
24	The Development and Validation of Expert Systems for Predicting Toxicity. ATLA Alternatives To Laboratory Animals, 1997, 25, 223-251.	0.7	96
25	Quantitative structureâ€"permeability relationships for percutaneous absorption: re-analysis of steroid data. International Journal of Pharmaceutics, 2002, 238, 105-109.	2.6	91
26	Read-across approaches - misconceptions, promises and challenges ahead. ALTEX: Alternatives To Animal Experimentation, 2014, 31, 387-396.	0.9	90
27	Structureâ^'Toxicity Relationships for the Effects toTetrahymena pyriformisof Aliphatic, Carbonyl-Containing, Î±,Î²-Unsaturated Chemicals. Chemical Research in Toxicology, 2005, 18, 330-341.	1.7	89
28	Chemical Safety Assessment Using Read-Across: Assessing the Use of Novel Testing Methods to Strengthen the Evidence Base for Decision Making. Environmental Health Perspectives, 2015, 123, 1232-1240.	2.8	89
29	Consensus QSAR Models:â€‰ Do the Benefits Outweigh the Complexity?. Journal of Chemical Information and Modeling, 2007, 47, 1460-1468.	2.5	86
30	Adverse Outcome Pathways can drive nonâ€animal approaches for safety assessment. Journal of Applied Toxicology, 2015, 35, 971-975.	1.4	82
31	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.	2.4	81
32	The present status of QSAR in toxicology. Computational and Theoretical Chemistry, 2003, 622, 23-38.	1.5	79
33	Electrophilic Reaction Chemistry of Low Molecular Weight Respiratory Sensitizers. Chemical Research in Toxicology, 2009, 22, 1447-1453.	1.7	78
34	Assessing Applicability Domains of Toxicological QSARs: Definition, Confidence in Predicted Values, and the Role of Mechanisms of Action. QSAR and Combinatorial Science, 2007, 26, 238-254.	1.5	76
35	The identification of nuclear receptors associated with hepatic steatosis to develop and extend adverse outcome pathways. Critical Reviews in Toxicology, 2016, 46, 138-152.	1.9	76
36	Validation of Vibrio fisheri acute toxicity data: mechanism of action-based QSARs for non-polar narcotics and polar narcotic phenols. Science of the Total Environment, 1997, 204, 75-88.	3.9	73

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37	In silicomodels for drug-induced liver injury â€“ current status. Expert Opinion on Drug Metabolism and Toxicology, 2012, 8, 201-217.	1.5	73
38	Structureâ^'Toxicity Relationships for Aliphatic Chemicals Evaluated with Tetrahymena pyriformis. Chemical Research in Toxicology, 2002, 15, 1602-1609.	1.7	72
39	Assessment and Modeling of the Toxicity of Organic Chemicals to Chlorella vulgaris:â€‰ Development of a Novel Database. Chemical Research in Toxicology, 2004, 17, 545-554.	1.7	71
40	Formation of Categories from Structureâ^'Activity Relationships To Allow Read-Across for Risk Assessment: Toxicity of Î±,Î²-Unsaturated Carbonyl Compounds. Chemical Research in Toxicology, 2008, 21, 2300-2312.	1.7	70
41	Structure-activity relationships for gene activation oestrogenicity: Evaluation of a diverse set of aromatic chemicals. Environmental Toxicology, 2002, 17, 14-23.	2.1	69
42	The use of discriminant analysis, logistic regression and classification tree analysis in the development of classification models for human health effects. Computational and Theoretical Chemistry, 2003, 622, 97-111.	1.5	69
43	Quantitative structure-skin permeability relationships. Toxicology, 2017, 387, 27-42.	2.0	69
44	Quantitative adverse outcome pathway (qAOP) models for toxicity prediction. Archives of Toxicology, 2020, 94, 1497-1510.	1.9	65
45	QSAR Study of the Toxicity of Nitrobenzenes toTetrahymena pyriformis. QSAR and Combinatorial Science, 1995, 14, 427-432.	1.4	61
46	Novel approach for efficient predictions properties of large pool of nanomaterials based on limited set of species: nano-read-across. Nanotechnology, 2015, 26, 015701.	1.3	61
47	Development and analysis of an adverse outcome pathway network for human neurotoxicity. Archives of Toxicology, 2019, 93, 2759-2772.	1.9	61
48	Lessons learned from read-across case studies for repeated-dose toxicity. Regulatory Toxicology and Pharmacology, 2017, 88, 185-191.	1.3	58
