Mark T D Cronin

List of Publications by Citations

207 papers	18,102 citations	46 h-index	133 g-index
238 ext. papers	20,247 ext. citations	4.8 avg, IF	6.57 L-index

#	Paper	IF	Citations
207	Free radicals and antioxidants in normal physiological functions and human disease. *International Journal of Biochemistry and Cell Biology*, **2007**, 39, 44-84	5.6	8827
206	QSAR modeling: where have you been? Where are you going to?. *Journal of Medicinal Chemistry*, **2014**, 57, 4977-5010	8.3	996
205	Methods for reliability and uncertainty assessment and for applicability evaluations of classification- and regression-based QSARs. *Environmental Health Perspectives*, **2003**, 111, 1361-75	8.4	957
204	Alternative (non-animal) methods for cosmetics testing: current status and future prospects-2010. *Archives of Toxicology*, **2011**, 85, 367-485	5.8	398
203	Pitfalls in QSAR. *Computational and Theoretical Chemistry*, **2003**, 622, 39-51		260
202	Use of QSARs in international decision-making frameworks to predict health effects of chemical substances. *Environmental Health Perspectives*, **2003**, 111, 1391-401	8.4	205
201	Use of QSARs in international decision-making frameworks to predict ecologic effects and environmental fate of chemical substances. *Environmental Health Perspectives*, **2003**, 111, 1376-90	8.4	169
200	Quantitative structure□ctivity relationships (QSARs) in toxicology: a historical perspective. *Computational and Theoretical Chemistry*, **2003**, 622, 1-22		169
199	Measurement and estimation of electrophilic reactivity for predictive toxicology. *Chemical Reviews*, **2011**, 111, 2562-96	68.1	152
198	Quantitative structure-activity relationships (QSARs) for the prediction of skin permeation of exogenous chemicals. *Chemosphere*, **2002**, 48, 603-13	8.4	146
197	Comparative assessment of methods to develop QSARs for the prediction of the toxicity of phenols to Tetrahymena pyriformis. *Chemosphere*, **2002**, 49, 1201-21	8.4	132
196	A European perspective on alternatives to animal testing for environmental hazard identification and risk assessment. *Regulatory Toxicology and Pharmacology*, **2013**, 67, 506-30	3.4	121
195	QSAR in Toxicology. 1. Prediction of Aquatic Toxicity. *QSAR and Combinatorial Science*, **1995**, 14, 1-7		112
194	Structure-toxicity relationships for phenols to Tetrahymena pyriformis. *Chemosphere*, **1996**, 32, 1453-68	8.4	110
193	The Role of Omics in the Application of Adverse Outcome Pathways for Chemical Risk Assessment. *Toxicological Sciences*, **2017**, 158, 252-262	4.4	107
192	In silico toxicology protocols. *Regulatory Toxicology and Pharmacology*, **2018**, 96, 1-17	3.4	104
191	Prediction of michael-type acceptor reactivity toward glutathione. *Chemical Research in Toxicology*, **2010**, 23, 1576-85	4	102

