List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/4934656/publications.pdf Version: 2024-02-01

		30047	32815
201	11,493	54	100
papers	citations	h-index	g-index
210	210	210	0.000
219	219	219	9692
all docs	docs citations	times ranked	citing authors

#	Article	IF	CITATIONS
1	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
2	Alternative (non-animal) methods for cosmetics testing: current status and future prospects—2010. Archives of Toxicology, 2011, 85, 367-485.	1.9	488
3	An evaluation of the implementation of the Cramer classification scheme in the Toxtree software. SAR and QSAR in Environmental Research, 2008, 19, 495-524.	1.0	359
4	Applying Adverse Outcome Pathways (AOPs) to support Integrated Approaches to Testing and Assessment (IATA). Regulatory Toxicology and Pharmacology, 2014, 70, 629-640.	1.3	291
5	A theoretical framework for predicting the oxidative stress potential of oxide nanoparticles. Nanotoxicology, 2011, 5, 228-235.	1.6	289
6	A Modular Approach to the ECVAM Principles on Test Validity. ATLA Alternatives To Laboratory Animals, 2004, 32, 467-472.	0.7	275
7	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	2.8	264
8	In vivo kinetics of human natural killer cells: the effects of ageing and acute and chronic viral infection. Immunology, 2007, 121, 258-265.	2.0	257
9	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
10	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
11	The ECVAM International Validation Study on in Vitro Tests for Acute Skin Irritation: Report on the Validity of the EPISKIN and EpiDerm Assays and on the Skin Integrity Function Test. ATLA Alternatives To Laboratory Animals, 2007, 35, 559-601.	0.7	185
12	Regulatory assessment of chemical mixtures: Requirements, current approaches and future perspectives. Regulatory Toxicology and Pharmacology, 2016, 80, 321-334.	1.3	185
13	New Publicly Available Chemical Query Language, CSRML, To Support Chemotype Representations for Application to Data Mining and Modeling. Journal of Chemical Information and Modeling, 2015, 55, 510-528.	2.5	183
14	Metabolism: A Bottleneck in <i>In Vitro</i> Toxicological Test Development. ATLA Alternatives To Laboratory Animals, 2006, 34, 49-84.	0.7	161
15	B-cell kinetics in humans: rapid turnover of peripheral blood memory cells. Blood, 2005, 105, 3633-3640.	0.6	155
16	Applying quantitative structure–activity relationship approaches to nanotoxicology: Current status and future potential. Toxicology, 2013, 313, 15-23.	2.0	151
17	Regulatory assessment and risk management of chemical mixtures: challenges and ways forward. Critical Reviews in Toxicology, 2019, 49, 174-189.	1.9	135
18	The role of the European Chemicals Bureau in promoting the regulatory use of (Q)SAR methods. SAR and QSAR in Environmental Research, 2007, 18, 111-125.	1.0	130

#	Article	IF	CITATIONS
19	QSAR modeling of nanomaterials. Wiley Interdisciplinary Reviews: Nanomedicine and Nanobiotechnology, 2011, 3, 298-306.	3.3	121
20	The Registry of Cytotoxicity: Toxicity Testing in Cell Cultures to Predict Acute Toxicity (LD50) and to Reduce Testing in Animals. ATLA Alternatives To Laboratory Animals, 2003, 31, 89-89.	0.7	115
21	Measurement and modeling of human T cell kinetics. European Journal of Immunology, 2003, 33, 2316-2326.	1.6	114
22	Review of (Quantitative) Structure–Activity Relationships for Acute Aquatic Toxicity. QSAR and Combinatorial Science, 2008, 27, 77-90.	1.5	108
23	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
24	In vivo T lymphocyte dynamics in humans and the impact of human T-lymphotropic virus 1 infection. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 8035-8040.	3.3	105