49	Genetic toxicology in silico protocol. Regulatory Toxicology and Pharmacology, 2019, 107, 104403.	1.3	57
50	Legacy data sharing to improve drug safety assessment: the eTOX project. Nature Reviews Drug Discovery, 2017, 16, 811-812.	21.5	56
51	In Silico Toxicology Data Resources to Support Read-Across and (Q)SAR. Frontiers in Pharmacology, 2019, 10, 561.	1.6	56
52	Using Molecular Initiating Events to Develop a Structural Alert Based Screening Workflow for Nuclear Receptor Ligands Associated with Hepatic Steatosis. Chemical Research in Toxicology, 2016, 29, 203-212.	1.7	52
53	QSAR in Toxicology. 3. Prediction of Chronic Toxicities. QSAR and Combinatorial Science, 1995, 14, 329-334.	1.4	50
54	Essential and desirable characteristics of ecotoxicity quantitative structureâ€“activity relationships. Environmental Toxicology and Chemistry, 2003, 22, 599-607.	2.2	50

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55	Assessing the safety of cosmetic chemicals: Consideration of a flux decision tree to predict dermally delivered systemic dose for comparison with oral TTC (Threshold of Toxicological Concern). Regulatory Toxicology and Pharmacology, 2016, 76, 174-186.	1.3	50
56	Alternative Methods for Skin Sensitisation Testing. ATLA Alternatives To Laboratory Animals, 1996, 24, 683-705.	0.7	49
57	Structureâ€“Toxicity Relationships for Three Mechanisms of Action of Toxicity toVibrio fischeri. Ecotoxicology and Environmental Safety, 1998, 39, 65-69.	2.9	48
58	(Q)SARs for Predicting Effects Relating to Reproductive Toxicity. QSAR and Combinatorial Science, 2008, 27, 91-100.	1.5	48
59	Internationalization of read-across as a validated new approach method (NAM) for regulatory toxicology. ALTEX: Alternatives To Animal Experimentation, 2020, 37, 579-606.	0.9	48
60	Quantitative structureâ€“activityâ€“activity and quantitative structureâ€“activity investigations of human and rodent toxicity. Chemosphere, 2006, 65, 1878-1887.	4.2	46
61	QSAR in Toxicology. 2. Prediction of Acute Mammalian Toxicity and Interspecies Correlations. QSAR and Combinatorial Science, 1995, 14, 117-120.	1.4	45
62	Molecular Quantum Similarity Analysis of Estrogenic Activity. Journal of Chemical Information and Computer Sciences, 2003, 43, 1166-1176.	2.8	45
63	In silico resources to assist in the development and evaluation of physiologically-based kinetic models. Computational Toxicology, 2019, 11, 33-49.	1.8	45
64	Assessing uncertainty in read-across: Questions to evaluate toxicity predictions based on knowledge gained from case studies. Computational Toxicology, 2019, 9, 1-11.	1.8	45
65	Navigating through the minefield of read-across frameworks: A commentary perspective. Computational Toxicology, 2018, 6, 39-54.	1.8	44
66	QSAR Analysis of the Toxicity of Aromatic Compounds toChlorellavulgarisin a Novel Short-Term Assay. Journal of Chemical Information and Computer Sciences, 2004, 44, 258-265.	2.8	42
67	Quantitative Structure-Activity Relationships of Chemicals Acting by Non-polar Narcosisâ€”Theoretical Considerations. QSAR and Combinatorial Science, 1998, 17, 131-138.	1.4	42
68	Development of an in Silico Profiler for Mitochondrial Toxicity. Chemical Research in Toxicology, 2015, 28, 1891-1902.	1.7	41
69	(Q)SARs to predict environmental toxicities: current status and future needs. Environmental Sciences: Processes and Impacts, 2017, 19, 213-220.	1.7	41
70	The SEURAT-1 approach towards animal free human safety assessment. ALTEX: Alternatives To Animal Experimentation, 2015, 32, 9-24.	0.9	40
71	A framework for chemical safety assessment incorporating new approach methodologies within REACH. Archives of Toxicology, 2022, 96, 743-766.	1.9	39
72	QSAR in Toxicology. 4. Prediction of Non-lethal Mammalian Toxicological Endpoints, and Expert Systems for Toxicity Prediction. QSAR and Combinatorial Science, 1995, 14, 518-523.	1.4	38