190	Development of quantitative structure-activity relationships for the toxicity of aromatic compounds to Tetrahymena pyriformis: comparative assessment of the methodologies. *Chemical Research in Toxicology*, **2001**, 14, 1284-95	4	98
189	Toward Good Read-Across Practice (GRAP) guidance. *ALTEX: Alternatives To Animal Experimentation* , **2016**, 33, 149-66	4.3	98
188	The Development and Validation of Expert Systems for Predicting Toxicity: The Report and Recommendations of an ECVAM/ECB Workshop (ECVAM Workshop 24)1,2. *ATLA Alternatives To Laboratory Animals*, **1997**, 25, 223-251	2.1	86
187	Structure-toxicity relationships for the effects to Tetrahymena pyriformis of aliphatic, carbonyl-containing, alpha,beta-unsaturated chemicals. *Chemical Research in Toxicology*, **2005**, 18, 330-41	4	82
186	Statement on advancing the assessment of chemical mixtures and their risks for human health and the environment. *Environment International*, **2020**, 134, 105267	12.9	81
185	Quantitative structure-permeability relationships for percutaneous absorption: re-analysis of steroid data. *International Journal of Pharmaceutics*, **2002**, 238, 105-9	6.5	80
184	Quantifying intrinsic chemical reactivity of molecular structural features for protein binding and reactive toxicity, using the MOSES chemoinformatics system. *Journal of Cheminformatics*, **2012**, 4,	8.6	78
183	Consensus QSAR models: do the benefits outweigh the complexity?. *Journal of Chemical Information and Modeling*, **2007**, 47, 1460-8	6.1	77
182	Read-across approaches--misconceptions, promises and challenges ahead. *ALTEX: Alternatives To Animal Experimentation*, **2014**, 31, 387-96	4.3	75
181	Structure-based classification of antibacterial activity. *Journal of Chemical Information and Computer Sciences*, **2002**, 42, 869-78		74
180	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		70
179	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	10.2	68
178	Adverse Outcome Pathways can drive non-animal approaches for safety assessment. *Journal of Applied Toxicology*, **2015**, 35, 971-5	4.1	66
177	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, 1232-40	8.4	66
176	In silico models for drug-induced liver injury--current status. *Expert Opinion on Drug Metabolism and Toxicology*, **2012**, 8, 201-17	5.5	65
175	Formation of categories from structure-activity relationships to allow read-across for risk assessment: toxicity of alpha,beta-unsaturated carbonyl compounds. *Chemical Research in Toxicology*, **2008**, 21, 2300-12	4	65
174	Thresholds of Toxicological Concern for cosmetics-related substances: New database, thresholds, and enrichment of chemical space. *Food and Chemical Toxicology*, **2017**, 109, 170-193	4.7	64
173	The present status of QSAR in toxicology. *Computational and Theoretical Chemistry*, **2003**, 622, 23-38		64

172	Electrophilic reaction chemistry of low molecular weight respiratory sensitizers. *Chemical Research in Toxicology*, **2009**, 22, 1447-53	4	63
171	Structure-toxicity relationships for aliphatic chemicals evaluated with Tetrahymena pyriformis. *Chemical Research in Toxicology*, **2002**, 15, 1602-9	4	63
170	Assessment and modeling of the toxicity of organic chemicals to Chlorella vulgaris: development of a novel database. *Chemical Research in Toxicology*, **2004**, 17, 545-54	4	61
169	Structure-activity relationships for gene activation oestrogenicity: evaluation of a diverse set of aromatic chemicals. *Environmental Toxicology*, **2002**, 17, 14-23	4.2	55
168	The identification of nuclear receptors associated with hepatic steatosis to develop and extend adverse outcome pathways. *Critical Reviews in Toxicology*, **2016**, 46, 138-52	5.7	53
167	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		52
166	Novel approach for efficient predictions properties of large pool of nanomaterials based on limited set of species: nano-read-across. *Nanotechnology*, **2015**, 26, 015701	3.4	50
165	QSAR Study of the Toxicity of Nitrobenzenes to Tetrahymena pyriformis. *QSAR and Combinatorial Science*, **1995**, 14, 427-432		50
164	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, 203-12	4	46
163	Essential and desirable characteristics of ecotoxicity quantitative structure□activity relationships. *Environmental Toxicology and Chemistry*, **2003**, 22, 599-607	3.8	46
162	Lessons learned from read-across case studies for repeated-dose toxicity. *Regulatory Toxicology and Pharmacology*, **2017**, 88, 185-191	3.4	45
161	Quantitative structure-skin permeability relationships. *Toxicology*, **2017**, 387, 27-42	4.4	45
160	Structure-toxicity relationships for three mechanisms of action of toxicity to Vibrio fischeri. *Ecotoxicology and Environmental Safety*, **1998**, 39, 65-9	7	42
159	Alternative Methods for Skin Sensitisation Testing: The Report and Recommendations of ECVAM Workshop 191, 2. *ATLA Alternatives To Laboratory Animals*, **1996**, 24, 683-705	2.1	42
158	Genetic toxicology in silico protocol. *Regulatory Toxicology and Pharmacology*, **2019**, 107, 104403	3.4	41
157	Quantitative structure-activity-activity and quantitative structure-activity investigations of human and rodent toxicity. *Chemosphere*, **2006**, 65, 1878-87	8.4	41
156	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, 174-86	3.4	40
155	QSAR in Toxicology. 3. Prediction of Chronic Toxicities. *QSAR and Combinatorial Science*, **1995**, 14, 329-334		40

