Mark T D Cronin

List of Publications by Year
in descending order

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Version: 2024-02-01

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	Towards a qAOP framework for predictive toxicology - Linking data to decisions. Computational Toxicology, 2022, 21, 100195.	1.8	17
2	Evaluating confidence in toxicity assessments based on experimental data and in silico predictions. Computational Toxicology, 2022, 21, 100204.	1.8	10
3	A matter of trust: Learning lessons about causality will make qAOPs credible. Computational Toxicology, 2022, 21, 100205.	1.8	4
4	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
5	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
6	A framework for chemical safety assessment incorporating new approach methodologies within REACH. Archives of Toxicology, 2022, 96, 743-766.	1.9	39
7	A review of in silico toxicology approaches to support the safety assessment of cosmetics-related materials. Computational Toxicology, 2022, 21, 100213.	1.8	20
8	Probabilistic modelling of developmental neurotoxicity based on a simplified adverse outcome pathway network. Computational Toxicology, 2022, 21, 100206.	1.8	15
9	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
10	A strategy to define applicability domains for read-across. Computational Toxicology, 2022, 22, 100220.	1.8	4
11	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
12	Principles and procedures for assessment of acute toxicity incorporating in silico methods. Computational Toxicology, 2022, 24, 100237.	1.8	5
13	A Robust, Mechanistically Based In Silico Structural Profiler for Hepatic Cholestasis. Chemical Research in Toxicology, 2021, 34, 641-655.	1.7	6
14	Computational Approaches for Drug-Induced Liver Injury (DILI) Prediction: State of the Art and Challenges. , 2021, , 308-329.		4
15	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
16	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
17	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
18	Threshold of Toxicological Concernâ€"An Update for Non-Genotoxic Carcinogens. Frontiers in Toxicology, 2021, 3, 688321.	1.6	5

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19	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
20	Derivation, characterisation and analysis of an adverse outcome pathway network for human hepatotoxicity. Toxicology, 2021, 459, 152856.	2.0	25
21	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
22	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
23	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
24	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
25	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
26	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
27	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
28	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
29	In Silico Identification of Chemicals Capable of Binding to the Ecdysone Receptor. Environmental Toxicology and Chemistry, 2020, 39, 1438-1450.	2.2	5
30	Quantitative adverse outcome pathway (qAOP) models for toxicity prediction. Archives of Toxicology, 2020, 94, 1497-1510.	1.9	65
31	Skin sensitization in silico protocol. Regulatory Toxicology and Pharmacology, 2020, 116, 104688.	1.3	27
32	Potential of ToxCast Data in the Safety Assessment of Food Chemicals. Toxicological Sciences, 2020, 174, 326-340.	1.4	18
33	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
34	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
35	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
36	In Silico Toxicology Data Resources to Support Read-Across and (Q)SAR. Frontiers in Pharmacology, 2019, 10, 561.	1.6	56

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37	Development and analysis of an adverse outcome pathway network for human neurotoxicity. Archives of Toxicology, 2019, 93, 2759-2772.	1.9	61
38	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
39	Chemoinformatic Consideration of Novel Psychoactive Substances: Compilation and Preliminary Analysis of a Categorised Dataset. Molecular Informatics, 2019, 38, e1800142.	1.4	3
40	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
41	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
42	Genetic toxicology in silico protocol. Regulatory Toxicology and Pharmacology, 2019, 107, 104403.	1.3	57
43	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
44	In silico resources to assist in the development and evaluation of physiologically-based kinetic models. Computational Toxicology, 2019, 11, 33-49.	1.8	45
45	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
46	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
47	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
48	Interpretation of QSAR Models: Mining Structural Patterns Taking into Account Molecular Context. Molecular Informatics, 2019, 38, 1800084.	1.4	6
49	Computational Methods to Predict Toxicity. , 2019, , 287-300.		6
50	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
51	Optimizing drug discovery by Investigative Toxicology: Current and future trends. ALTEX: Alternatives To Animal Experimentation, 2019, 36, 289-313.	0.9	38
52	Navigating through the minefield of read-across frameworks: A commentary perspective. Computational Toxicology, 2018, 6, 39-54.	1.8	44
53	In silico toxicology protocols. Regulatory Toxicology and Pharmacology, 2018, 96, 1-17.	1.3	159
54	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