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73	Molecular Modelling Study of the PPARÎ³ Receptor in Relation to the Mode of Action/Adverse Outcome Pathway Framework for Liver Steatosis. International Journal of Molecular Sciences, 2014, 15, 7651-7666.	1.8	38
74	Investigation of the Verhaar scheme for predicting acute aquatic toxicity: Improving predictions obtained from Toxtree ver. 2.6. Chemosphere, 2015, 139, 146-154.	4.2	38
75	Adverse Outcome Pathway (AOP) Informed Modeling of Aquatic Toxicology: QSARs, Read-Across, and Interspecies Verification of Modes of Action. Environmental Science & Technology, 2016, 50, 3995-4007.	4.6	38
76	Optimizing drug discovery by Investigative Toxicology: Current and future trends. ALTEX: Alternatives To Animal Experimentation, 2019, 36, 289-313.	0.9	38
77	Structure-based methods for the prediction of drug metabolism. Expert Opinion on Drug Metabolism and Toxicology, 2006, 2, 545-557.	1.5	37
78	Proposed Integrated Decision-tree Testing Strategies for Mutagenicity and Carcinogenicity in Relation to the EU REACH Legislation. ATLA Alternatives To Laboratory Animals, 2007, 35, 267-287.	0.7	37
79	The In Chemicoâ€“In Silico Interface: Challenges for Integrating Experimental and Computational Chemistry to Identify Toxicity. ATLA Alternatives To Laboratory Animals, 2009, 37, 513-521.	0.7	37
80	Integrated Testing Strategies for Use in the EU REACH System. ATLA Alternatives To Laboratory Animals, 2006, 34, 407-427.	0.7	36
81	Identification and description of the uncertainty, variability, bias and influence in quantitative structure-activity relationships (QSARs) for toxicity prediction. Regulatory Toxicology and Pharmacology, 2019, 106, 90-104.	1.3	36
82	Effect of substituent size and dimensionality on potency of phenolic xenoestrogens evaluated with a recombinant yeast assay. Environmental Toxicology and Chemistry, 2000, 19, 2637-2642.	2.2	35
83	The use of pH measurements to predict the potential of chemicals to cause acute dermal and ocular toxicity. Toxicology, 2001, 169, 119-131.	2.0	35
84	Quantitative structureâ€activity relationships for weak acid respiratory uncouplers to Vibrio fisheri. Environmental Toxicology and Chemistry, 1997, 16, 357-360.	2.2	34
85	A review of the use ofin silicomethods to predict the chemistry of molecular initiating events related to drug toxicity. Expert Opinion on Drug Metabolism and Toxicology, 2011, 7, 1481-1495.	1.5	34
86	Chelators in Iron and Copper Toxicity. Current Pharmacology Reports, 2016, 2, 271-280.	1.5	34
87	How Does the Quality of Phospholipidosis Data Influence the Predictivity of Structural Alerts?. Journal of Chemical Information and Modeling, 2014, 54, 2224-2232.	2.5	33
88	New ideas for non-animal approaches to predict repeated-dose systemic toxicity: Report from an EPAA Blue Sky Workshop. Regulatory Toxicology and Pharmacology, 2020, 114, 104668.	1.3	33
89	Comparing the CORAL and Random Forest Approaches for Modelling the In Vitro Cytotoxicity of Silica Nanomaterials. ATLA Alternatives To Laboratory Animals, 2016, 44, 533-556.	0.7	31
90	Comparative Quantitative Structureâ€“Activityâ€“Activity Relationships for Toxicity to Tetrahymena pyriformis and Pimephales promelas. ATLA Alternatives To Laboratory Animals, 2007, 35, 15-24.	0.7	30

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91	The Use of a Chemistry-based Profiler for Covalent DNA Binding in the Development of Chemical Categories for Read-across for Genotoxicity. ATLA Alternatives To Laboratory Animals, 2011, 39, 131-145.	0.7	30
92	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.	1.3	30
93	Assessment and Reproducibility of Quantitative Structureâ€“Activity Relationship Models by the Nonexpert. Journal of Chemical Information and Modeling, 2018, 58, 673-682.	2.5	29
94	QUANTITATIVE STRUCTUREâ€“ACTIVITY RELATIONSHIPS FOR WEAK ACID RESPIRATORY UNCOUPLERS TO VIBRIO FISHERI. Environmental Toxicology and Chemistry, 1997, 16, 357.	2.2	29
95	A 10-step framework for use of read-across (RAX) in next generation risk assessment (NGRA) for cosmetics safety assessment. Regulatory Toxicology and Pharmacology, 2022, 129, 105094.	1.3	29