154	Quantitative adverse outcome pathway (qAOP) models for toxicity prediction. *Archives of Toxicology*, **2020**, 94, 1497-1510	5.8	38
153	Toxicology Data Resources to Support Read-Across and (Q)SAR. *Frontiers in Pharmacology*, **2019**, 10, 561	5.6	38
152	Legacy data sharing to improve drug safety assessment: the eTOX project. *Nature Reviews Drug Discovery*, **2017**, 16, 811-812	64.1	37
151	(Q)SARs for Predicting Effects Relating to Reproductive Toxicity. *QSAR and Combinatorial Science*, **2008**, 27, 91-100		37
150	A Review of Tools as Alternatives to Animal Testing: Principles, Resources and Applications. *ATLA Alternatives To Laboratory Animals*, **2020**, 48, 146-172	2.1	37
149	Development of an in Silico Profiler for Mitochondrial Toxicity. *Chemical Research in Toxicology*, **2015**, 28, 1891-902	4	36
148	Molecular quantum similarity analysis of estrogenic activity. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1166-76		36
147	QSAR in Toxicology. 2. Prediction of Acute Mammalian Toxicity and Interspecies Correlations. *QSAR and Combinatorial Science*, **1995**, 14, 117-120		36
146	QSAR analysis of the toxicity of aromatic compounds to Chlorella vulgaris in a novel short-term assay. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 258-65		35
145	Molecular modelling study of the PPAR□receptor in relation to the mode of action/adverse outcome pathway framework for liver steatosis. *International Journal of Molecular Sciences*, **2014**, 15, 7651-66	6.3	34
144	Integrated testing strategies for use in the EU REACH system. *ATLA Alternatives To Laboratory Animals*, **2006**, 34, 407-27	2.1	34
143	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	10.3	34
142	Assessing uncertainty in read-across: Questions to evaluate toxicity predictions based on knowledge gained from case studies. *Computational Toxicology*, **2019**, 9, 1-11	3.1	34
141	Quantitative Structure-Activity Relationships of Chemicals Acting by Non-polar Narcosis□heoretical Considerations. *QSAR and Combinatorial Science*, **1998**, 17, 131-138		34
140	Development and analysis of an adverse outcome pathway network for human neurotoxicity. *Archives of Toxicology*, **2019**, 93, 2759-2772	5.8	33
139	Proposed integrated decision-tree testing strategies for mutagenicity and carcinogenicity in relation to the EU REACH legislation. *ATLA Alternatives To Laboratory Animals*, **2007**, 35, 267-87	2.1	32
138	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	3.8	32
137	(Q)SARs to predict environmental toxicities: current status and future needs. *Environmental Sciences: Processes and Impacts*, **2017**, 19, 213-220	4.3	31