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55	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
56	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
57	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
58	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
59	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
60	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
61	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
62	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
63	(Q)SARs to predict environmental toxicities: current status and future needs. Environmental Sciences: Processes and Impacts, 2017, 19, 213-220.	1.7	41
64	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
65	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
66	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
67	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
68	Legacy data sharing to improve drug safety assessment: the eTOX project. Nature Reviews Drug Discovery, 2017, 16, 811-812.	21.5	56
69	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
70	Relationship Between Adverse Outcome Pathways and Chemistry-BasedIn SilicoModels to Predict Toxicity. Applied in Vitro Toxicology, 2017, 3, 286-297.	0.6	26
71	The Role of Omics in the Application of Adverse Outcome Pathways for Chemical Risk Assessment. Toxicological Sciences, 2017, 158, 252-262.	1.4	161
72	Lessons learned from read-across case studies for repeated-dose toxicity. Regulatory Toxicology and Pharmacology, 2017, 88, 185-191.	1.3	58

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73	Quantitative structure-skin permeability relationships. Toxicology, 2017, 387, 27-42.	2.0	69
74	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
75	In SilicoPrediction of Organ Level Toxicity: Linking Chemistry to Adverse Effects. Toxicological Research, 2017, 33, 173-182.	1.1	26
76	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
77	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
78	Development of a Fragment-Based in Silico Profiler for Michael Addition Thiol Reactivity. Chemical Research in Toxicology, 2016, 29, 1073-1081.	1.7	17
79	Chelators in Iron and Copper Toxicity. Current Pharmacology Reports, 2016, 2, 271-280.	1.5	34
80	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
81	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
82	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
83	Toward Good Read-Across Practice (GRAP) guidance. ALTEX: Alternatives To Animal Experimentation, 2016, 33, 149-166.	0.9	134
84	Adverse Outcome Pathways can drive nonâ€animal approaches for safety assessment. Journal of Applied Toxicology, 2015, 35, 971-975.	1.4	82
85	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
86	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
87	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
88	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
89	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
90	Development of an in Silico Profiler for Mitochondrial Toxicity. Chemical Research in Toxicology, 2015, 28, 1891-1902.	1.7	41

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91	Systems Biology Approach Reveals a Calcium-Dependent Mechanism for Basal Toxicity in Daphnia magna. Environmental Science & Technology, 2015, 49, 11132-11140.	4.6	28
92	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
93	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
94	The SEURAT-1 approach towards animal free human safety assessment. ALTEX: Alternatives To Animal Experimentation, 2015, 32, 9-24.	0.9	40
95	Development of an In Silico Profiler for Respiratory Sensitisation. ATLA Alternatives To Laboratory Animals, 2014, 42, 367-375.	0.7	13
96	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
97	Feature Selection Modelling for Percutaneous Absorption across Synthetic Membranes. , 2014, , .		0
98	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
99	QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010.	2.9	1,401
100	Description of the MoA/AOP linked with PPARgamma receptor dysregulation leading to liver fibrosis. Toxicology Letters, 2014, 229, S49.	0.4	0
101	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
102	Read-across approaches - misconceptions, promises and challenges ahead. ALTEX: Alternatives To Animal Experimentation, 2014, 31, 387-396.	0.9	90
103	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
104	Towards a Fuzzy Expert System on Toxicological Data Quality Assessment. Molecular Informatics, 2013, 32, 65-78.	1.4	24
105	Toward better understanding of liver steatosis MoA: Molecular modelling study of PPAR gamma receptor. Toxicology Letters, 2013, 221, S85.	0.4	2
106	Data mining toxicity effects through an ontology approach to investigate toxicity mode of action. Toxicology Letters, 2013, 221, S80.	0.4	0
107	Development of integrated in silico models for toxicity prediction focussing on cosmetic ingredients. Toxicology Letters, 2013, 221, S81.	0.4	0
108	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

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109	Pragmatic Approaches to Using Computational Methods To Predict Xenobiotic Metabolism. Journal of Chemical Information and Modeling, 2013, 53, 1282-1293.	2.5	24
110	International QSAR Award Winner 2012: Prof Terry Wayne Schultz. SAR and QSAR in Environmental Research, 2013, 24, 255-257.	1.0	1
111	In silicomodels for drug-induced liver injury â€“ current status. Expert Opinion on Drug Metabolism and Toxicology, 2012, 8, 201-217.	1.5	73
112	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
113	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
114	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
115	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
116	Modelling acute oral mammalian toxicity. 1. Definition of a quantifiable baseline effect. Toxicology in Vitro, 2011, 25, 1281-1293.	1.1	25
117	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
118	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
119	Measurement and Estimation of Electrophilic Reactivity for Predictive Toxicology. Chemical Reviews, 2011, 111, 2562-2596.	23.0	178
120	Alternative (non-animal) methods for cosmetics testing: current status and future prospectsâ€”2010. Archives of Toxicology, 2011, 85, 367-485.	1.9	488
121	In Silico Studies of the Relationship Between Chemical Structure and Drug Induced Phospholipidosis. Molecular Informatics, 2011, 30, 415-429.	1.4	22
122	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
123	Using In Silico Tools in a Weight of Evidence Approach to Aid Toxicological Assessment. Molecular Informatics, 2010, 29, 97-110.	1.4	25
124	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
125	Quantitative Structureâ€“Activity Relationships (QSARs) â€“ Applications and Methodology. Challenges and Advances in Computational Chemistry and Physics, 2010, , 3-11.	0.6	20
126	Prediction of Michael-Type Acceptor Reactivity toward Glutathione. Chemical Research in Toxicology, 2010, 23, 1576-1585.	1.7	115