96	Systems Biology Approach Reveals a Calcium-Dependent Mechanism for Basal Toxicity in Daphnia magna. Environmental Science & Technology, 2015, 49, 11132-11140.	4.6	28
97	Strategies for the optimisation of in vivo experiments in accordance with the 3Rs philosophy. Regulatory Toxicology and Pharmacology, 2012, 63, 140-154.	1.3	27
98	Perspectives from the NanoSafety Modelling Cluster on the validation criteria for (Q)SAR models used in nanotechnology. Food and Chemical Toxicology, 2018, 112, 478-494.	1.8	27
99	Skin sensitization in silico protocol. Regulatory Toxicology and Pharmacology, 2020, 116, 104688.	1.3	27
100	Relationship Between Adverse Outcome Pathways and Chemistry-BasedIn SilicoModels to Predict Toxicity. Applied in Vitro Toxicology, 2017, 3, 286-297.	0.6	26
101	Development of thresholds of excess toxicity for environmental species and their application to identification of modes of acute toxic action. Science of the Total Environment, 2018, 616-617, 491-499.	3.9	26
102	In SilicoPrediction of Organ Level Toxicity: Linking Chemistry to Adverse Effects. Toxicological Research, 2017, 33, 173-182.	1.1	26
103	The Current Status and Future Applicability of Quantitative Structureâ€“activity Relationships (QSARs) in Predicting Toxicity. ATLA Alternatives To Laboratory Animals, 2002, 30, 81-84.	0.7	25
104	Quantitative structureâ€“activity relationships for the toxicity of organophosphorus and carbamate pesticides to the Rainbow troutOnchorhyncus mykiss. Pest Management Science, 2006, 62, 819-831.	1.7	25
105	Using In Silico Tools in a Weight of Evidence Approach to Aid Toxicological Assessment. Molecular Informatics, 2010, 29, 97-110.	1.4	25
106	Modelling acute oral mammalian toxicity. 1. Definition of a quantifiable baseline effect. Toxicology in Vitro, 2011, 25, 1281-1293.	1.1	25
107	An ISA-TAB-Nano based data collection framework to support data-driven modelling of nanotoxicology. Beilstein Journal of Nanotechnology, 2015, 6, 1978-1999.	1.5	25
108	Derivation, characterisation and analysis of an adverse outcome pathway network for human hepatotoxicity. Toxicology, 2021, 459, 152856.	2.0	25

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109	Integrated Decision-tree Testing Strategies for Acute Systemic Toxicity and Toxicokinetics with Respect to the Requirements of the EU REACH Legislation. ATLA Alternatives To Laboratory Animals, 2008, 36, 45-63.	0.7	24
110	Towards a Fuzzy Expert System on Toxicological Data Quality Assessment. Molecular Informatics, 2013, 32, 65-78.	1.4	24
111	Pragmatic Approaches to Using Computational Methods To Predict Xenobiotic Metabolism. Journal of Chemical Information and Modeling, 2013, 53, 1282-1293.	2.5	24
112	Read-across of 90-day rat oral repeated-dose toxicity: A case study for selected Î²-olefinic alcohols. Computational Toxicology, 2017, 1, 22-32.	1.8	24
113	Estrogenicity and acute toxicity of selected anilines using a recombinant yeast assay. Chemosphere, 2003, 52, 1173-1181.	4.2	23
114	In Silico Studies of the Relationship Between Chemical Structure and Drug Induced Phospholipidosis. Molecular Informatics, 2011, 30, 415-429.	1.4	22
115	The application of molecular modelling in the safety assessment of chemicals: A case study on ligand-dependent PPARÎ³ dysregulation. Toxicology, 2017, 392, 140-154.	2.0	21
116	New framework for a non-animal approach adequately assures the safety of cosmetic ingredients â€“ A case study on caffeine. Regulatory Toxicology and Pharmacology, 2021, 123, 104931.	1.3	21
117	An Integrated Decision-tree Testing Strategy for Skin Sensitisation with Respect to the Requirements of the EU REACH Legislation. ATLA Alternatives To Laboratory Animals, 2007, 35, 683-697.	0.7	20
118	Quantitative Structureâ€“Activity Relationships (QSARs) â€“ Applications and Methodology. Challenges and Advances in Computational Chemistry and Physics, 2010, , 3-11.	0.6	20