136	Investigation of the Verhaar scheme for predicting acute aquatic toxicity: improving predictions obtained from Toxtree ver. 2.6. *Chemosphere*, **2015**, 139, 146-54	8.4	31
135	Quantitative structure-activity relationships for weak acid respiratory uncouplers to Vibrio fisheri. *Environmental Toxicology and Chemistry*, **1997**, 16, 357-360	3.8	31
134	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		31
133	The SEURAT-1 approach towards animal free human safety assessment. *ALTEX: Alternatives To Animal Experimentation*, **2015**, 32, 9-24	4.3	31
132	A review of the use of in silico methods to predict the chemistry of molecular initiating events related to drug toxicity. *Expert Opinion on Drug Metabolism and Toxicology*, **2011**, 7, 1481-95	5.5	30
131	Structure-based methods for the prediction of drug metabolism. *Expert Opinion on Drug Metabolism and Toxicology*, **2006**, 2, 545-57	5.5	30
130	Comparative quantitative structure-activity-activity relationships for toxicity to Tetrahymena pyriformis and Pimephales promelas. *ATLA Alternatives To Laboratory Animals*, **2007**, 35, 15-24	2.1	29
129	In silico resources to assist in the development and evaluation of physiologically-based kinetic models. *Computational Toxicology*, **2019**, 11, 33-49	3.1	28
128	How does the quality of phospholipidosis data influence the predictivity of structural alerts?. *Journal of Chemical Information and Modeling*, **2014**, 54, 2224-32	6.1	28
127	The use of pH measurements to predict the potential of chemicals to cause acute dermal and ocular toxicity. *Toxicology*, **2001**, 169, 119-31	4.4	28
126	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, 131-45	2.1	27
125	Internationalization of read-across as a validated new approach method (NAM) for regulatory toxicology. *ALTEX: Alternatives To Animal Experimentation*, **2020**, 37, 579-606	4.3	27
124	. *Environmental Toxicology and Chemistry*, **1997**, 16, 357	3.8	26
123	Chelators in Iron and Copper Toxicity. *Current Pharmacology Reports*, **2016**, 2, 271-280	5.5	26
122	Systems Biology Approach Reveals a Calcium-Dependent Mechanism for Basal Toxicity in Daphnia magna. *Environmental Science & Technology*, **2015**, 49, 11132-40	10.3	25
121	Assessment and Reproducibility of Quantitative Structure-Activity Relationship Models by the Nonexpert. *Journal of Chemical Information and Modeling*, **2018**, 58, 673-682	6.1	25
120	Strategies for the optimisation of in vivo experiments in accordance with the 3Rs philosophy. *Regulatory Toxicology and Pharmacology*, **2012**, 63, 140-54	3.4	24
119	Using In Silico Tools in a Weight of Evidence Approach to Aid Toxicological Assessment. *Molecular Informatics*, **2010**, 29, 97-110	3.8	24

118	The in chemico-in silico interface: challenges for integrating experimental and computational chemistry to identify toxicity. *ATLA Alternatives To Laboratory Animals*, **2009**, 37, 513-21	2.1	24
117	Optimizing drug discovery by Investigative Toxicology: Current and future trends. *ALTEX: Alternatives To Animal Experimentation*, **2019**, 36, 289-313	4.3	24
116	GRADE Guidelines 30: the GRADE approach to assessing the certainty of modeled evidence-An overview in the context of health decision-making. *Journal of Clinical Epidemiology*, **2021**, 129, 138-150	5.7	24
115	Navigating through the minefield of read-across frameworks: A commentary perspective. *Computational Toxicology*, **2018**, 6, 39-54	3.1	23
114	An ISA-TAB-Nano based data collection framework to support data-driven modelling of nanotoxicology. *Beilstein Journal of Nanotechnology*, **2015**, 6, 1978-99	3	23
113	Quantitative structure-activity relationships for the toxicity of organophosphorus and carbamate pesticides to the Rainbow trout Onchorhyncus mykiss. *Pest Management Science*, **2006**, 62, 819-31	4.6	23
112	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	2.1	23
111	Read-across of 90-day rat oral repeated-dose toxicity: A case study for selected olefinic alcohols. *Computational Toxicology*, **2017**, 1, 22-32	3.1	22
110	Towards a Fuzzy Expert System on Toxicological Data Quality Assessment. *Molecular Informatics*, **2013**, 32, 65-78	3.8	22
109	Relationship Between Adverse Outcome Pathways and Chemistry-BasedIn SilicoModels to Predict Toxicity. *Applied in Vitro Toxicology*, **2017**, 3, 286-297	1.3	22
108	The current status and future applicability of quantitative structure-activity relationships (QSARs) in predicting toxicity. *ATLA Alternatives To Laboratory Animals*, **2002**, 30 Suppl 2, 81-4	2.1	22
107	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	4.7	21
106	Pragmatic approaches to using computational methods to predict xenobiotic metabolism. *Journal of Chemical Information and Modeling*, **2013**, 53, 1282-93	6.1	21
105	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	2.1	21
104	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	3.4	20
103	Modelling acute oral mammalian toxicity. 1. Definition of a quantifiable baseline effect. *Toxicology in Vitro*, **2011**, 25, 1281-93	3.6	20
102	Prediction of Organ Level Toxicity: Linking Chemistry to Adverse Effects. *Toxicological Research*, **2017**, 33, 173-182	3.7	20
101	The application of molecular modelling in the safety assessment of chemicals: A case study on ligand-dependent PPAR dysregulation. *Toxicology*, **2017**, 392, 140-154	4.4	18