25	Strategies to improve the regulatory assessment of developmental neurotoxicity (DNT) using in vitro methods. Toxicology and Applied Pharmacology, 2018, 354, 7-18.	1.3	105
26	Direct Measurement of T Cell Subset Kinetics In Vivo in Elderly Men and Women. Journal of Immunology, 2004, 173, 1787-1794.	0.4	104
27	Applying 'omics technologies in chemicals risk assessment: Report of an ECETOC workshop. Regulatory Toxicology and Pharmacology, 2017, 91, S3-S13.	1.3	102
28	Structure-Based Classification of Antibacterial Activity. Journal of Chemical Information and Computer Sciences, 2002, 42, 869-878.	2.8	97
29	The Development and Validation of Expert Systems for Predicting Toxicity. ATLA Alternatives To Laboratory Animals, 1997, 25, 223-251.	0.7	96
30	Investigating the influence of data splitting on the predictive ability of QSAR/QSPR models. Structural Chemistry, 2011, 22, 795-804.	1.0	91
31	Next generation physiologically based kinetic (NG-PBK) models in support of regulatory decision making. Computational Toxicology, 2019, 9, 61-72.	1.8	91
32	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
33	The Adverse Outcome Pathway approach in nanotoxicology. Computational Toxicology, 2017, 1, 3-11.	1.8	82
34	Modeling the structureâ€property relationships of nanoneedles: A journey toward nanomedicine. Journal of Computational Chemistry, 2009, 30, 275-284.	1.5	76
35	Towards an alternative testing strategy for nanomaterials used in nanomedicine: Lessons from NanoTEST. Nanotoxicology, 2015, 9, 118-132.	1.6	75
36	Ab initio chemical safety assessment: A workflow based on exposure considerations and non-animal methods. Computational Toxicology, 2017, 4, 31-44.	1.8	75

#	Article	IF	CITATIONS
37	Carcinogenicity assessment: Addressing the challenges of cancer and chemicals in the environment. Environment International, 2019, 128, 417-429.	4.8	71
38	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
39	Quantitative structure-skin permeability relationships. Toxicology, 2017, 387, 27-42.	2.0	69
40	Follow-up to the ECVAM Prevalidation Study on <i>In Vitro</i> Tests for Acute Skin Irritation. ATLA Alternatives To Laboratory Animals, 2002, 30, 109-129.	0.7	66
41	Quantitative adverse outcome pathway (qAOP) models for toxicity prediction. Archives of Toxicology, 2020, 94, 1497-1510.	1.9	65
42	Toxmatch–a new software tool to aid in the development and evaluation of chemically similar groups. SAR and QSAR in Environmental Research, 2008, 19, 397-412.	1.0	64
43	Computational methods to predict the reactivity of nanoparticles through structure–property relationships. Expert Opinion on Drug Delivery, 2010, 7, 295-305.	2.4	64
44	Establishment of an in vitro reporter gene assay for developmental cardiac toxicity. Toxicology in Vitro, 2001, 15, 215-223.	1.1	62
45	Development and analysis of an adverse outcome pathway network for human neurotoxicity. Archives of Toxicology, 2019, 93, 2759-2772.	1.9	61
46	Grouping of nanomaterials to read-across hazard endpoints: a review. Nanotoxicology, 2019, 13, 100-118.	1.6	61
47	Assessment of developmental neurotoxicity induced by chemical mixtures using an adverse outcome pathway concept. Environmental Health, 2020, 19, 23.	1.7	61
48	The ECVAM International Validation Study on In Vitro Tests for Skin Corrosivity. 1. Selection and Distribution of the Test Chemicals. Toxicology in Vitro, 1998, 12, 471-482.	1.1	59
49	Review of Estimation Models for Biodegradation. QSAR and Combinatorial Science, 2008, 27, 32-40.	1.5	58
50	The importance of hydrophobicity and electrophilicity descriptors in mechanistically-based QSARs for toxicological endpoints. SAR and QSAR in Environmental Research, 2002, 13, 167-176.	1.0	57