119	Read-across of 90-day rat oral repeated-dose toxicity: A case study for selected n-alkanols. Computational Toxicology, 2017, 2, 12-19.	1.8	20
120	Unlocking the potential of in silico chemical safety assessment â€“ A report on a cross-sector symposium on current opportunities and future challenges. Computational Toxicology, 2019, 10, 38-43.	1.8	20
121	A review of in silico toxicology approaches to support the safety assessment of cosmetics-related materials. Computational Toxicology, 2022, 21, 100213.	1.8	20
122	Read-across for rat oral gavage repeated-dose toxicity for short-chain mono-alkylphenols: A case study. Computational Toxicology, 2017, 2, 1-11.	1.8	19
123	A mode-of-action ontology model for safety evaluation of chemicals: Outcome of a series of workshops on repeated dose toxicity. Toxicology in Vitro, 2019, 59, 44-50.	1.1	19
124	Physico-chemical interpretation and prediction of the dimyristoyl phosphatidyl cholineâ€“water partition coefficient. Computational and Theoretical Chemistry, 2002, 593, 9-18.	1.5	18
125	In vitro and in silico studies of the membrane permeability of natural flavonoids from Silybum marianum (L.) Gaertn. and their derivatives. Phytomedicine, 2019, 53, 79-85.	2.3	18
126	Potential of ToxCast Data in the Safety Assessment of Food Chemicals. Toxicological Sciences, 2020, 174, 326-340.	1.4	18

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127	Integrated decision-tree testing strategies for developmental and reproductive toxicity with respect to the requirements of the EU REACH legislation. ATLA Alternatives To Laboratory Animals, 2008, 36, 65-80.	0.7	18
128	Read-across and new approach methodologies applied in a 10-step framework for cosmetics safety assessment â€“ A case study with parabens. Regulatory Toxicology and Pharmacology, 2022, 132, 105161.	1.3	18
129	An Integrated Decision-tree Testing Strategy for Repeat Dose Toxicity with Respect to the Requirements of the EU REACH Legislation. ATLA Alternatives To Laboratory Animals, 2008, 36, 93-101.	0.7	17
130	Ensuring confidence in predictions: A scheme to assess the scientific validity of in silico models. Advanced Drug Delivery Reviews, 2015, 86, 101-111.	6.6	17
131	Development of a Fragment-Based in Silico Profiler for Michael Addition Thiol Reactivity. Chemical Research in Toxicology, 2016, 29, 1073-1081.	1.7	17
132	Towards a qAOP framework for predictive toxicology - Linking data to decisions. Computational Toxicology, 2022, 21, 100195.	1.8	17
133	Embedded Cluster Modelling-A novel method for analysing embedded data sets. QSAR and Combinatorial Science, 1999, 18, 229-235.	1.4	16
134	Structureâ€“permeability Relationships for Transcorneal Penetration. ATLA Alternatives To Laboratory Animals, 2000, 28, 403-413.	0.7	16
135	A Novel Index for the Description of Molecular Linearity. Journal of Chemical Information and Computer Sciences, 2001, 41, 1228-1236.	2.8	16
136	The Use of Bootstrap Resampling to Assess the Variability of Draize Tissue Scores. ATLA Alternatives To Laboratory Animals, 2001, 29, 557-573.	0.7	15
137	Read-across of 90-day rat oral repeated-dose toxicity: A case study for selected 2-alkyl-1-alkanols. Computational Toxicology, 2017, 2, 28-38.	1.8	15
138	Probabilistic modelling of developmental neurotoxicity based on a simplified adverse outcome pathway network. Computational Toxicology, 2022, 21, 100206.	1.8	15
139	Investigation of Critical Body Residues and Modes of Toxic Action Based on Injection and Aquatic Exposure in Fish. Water, Air, and Soil Pollution, 2015, 226, 1.	1.1	14
140	Incorporating lines of evidence from New Approach Methodologies (NAMs) to reduce uncertainties in a category based read-across: A case study for repeated dose toxicity. Regulatory Toxicology and Pharmacology, 2021, 120, 104855.	1.3	14
141	The Use of Bootstrap Resampling to Assess the Uncertainty of Cooper Statistics. ATLA Alternatives To Laboratory Animals, 2001, 29, 447-459.	0.7	13
142	Integrated Decision-tree Testing Strategies for Environmental Toxicity with Respect to the Requirements of the EU REACH Legislation. ATLA Alternatives To Laboratory Animals, 2006, 34, 651-664.	0.7	13