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127	Prediction of Harmful Human Health Effects of Chemicals from Structure. Challenges and Advances in Computational Chemistry and Physics, 2010, , 305-325.	0.6	5
128	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
129	Electrophilic Reaction Chemistry of Low Molecular Weight Respiratory Sensitizers. Chemical Research in Toxicology, 2009, 22, 1447-1453.	1.7	78
130	A computational investigation of the reactivity of electrophilic toxicants. Toxicology Letters, 2009, 189, S259.	0.4	1
131	(Q)SARs for Predicting Effects Relating to Reproductive Toxicity. QSAR and Combinatorial Science, 2008, 27, 91-100.	1.5	48
132	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
133	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
134	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
135	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
136	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
137	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
138	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
139	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
140	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
141	Development of Integrated Testing Strategies for REACH: Motivation, Background and Introduction. ATLA Alternatives To Laboratory Animals, 2008, 36, i-iii.	0.7	2
142	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
143	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
144	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

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145	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
146	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
147	Consensus QSAR Models:â€‰ Do the Benefits Outweigh the Complexity?. Journal of Chemical Information and Modeling, 2007, 47, 1460-1468.	2.5	86
148	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
149	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
150	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
151	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
152	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
153	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
154	Quantitative structureâ€“activityâ€“activity and quantitative structureâ€“activity investigations of human and rodent toxicity. Chemosphere, 2006, 65, 1878-1887.	4.2	46
155	Integrated Testing Strategies for Use in the EU REACH System. ATLA Alternatives To Laboratory Animals, 2006, 34, 407-427.	0.7	36
156	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
157	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
158	Structure-based methods for the prediction of drug metabolism. Expert Opinion on Drug Metabolism and Toxicology, 2006, 2, 545-557.	1.5	37
159	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
160	A Study on Feature Selection for Toxicity Prediction. Lecture Notes in Computer Science, 2005, , 31-34.	1.0	4
161	Using kNN Model for Automatic Feature Selection. Lecture Notes in Computer Science, 2005, , 410-419.	1.0	8
162	The Prediction of Skin Permeability Using Quantitative Structureâ€“Activity Relationship Methods. , 2005, , 113-134.		3

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163	Toxicological Information for Use in Predictive Modeling. , 2005, , 93-133.		10
164	The Endocrine Disrupting Activity of Pesticides. Outlooks on Pest Management, 2004, 15, 211-214.	0.1	0
165	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
166	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
167	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
168	A Framework for Promoting the Acceptance and Regulatory Use of (Quantitative) Structure- Activity Relationships. , 2004, , .		3
169	Predicting Chemical Toxicity and Fate in Humans and the Environment â€šÃ„Ã® An Introduction. , 2004, , .		1
170	Validation of (Q)SARs Models: Jaworska et al.'s Response. Environmental Health Perspectives, 2004, 112, a86-a87.	2.8	0
171	The Use by Governmental Regulatory Agencies of Quantitative Structure- Activity Relationships and Expert Systems to Predict Toxicity. , 2004, , .		1
172	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
173	Essential and desirable characteristics of ecotoxicity quantitative structureâ€“activity relationships. Environmental Toxicology and Chemistry, 2003, 22, 599-607.	2.2	50
174	Quantitative structureâ€“activity relationships (QSARs) in toxicology: a historical perspective. Computational and Theoretical Chemistry, 2003, 622, 1-22.	1.5	205
175	The present status of QSAR in toxicology. Computational and Theoretical Chemistry, 2003, 622, 23-38.	1.5	79
176	Pitfalls in QSAR. Computational and Theoretical Chemistry, 2003, 622, 39-51.	1.5	300
177	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
178	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
179	Molecular Quantum Similarity Analysis of Estrogenic Activity. Journal of Chemical Information and Computer Sciences, 2003, 43, 1166-1176.	2.8	45
180	Estrogenicity and acute toxicity of selected anilines using a recombinant yeast assay. Chemosphere, 2003, 52, 1173-1181.	4.2	23