51	Publicly-accessible QSAR software tools developed by the Joint Research Centre. SAR and QSAR in Environmental Research, 2008, 19, 785-799.	1.0	57
52	Testing strategies for the safety of nanoparticles used in medical applications. Nanomedicine, 2009, 4, 605-607.	1.7	57
53	Human cytomegalovirus-specific CD8+ T-cell expansions contain long-lived cells that retain functional capacity in both young and elderly subjects. Immunology, 2011, 132, 27-38.	2.0	56
54	3.3. Eye Irritation. ATLA Alternatives To Laboratory Animals, 2005, 33, 47-81.	0.7	55

#	Article	IF	CITATIONS
55	Current EU regulatory requirements for the assessment of chemicals and cosmetic products: challenges and opportunities for introducing new approach methodologies. Archives of Toxicology, 2021, 95, 1867-1897.	1.9	55
56	The prospects for using (Q)SARs in a changing political environmenthigh expectations and a key role for the european commission's joint research centre. SAR and QSAR in Environmental Research, 2004, 15, 331-343.	1.0	53
57	Structural analysis and predictive value of the rodent in vivo micronucleus assay results. Mutagenesis, 2010, 25, 335-341.	1.0	53
58	Review of Literatureâ€Based Quantitative Structure–Activity Relationship Models for Bioconcentration. QSAR and Combinatorial Science, 2008, 27, 21-31.	1.5	51
59	A Mini Review of Mammalian Toxicity (Q)SAR Models. QSAR and Combinatorial Science, 2008, 27, 41-48.	1.5	51
60	Computer models versus reality: How well do in silico models currently predict the sensitization potential of a substance. Regulatory Toxicology and Pharmacology, 2013, 67, 468-485.	1.3	51
61	ECVAM's Response to the Changing Political Environment for Alternatives: Consequences of the European Union Chemicals and Cosmetics Policies. ATLA Alternatives To Laboratory Animals, 2003, 31, 473-481.	0.7	50
62	Validation of counter propagation neural network models for predictive toxicology according to the OECD principles: a case study. SAR and QSAR in Environmental Research, 2006, 17, 265-284.	1.0	50
63	The Importance of the Prediction Model in the Validation of Alternative Tests. ATLA Alternatives To Laboratory Animals, 2001, 29, 135-143.	0.7	48
64	(Q)SARs for Predicting Effects Relating to Reproductive Toxicity. QSAR and Combinatorial Science, 2008, 27, 91-100.	1.5	48
65	Quantitative structure–activity–activity and quantitative structure–activity investigations of human and rodent toxicity. Chemosphere, 2006, 65, 1878-1887.	4.2	46
66	Predicting toxicity of nanoparticles. Nature Nanotechnology, 2011, 6, 138-139.	15.6	46
67	Consensus of classification trees for skin sensitisation hazard prediction. Toxicology in Vitro, 2016, 36, 197-209.	1.1	45
68	Validation of a QSAR model for acute toxicity. SAR and QSAR in Environmental Research, 2006, 17, 147-171.	1.0	44
69	Establishing the level of safety concern for chemicals in food without the need for toxicity testing. Regulatory Toxicology and Pharmacology, 2014, 68, 275-296.	1.3	44
70	Analysis of the Local Lymph Node Assay (LLNA) variability for assessing the prediction of skin sensitisation potential and potency of chemicals with non-animal approaches. Toxicology in Vitro, 2016, 34, 220-228.	1.1	44
71	Investigating the state of physiologically based kinetic modelling practices and challenges associated with gaining regulatory acceptance of model applications. Regulatory Toxicology and Pharmacology, 2017, 90, 104-115.	1.3	42
72	Prediction of estrogenicity: validation of a classification model. SAR and QSAR in Environmental Research, 2006, 17, 195-223.	1.0	40