143	Development of an In Silico Profiler for Respiratory Sensitisation. ATLA Alternatives To Laboratory Animals, 2014, 42, 367-375.	0.7	13
144	Methods for assigning confidence to toxicity data with multiple values â€” Identifying experimental outliers. Science of the Total Environment, 2014, 482-483, 358-365.	3.9	13

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145	Exploring the Potential of ToxCast Data in Supporting Read-Across for Evaluation of Food Chemical Safety. Chemical Research in Toxicology, 2021, 34, 300-312.	1.7	13
146	An Integrated Decision-tree Testing Strategy for Eye Irritation with Respect to the Requirements of the EU REACH Legislation. ATLA Alternatives To Laboratory Animals, 2008, 36, 81-92.	0.7	12
147	Integrated Decision-tree Testing Strategies for Developmental and Reproductive Toxicity with Respect to the Requirements of the EU REACH Legislation. ATLA Alternatives To Laboratory Animals, 2008, 36, 123-138.	0.7	12
148	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
149	Advances in the prediction of gastrointestinal absorption: Quantitative Structure-Activity Relationship (QSAR) modelling of PAMPA permeability. Computational Toxicology, 2019, 10, 51-59.	1.8	12
150	Integrated Decision-tree Testing Strategies for Skin Corrosion and Irritation with Respect to the Requirements of the EU REACH Legislation. ATLA Alternatives To Laboratory Animals, 2007, 35, 673-682.	0.7	11
151	A Comparative Study of Machine Learning Algorithms Applied to Predictive Toxicology Data Mining. ATLA Alternatives To Laboratory Animals, 2007, 35, 25-32.	0.7	11
152	Data Quality in the Human and Environmental Health Sciences: Using Statistical Confidence Scoring to Improve QSAR/QSPR Modeling. Journal of Chemical Information and Modeling, 2015, 55, 1739-1746.	2.5	11
153	In silico approaches in organ toxicity hazard assessment: Current status and future needs for predicting heart, kidney and lung toxicities. Computational Toxicology, 2021, 20, 100188.	1.8	11
154	Correlation between bond dissociation energies and spin distribution for the radicals of ethers: A DFT study. Computational and Theoretical Chemistry, 2010, 955, 165-170.	1.5	10
155	Application of a computational model for Michael addition reactivity in the prediction of toxicity to Tetrahymena pyriformis. Chemosphere, 2011, 85, 1066-1074.	4.2	10
156	In silico approaches in organ toxicity hazard assessment: Current status and future needs in predicting liver toxicity. Computational Toxicology, 2021, 20, 100187.	1.8	10
157	Toxicological Information for Use in Predictive Modeling. , 2005, , 93-133.		10
158	Formation of mechanistic categories and local models to facilitate the prediction of toxicity. ALTEX: Alternatives To Animal Experimentation, 2011, 28, 45-49.	0.9	10
159	Evaluating confidence in toxicity assessments based on experimental data and in silico predictions. Computational Toxicology, 2022, 21, 100204.	1.8	10
160	An Integrated Decision-tree Testing Strategy for Skin Sensitisation with Respect to the Requirements of the EU REACH Legislation. ATLA Alternatives To Laboratory Animals, 2008, 36, 75-89.	0.7	9
161	Integrated Decision-tree Testing Strategies for Mutagenicity and Carcinogenicity with Respect to the Requirements of the EU REACH Legislation. ATLA Alternatives To Laboratory Animals, 2008, 36, 43-63.	0.7	9
162	Development of an Enhanced Mechanistically Driven Mode of Action Classification Scheme for Adverse Effects on Environmental Species. Environmental Science & Technology, 2021, 55, 1897-1907.	4.6	9

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163	Determination of â€œfitness-for-purposeâ€•of quantitative structure-activity relationship (QSAR) models to predict (eco-)toxicological endpoints for regulatory use. Regulatory Toxicology and Pharmacology, 2021, 123, 104956.	1.3	9