100	Read-across for rat oral gavage repeated-dose toxicity for short-chain mono-alkylphenols: A case study. *Computational Toxicology*, **2017**, 2, 1-11	3.1	18
99	Read-across of 90-day rat oral repeated-dose toxicity: A case study for selected n -alkanols. *Computational Toxicology*, **2017**, 2, 12-19	3.1	18
98	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	3.4	18
97	In Silico Studies of the Relationship Between Chemical Structure and Drug Induced Phospholipidosis. *Molecular Informatics*, **2011**, 30, 415-29	3.8	18
96	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, 683-97	2.1	18
95	Estrogenicity and acute toxicity of selected anilines using a recombinant yeast assay. *Chemosphere*, **2003**, 52, 1173-81	8.4	18
94	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	10.2	18
93	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	2.1	18
92	Unlocking the potential of chemical safety assessment - A report on a cross-sector symposium on current opportunities and future challenges. *Computational Toxicology*, **2019**, 10, 38-43	3.1	16
91	Skin sensitization in silico protocol. *Regulatory Toxicology and Pharmacology*, **2020**, 116, 104688	3.4	16
90	Quantitative Structure□Activity Relationships (QSARs) □Applications and Methodology. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 3-11	0.7	16
89	Physico-chemical interpretation and prediction of the dimyristoyl phosphatidyl choline□water partition coefficient. *Computational and Theoretical Chemistry*, **2002**, 593, 9-18		16
88	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	3.1	15
87	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	3.4	15
86	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	2.1	15
85	Structure-permeability Relationships for Transcorneal Penetration. *ATLA Alternatives To Laboratory Animals*, **2000**, 28, 403-13	2.1	14
84	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	6.5	14
83	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	3.6	13

82	Ensuring confidence in predictions: A scheme to assess the scientific validity of in silico models. *Advanced Drug Delivery Reviews*, **2015**, 86, 101-11	18.5	13
81	Methods for assigning confidence to toxicity data with multiple values--Identifying experimental outliers. *Science of the Total Environment*, **2014**, 482-483, 358-65	10.2	13
80	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, 651-64	2.1	13
79	Embedded Cluster Modelling□A novel method for analysing embedded data sets. *QSAR and Combinatorial Science*, **1999**, 18, 229-235		13
78	The use of bootstrap resampling to assess the uncertainty of cooper statistics. *ATLA Alternatives To Laboratory Animals*, **2001**, 29, 447-59	2.1	12
77	Development of a Fragment-Based in Silico Profiler for Michael Addition Thiol Reactivity. *Chemical Research in Toxicology*, **2016**, 29, 1073-81	4	12
76	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	2.6	11
75	A novel index for the description of molecular linearity. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 1228-36		11
74	The use of bootstrap resampling to assess the variability of Draize tissue scores. *ATLA Alternatives To Laboratory Animals*, **2001**, 29, 557-73	2.1	11
73	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, 1739-46	6.1	10
72	Potential of ToxCast Data in the Safety Assessment of Food Chemicals. *Toxicological Sciences*, **2020**, 174, 326-340	4.4	10
71	Application of a computational model for Michael addition reactivity in the prediction of toxicity to Tetrahymena pyriformis. *Chemosphere*, **2011**, 85, 1066-74	8.4	10
70	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	2.1	10
69	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 Suppl 1, 123-38	2.1	10
68	A mechanistic framework for integrating chemical structure and high-throughput screening results to improve toxicity predictions. *Computational Toxicology*, **2018**, 8, 1-12	3.1	9
67	Correlation between bond dissociation energies and spin distribution for the radicals of ethers: A DFT study. *Computational and Theoretical Chemistry*, **2010**, 955, 165-170		9
66	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, 673-82	2.1	9
65	Toxicological Information for Use in Predictive Modeling **2005**, 93-133		9