#	Article	IF	CITATIONS
73	The ECVAM International Validation Study on In Vitro Tests for Acute Skin Irritation: Selection of Test Chemicals. ATLA Alternatives To Laboratory Animals, 2007, 35, 603-619.	0.7	40
74	In vitro-to-in vivo correlation of the skin penetration, liver clearance and hepatotoxicity of caffeine. Food and Chemical Toxicology, 2015, 75, 39-49.	1.8	40
75	COMPARISON OF THE APPLICABILITY DOMAIN OF A QUANTITATIVE STRUCTURE–ACTIVITY RELATIONSHIP FOR ESTROGENICITY WITH A LARGE CHEMICAL INVENTORY. Environmental Toxicology and Chemistry, 2006, 25, 1223.	2.2	39
76	Grouping of nanomaterials to read-across hazard endpoints: from data collection to assessment of the grouping hypothesis by application of chemoinformatic techniques. Particle and Fibre Toxicology, 2018, 15, 37.	2.8	39
77	A feasibility study developing an integrated testing strategy assessing skin irritation potential of chemicals. Toxicology Letters, 2008, 180, 9-20.	0.4	38
78	QUANTITATIVE STRUCTURE–ACTIVITY RELATIONSHIPS FOR HUMAN HEALTH EFFECTS: COMMONALITIES WITH OTHER ENDPOINTS. Environmental Toxicology and Chemistry, 2003, 22, 1829.	2.2	37
79	Validation of in vitro methods for human cytochrome P450 enzyme induction: Outcome of a multi-laboratory study. Toxicology in Vitro, 2019, 60, 212-228.	1.1	36
80	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
81	Review of the Availability of <i>In Vitro</i> and <i>In Silico</i> Methods for Assessing Dermal Bioavailability. Applied in Vitro Toxicology, 2015, 1, 147-164.	0.6	35
82	The influence of inter-particle forces on diffusion at the nanoscale. Scientific Reports, 2019, 9, 12689.	1.6	35
83	A Review of (Q)SAR Models for Skin and Eye Irritation and Corrosion. QSAR and Combinatorial Science, 2008, 27, 49-59.	1.5	32
84	Toxmatch—A chemical classification and activity prediction tool based on similarity measures. Regulatory Toxicology and Pharmacology, 2008, 52, 77-84.	1.3	32
85	Theoretical and mathematical foundation of the Virtual Cell Based Assay – A review. Toxicology in Vitro, 2017, 45, 209-221.	1.1	31
86	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
87	Computational models for the assessment of manufactured nanomaterials: Development of model reporting standards and mapping of the model landscape. Computational Toxicology, 2019, 9, 143-151.	1.8	30
88	Qsar investigation of a large data set for fish, algae and Daphnia toxicity. SAR and QSAR in Environmental Research, 2004, 15, 413-431.	1.0	29
89	The Integrated Use of Models for the Properties and Effects of Chemicals by means of a Structured Workflow. QSAR and Combinatorial Science, 2008, 27, 6-20.	1.5	29
90	Overcoming Barriers to Validation of Non-animal Partial Replacement Methods/Integrated Testing Strategies: The Report of an EPAA–ECVAM Workshop. ATLA Alternatives To Laboratory Animals, 2009, 37, 437-444.	0.7	29

#	Article	IF	CITATIONS
91	Computational toxicology at the European Commission's Joint Research Centre. Expert Opinion on Drug Metabolism and Toxicology, 2010, 6, 785-792.	1.5	29
92	The Role of ECVAM in Promoting the Regulatory Acceptance of Alternative Methods in the European Union. ATLA Alternatives To Laboratory Animals, 2001, 29, 525-535.	0.7	28
93	The margin of internal exposure (MOIE) concept for dermal risk assessment based on oral toxicity data – A case study with caffeine. Toxicology, 2017, 392, 119-129.	2.0	28
94	Artificial Intelligence for chemical risk assessment. Computational Toxicology, 2020, 13, 100114.	1.8	27
95	The role of the European centre for the validation of alternative methods (ECVAM) in the validation of (Q)SARs. SAR and QSAR in Environmental Research, 2004, 15, 345-358.	1.0	26