164	Prediction of the Neurotoxic Potential of Chemicals Based on Modelling of Molecular Initiating Events Upstream of the Adverse Outcome Pathways of (Developmental) Neurotoxicity. International Journal of Molecular Sciences, 2022, 23, 3053.	1.8	9
165	Correspondence Analysis of the Skin Sensitization Potential of Organic Chemicals. QSAR and Combinatorial Science, 1997, 16, 33-37.	1.4	8
166	An Integrated Decision-tree Testing Strategy for Eye Irritation with Respect to the Requirements of the EU REACH Legislation. ATLA Alternatives To Laboratory Animals, 2008, 36, 111-122.	0.7	8
167	Compilation of Data and Modelling of Nanoparticle Interactions and Toxicity in the NanoPUZZLES Project. Advances in Experimental Medicine and Biology, 2017, 947, 303-324.	0.8	8
168	Read-across of 90-day rodent repeated-dose toxicity: A case study for selected simple aryl alcohol alkyl carboxylic acid esters. Computational Toxicology, 2018, 7, 1-8.	1.8	8
169	Using kNN Model for Automatic Feature Selection. Lecture Notes in Computer Science, 2005, , 410-419.	1.0	8
170	Quantitative Structure-Activity Relationships for Acute Aquatic Toxicity. , 2003, , .		7
171	Validation of a Fragment-Based Profiler for Thiol Reactivity for the Prediction of Toxicity: Skin Sensitization and Tetrahymena pyriformis. Chemical Research in Toxicology, 2017, 30, 604-613.	1.7	6
172	A critical review of adverse effects to the kidney: mechanisms, data sources, andin silicotools to assist prediction. Expert Opinion on Drug Metabolism and Toxicology, 2018, 14, 1225-1253.	1.5	6
173	Interpretation of QSAR Models: Mining Structural Patterns Taking into Account Molecular Context. Molecular Informatics, 2019, 38, 1800084.	1.4	6
174	Computational Methods to Predict Toxicity. , 2019, , 287-300.		6
175	A Robust, Mechanistically Based In Silico Structural Profiler for Hepatic Cholestasis. Chemical Research in Toxicology, 2021, 34, 641-655.	1.7	6
176	Integrated Testing Strategies for Use with Respect to the Requirements of the EU REACH Legislation. ATLA Alternatives To Laboratory Animals, 2008, 36, 7-27.	0.7	5
177	An Integrated Decision-tree Testing Strategy for Repeat Dose Toxicity with Respect to the Requirements of the EU REACH Legislation. ATLA Alternatives To Laboratory Animals, 2008, 36, 139-147.	0.7	5
178	In Silico Identification of Chemicals Capable of Binding to the Ecdysone Receptor. Environmental Toxicology and Chemistry, 2020, 39, 1438-1450.	2.2	5
179	Threshold of Toxicological Concernâ€”An Update for Non-Genotoxic Carcinogens. Frontiers in Toxicology, 2021, 3, 688321.	1.6	5
180	Prediction of Harmful Human Health Effects of Chemicals from Structure. Challenges and Advances in Computational Chemistry and Physics, 2010, , 305-325.	0.6	5

#	Article	IF	Citations
181	Computer-aided prediction of drug toxicity and metabolism. , 2003, , 259-278.		5
182	Principles and procedures for assessment of acute toxicity incorporating in silico methods. Computational Toxicology, 2022, 24, 100237.	1.8	5
183	Integrated Decision-tree Testing Strategies for Acute Systemic Toxicity and Toxicokinetics with Respect to the Requirements of the EU REACH Legislation. ATLA Alternatives To Laboratory Animals, 2008, 36, 91-109.	0.7	4
184	Robustness of an Immobilized Artificial Membrane High-Performance Liquid Chromatography Method for the Determination of Lipophilicity. Journal of Chemical & Engineering Data, 2012, 57, 3696-3700.	1.0	4
185	Finding synergies for the 3Rs â€“ Repeated Dose Toxicity testing: Report from an EPAA Partners' Forum. Regulatory Toxicology and Pharmacology, 2019, 108, 104470.	1.3	4
186	Computational Approaches for Drug-Induced Liver Injury (DILI) Prediction: State of the Art and Challenges. , 2021, , 308-329.		4
187	A Study on Feature Selection for Toxicity Prediction. Lecture Notes in Computer Science, 2005, , 31-34.	1.0	4
188	A matter of trust: Learning lessons about causality will make qAOPs credible. Computational Toxicology, 2022, 21, 100205.	1.8	4
189	The use of Bayesian methodology in the development and validation of a tiered assessment approach towards prediction of rat acute oral toxicity. Archives of Toxicology, 2022, 96, 817-830.	1.9	4