64	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	3.1	8
63	Development of an in silico profiler for respiratory sensitisation. *ATLA Alternatives To Laboratory Animals*, **2014**, 42, 367-75	2.1	8
62	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	3.4	8
61	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 Suppl 1, 75-89	2.1	7
60	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 Suppl 1, 43-63	2.1	7
59	Formation of mechanistic categories and local models to facilitate the prediction of toxicity. *ALTEX: Alternatives To Animal Experimentation*, **2011**, 28, 45-9	4.3	7
58	Advances in the prediction of gastrointestinal absorption: Quantitative Structure-Activity Relationship (QSAR) modelling of PAMPA permeability. *Computational Toxicology*, **2019**, 10, 51-59	3.1	7
57	Correspondence Analysis of the Skin Sensitization Potential of Organic Chemicals. *QSAR and Combinatorial Science*, **1997**, 16, 33-37		6
56	A comparative study of machine learning algorithms applied to predictive toxicology data mining. *ATLA Alternatives To Laboratory Animals*, **2007**, 35, 25-32	2.1	6
55	Derivation, characterisation and analysis of an adverse outcome pathway network for human hepatotoxicity. *Toxicology*, **2021**, 459, 152856	4.4	6
54	In Silico Identification of Chemicals Capable of Binding to the Ecdysone Receptor. *Environmental Toxicology and Chemistry*, **2020**, 39, 1438-1450	3.8	5
53	Integrated testing strategies for use with respect to the requirements of the EU REACH legislation. *ATLA Alternatives To Laboratory Animals*, **2008**, 36 Suppl 1, 7-27	2.1	5
52	Development of an Enhanced Mechanistically Driven Mode of Action Classification Scheme for Adverse Effects on Environmental Species. *Environmental Science & Technology*, **2021**, 55, 1897-1907	10.3	5
51	A critical review of adverse effects to the kidney: mechanisms, data sources, and in silico tools to assist prediction. *Expert Opinion on Drug Metabolism and Toxicology*, **2018**, 14, 1225-1253	5.5	5
50	Prediction of Harmful Human Health Effects of Chemicals from Structure. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 305-325	0.7	5
49	Compilation of Data and Modelling of Nanoparticle Interactions and Toxicity in the NanoPUZZLES Project. *Advances in Experimental Medicine and Biology*, **2017**, 947, 303-324	3.6	4
48	Finding synergies for the 3Rs - Repeated Dose Toxicity testing: Report from an EPAA PartnersT Forum. *Regulatory Toxicology and Pharmacology*, **2019**, 108, 104470	3.4	4
47	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	2.8	4

46	Quantitative Structure-Activity Relationships for Acute Aquatic Toxicity **2003**,		4
45	Evaluating Confidence in Toxicity Assessments Based on Experimental Data and Predictions.. *Computational Toxicology*, **2022**, 21,	3.1	4
44	Exploring the Potential of ToxCast Data in Supporting Read-Across for Evaluation of Food Chemical Safety. *Chemical Research in Toxicology*, **2021**, 34, 300-312	4	4
43	Computational Methods to Predict Toxicity **2019**, 287-300		4
42	New framework for a non-animal approach adequately assures the safety of cosmetic ingredients - A case study on caffeine. *Regulatory Toxicology and Pharmacology*, **2021**, 123, 104931	3.4	4
41	Using kNN Model for Automatic Feature Selection. *Lecture Notes in Computer Science*, **2005**, 410-419	0.9	4
40	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	4	3
39	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 Suppl 1, 91-109	2.1	3
38	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 Suppl 1, 111-22	2.1	3
37	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	5.8	3
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