96	Multiscale modelling approaches for assessing cosmetic ingredients safety. Toxicology, 2017, 392, 130-139.	2.0	26
97	A rule for designing safer nanomaterials: do not interfere with the cellular redox equilibrium. Nanotoxicology, 2015, 9, 116-117.	1.6	25
98	The Role of Qsar Methodology in the Regulatory Assessment of Chemicals. Challenges and Advances in Computational Chemistry and Physics, 2010, , 367-382.	0.6	24
99	Report of the EPAA–ECVAM Workshop on the Validation of Integrated Testing Strategies (ITS). ATLA Alternatives To Laboratory Animals, 2012, 40, 175-181.	0.7	24
100	Role of <i>in silico</i> genotoxicity tools in the regulatory assessment of pharmaceutical impurities. SAR and QSAR in Environmental Research, 2012, 23, 257-277.	1.0	24
101	Physiologically based kinetic (PBK) modelling and human biomonitoring data for mixture risk assessment. Environment International, 2020, 143, 105978.	4.8	24
102	Evaluation of SARs for the prediction of skin irritation/corrosion potential–structural inclusion rules in the BfR decision support systemâ€. SAR and QSAR in Environmental Research, 2007, 18, 331-342.	1.0	23
103	Application of physiologically-based toxicokinetic modelling in oral-to-dermal extrapolation of threshold doses of cosmetic ingredients. Toxicology Letters, 2014, 227, 189-202.	0.4	23
104	3.4. Skin Sensitisation. ATLA Alternatives To Laboratory Animals, 2005, 33, 83-103.	0.7	22
105	The role of validation in establishing the scientific credibility of predictive toxicology approaches intended for regulatory application. Computational Toxicology, 2021, 17, 100144.	1.8	22
106	The application of molecular modelling in the safety assessment of chemicals: A case study on ligand-dependent PPARÎ <sup>3</sup> dysregulation. Toxicology, 2017, 392, 140-154.	2.0	21
107	Evaluation of SARs for the prediction of eye irritation/corrosion potential–structural inclusion rules in the BfR decision support systemâ€. SAR and QSAR in Environmental Research, 2007, 18, 221-235.	1.0	20
108	Application of new statistical distribution approaches for environmental mixture risk assessment: A case study. Science of the Total Environment, 2019, 693, 133510.	3.9	20

#	Article	IF	CITATIONS
109	Grouping of multi-walled carbon nanotubes to read-across genotoxicity: A case study to evaluate the applicability of regulatory guidance. Computational Toxicology, 2019, 9, 22-35.	1.8	20
110	Unlocking the potential of in silico chemical safety assessment – A report on a cross-sector symposium on current opportunities and future challenges. Computational Toxicology, 2019, 10, 38-43.	1.8	20
111	Investigating cell type specific mechanisms contributing to acute oral toxicity. ALTEX: Alternatives To Animal Experimentation, 2019, 36, 39-64.	0.9	20
112	Prediction of acute toxicity to mice by the Arithmetic Mean Toxicity (AMT) modelling approach. SAR and QSAR in Environmental Research, 2010, 21, 265-275.	1.0	19
113	Physiologically based mathematical models of nanomaterials for regulatory toxicology: A review. Computational Toxicology, 2019, 9, 133-142.	1.8	19
114	Combining in vitro assays and mathematical modelling to study developmental neurotoxicity induced by chemical mixtures. Reproductive Toxicology, 2021, 105, 101-119.	1.3	19
115	An Evaluation of the Proposed OECD Testing Strategy for Skin Corrosion. ATLA Alternatives To Laboratory Animals, 1998, 26, 709-720.	0.7	18
116	Membrane transporter data to support kinetically-informed chemical risk assessment using non-animal methods: Scientific and regulatory perspectives. Environment International, 2019, 126, 659-671.	4.8	18