190	A strategy to define applicability domains for read-across. Computational Toxicology, 2022, 22, 100220.	1.8	4
191	Comparison of electrotopological-state indices versus atomic charge and superdelocalisability indices in a QSAR study of the receptor binding properties of halogenated estradiol derivatives. Molecular Diversity, 2004, 8, 343-355.	2.1	3
192	Chemoinformatic Consideration of Novel Psychoactive Substances: Compilation and Preliminary Analysis of a Categorised Dataset. Molecular Informatics, 2019, 38, e1800142.	1.4	3
193	A mechanistic model to study the kinetics and toxicity of salicylic acid in the kidney of four virtual individuals. Computational Toxicology, 2021, 19, 100172.	1.8	3
194	The Prediction of Skin Permeability Using Quantitative Structureâ€“Activity Relationship Methods. , 2005, , 113-134.		3
195	A Framework for Promoting the Acceptance and Regulatory Use of (Quantitative) Structure- Activity Relationships. , 2004, , .		3
196	Integrated Decision-tree Testing Strategies for Environmental Toxicity with Respect to the Requirements of the EU REACH Legislation. ATLA Alternatives To Laboratory Animals, 2008, 36, 29-42.	0.7	2
197	Development of Integrated Testing Strategies for REACH: Motivation, Background and Introduction. ATLA Alternatives To Laboratory Animals, 2008, 36, i-iii.	0.7	2
198	Toward better understanding of liver steatosis MoA: Molecular modelling study of PPAR gamma receptor. Toxicology Letters, 2013, 221, S85.	0.4	2

#	Article	IF	Citations
199	Threshold of toxicological concern (TTC) task force: a strategy to support application of TTC to dermally applied cosmetic ingredients. Toxicology Letters, 2013, 221, S35.	0.4	2
200	Re: A call for action on the development and implementation of new methodologies for safety assessment of chemical-based products in the EU â€“ A short communication. Regulatory Toxicology and Pharmacology, 2021, 122, 104911.	1.3	2
201	A computational investigation of the reactivity of electrophilic toxicants. Toxicology Letters, 2009, 189, S259.	0.4	1
202	International QSAR Award Winner 2012: Prof Terry Wayne Schultz. SAR and QSAR in Environmental Research, 2013, 24, 255-257.	1.0	1
203	Supporting data-mining, read-across and chemical space analysis for toxicity data gap filling using the COSMOS database. Toxicology Letters, 2017, 280, S285.	0.4	1
204	Development of Baseline Quantitative Structure-Activity Relationships (QSARs) for the Effects of Active Pharmaceutical Ingredients (APIs) to Aquatic Species. Methods in Pharmacology and Toxicology, 2020, , 331-356.	0.1	1
205	QSARs of fathead minnow and Microtox toxicity data using canonical correlation analysis. , 1993, , 541-542.		1
206	Predicting Chemical Toxicity and Fate in Humans and the Environment â€šÃ„Ã® An Introduction. , 2004, , .		1
207	The Use by Governmental Regulatory Agencies of Quantitative Structure- Activity Relationships and Expert Systems to Predict Toxicity. , 2004, , .		1
208	The Endocrine Disrupting Activity of Pesticides. Outlooks on Pest Management, 2004, 15, 211-214.	0.1	0
209	Quantifying intrinsic chemical reactivity of molecular structural features for protein binding and reactive toxicity, using the MOSES chemoinformatics system. Journal of Cheminformatics, 2012, 4, .	2.8	0
210	Data mining toxicity effects through an ontology approach to investigate toxicity mode of action. Toxicology Letters, 2013, 221, S80.	0.4	0
211	Development of integrated in silico models for toxicity prediction focussing on cosmetic ingredients. Toxicology Letters, 2013, 221, S81.	0.4	0
212	Feature Selection Modelling for Percutaneous Absorption across Synthetic Membranes. , 2014, , .		0
213	Description of the MoA/AOP linked with PPARgamma receptor dysregulation leading to liver fibrosis. Toxicology Letters, 2014, 229, S49.	0.4	0
214	Validation of (Q)SARs Models: Jaworska et al.'s Response. Environmental Health Perspectives, 2004, 112, a86-a87.	2.8	0