#	Article	IF	Citations
181	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
182	Computer-aided prediction of drug toxicity and metabolism. , 2003, , 259-278.		5
183	Quantitative Structure-Activity Relationships for Acute Aquatic Toxicity. , 2003, , .		7
184	Structureâ^'Toxicity Relationships for Aliphatic Chemicals Evaluated with Tetrahymena pyriformis. Chemical Research in Toxicology, 2002, 15, 1602-1609.	1.7	72
185	Structure-Based Classification of Antibacterial Activity. Journal of Chemical Information and Computer Sciences, 2002, 42, 869-878.	2.8	97
186	Quantitative structureâ€"activity relationships (QSARs) for the prediction of skin permeation of exogenous chemicals. Chemosphere, 2002, 48, 603-613.	4.2	168
187	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
188	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
189	Physico-chemical interpretation and prediction of the dimyristoyl phosphatidyl cholineâ€"water partition coefficient. Computational and Theoretical Chemistry, 2002, 593, 9-18.	1.5	18
190	Quantitative structureâ€"permeability relationships for percutaneous absorption: re-analysis of steroid data. International Journal of Pharmaceutics, 2002, 238, 105-109.	2.6	91
191	Structure-activity relationships for gene activation oestrogenicity: Evaluation of a diverse set of aromatic chemicals. Environmental Toxicology, 2002, 17, 14-23.	2.1	69
192	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
193	A Novel Index for the Description of Molecular Linearity. Journal of Chemical Information and Computer Sciences, 2001, 41, 1228-1236.	2.8	16
194	The Use of Bootstrap Resampling to Assess the Uncertainty of Cooper Statistics. ATLA Alternatives To Laboratory Animals, 2001, 29, 447-459.	0.7	13
195	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
196	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
197	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
198	Structureâ€"permeability Relationships for Transcorneal Penetration. ATLA Alternatives To Laboratory Animals, 2000, 28, 403-413.	0.7	16

#	Article	IF	Citations
199	Embedded Cluster Modelling-A novel method for analysing embedded data sets. QSAR and Combinatorial Science, 1999, 18, 229-235.	1.4	16
200	Structureâ€“Toxicity Relationships for Three Mechanisms of Action of Toxicity toVibrio fischeri. Ecotoxicology and Environmental Safety, 1998, 39, 65-69.	2.9	48
201	Quantitative Structure-Activity Relationships of Chemicals Acting by Non-polar Narcosisâ€”Theoretical Considerations. QSAR and Combinatorial Science, 1998, 17, 131-138.	1.4	42
202	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
203	Correspondence Analysis of the Skin Sensitization Potential of Organic Chemicals. QSAR and Combinatorial Science, 1997, 16, 33-37.	1.4	8
204	Quantitative structureâ€activity relationships for weak acid respiratory uncouplers to Vibrio fisheri. Environmental Toxicology and Chemistry, 1997, 16, 357-360.	2.2	34
205	The Development and Validation of Expert Systems for Predicting Toxicity. ATLA Alternatives To Laboratory Animals, 1997, 25, 223-251.	0.7	96
206	QUANTITATIVE STRUCTUREâ€“ACTIVITY RELATIONSHIPS FOR WEAK ACID RESPIRATORY UNCOUPLERS TO VIBRIO FISHERI. Environmental Toxicology and Chemistry, 1997, 16, 357.	2.2	29
207	Structure-toxicity relationships for phenols to Tetrahymena pyriformis. Chemosphere, 1996, 32, 1453-1468.	4.2	129
208	Alternative Methods for Skin Sensitisation Testing. ATLA Alternatives To Laboratory Animals, 1996, 24, 683-705.	0.7	49
209	QSAR in Toxicology. 1. Prediction of Aquatic Toxicity. QSAR and Combinatorial Science, 1995, 14, 1-7.	1.4	123
210	QSAR in Toxicology. 2. Prediction of Acute Mammalian Toxicity and Interspecies Correlations. QSAR and Combinatorial Science, 1995, 14, 117-120.	1.4	45
211	QSAR in Toxicology. 3. Prediction of Chronic Toxicities. QSAR and Combinatorial Science, 1995, 14, 329-334.	1.4	50
212	QSAR Study of the Toxicity of Nitrobenzenes toTetrahymena pyriformis. QSAR and Combinatorial Science, 1995, 14, 427-432.	1.4	61
213	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
214	QSARs of fathead minnow and Microtox toxicity data using canonical correlation analysis. , 1993, , 541-542.		1