117	Tuning the Electronic Properties by Width and Length Modifications of Narrow- Diameter Carbon Nanotubes for Nanomedicine. Current Medicinal Chemistry, 2012, 19, 5219-5225.	1.2	17
118	From in vitro to in vivo: Integration of the virtual cell based assay with physiologically based kinetic modelling. Toxicology in Vitro, 2017, 45, 241-248.	1.1	17
119	Towards a qAOP framework for predictive toxicology - Linking data to decisions. Computational Toxicology, 2022, 21, 100195.	1.8	17
120	Embedded Cluster Modelling-A novel method for analysing embedded data sets. QSAR and Combinatorial Science, 1999, 18, 229-235.	1.4	16
121	Structure–permeability Relationships for Transcorneal Penetration. ATLA Alternatives To Laboratory Animals, 2000, 28, 403-413.	0.7	16
122	Role of Physiologically Based Kinetic modelling in addressing environmental chemical mixtures – A review. Computational Toxicology, 2019, 10, 158-168.	1.8	16
123	Assessment of the predictive capacity of a physiologically based kinetic model using a read-across approach. Computational Toxicology, 2021, 18, 100159.	1.8	16
124	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
125	The Principles of Validation and the ECVAM Validation Process. ATLA Alternatives To Laboratory Animals, 2004, 32, 623-629.	0.7	15
126	Characterization of age-related changes in bovine CD8+ T-cells. Veterinary Immunology and Immunopathology, 2011, 140, 47-54.	0.5	15

#	Article	IF	CITATIONS
127	Establishing a systematic framework to characterise in vitro methods for human hepatic metabolic clearance. Toxicology in Vitro, 2018, 53, 233-244.	1.1	15
128	Integration of data across toxicity endpoints for improved safety assessment of chemicals: the example of carcinogenicity assessment. Archives of Toxicology, 2021, 95, 1971-1993.	1.9	15
129	COSMOS next generation – A public knowledge base leveraging chemical and biological data to support the regulatory assessment of chemicals. Computational Toxicology, 2021, 19, 100175.	1.8	15
130	QSAR and Metabolic Assessment Tools in the Assessment of Genotoxicity. Methods in Molecular Biology, 2013, 930, 125-162.	0.4	15
131	Integrated Approaches to Testing and Assessment. Advances in Experimental Medicine and Biology, 2016, 856, 317-342.	0.8	15
132	Probabilistic modelling of developmental neurotoxicity based on a simplified adverse outcome pathway network. Computational Toxicology, 2022, 21, 100206.	1.8	15
133	Thresholds of toxicological concern for endocrine active substances in the aquatic environment. Integrated Environmental Assessment and Management, 2010, 6, 2-11.	1.6	14
134	Use of computational tools in the field of food safety. Regulatory Toxicology and Pharmacology, 2011, 60, 354-362.	1.3	14
135	Prediction of Acute Rodent Toxicity on the Basis of Chemical Structure and Physicochemical Similarity. Molecular Informatics, 2011, 30, 267-275.	1.4	14
136	Gaining acceptance in next generation PBK modelling approaches for regulatory assessments – An OECD international effort. Computational Toxicology, 2021, 18, 100163.	1.8	14
137	A General Approach for Evaluating Stepwise Testing Strategies. ATLA Alternatives To Laboratory Animals, 1999, 27, 161-177.	0.7	13
138	The Use of Bootstrap Resampling to Assess the Uncertainty of Cooper Statistics. ATLA Alternatives To Laboratory Animals, 2001, 29, 447-459.	0.7	13
139	Prediction Models for Eye Irritation Potential Based on Endpoints of the HETCAM and Neutral Red Uptake Tests. In Vitro & Molecular Toxicology, 2001, 14, 143-156.	0.6	13
140	An integrated approach for bioaccumulation assessment in mussels: Towards the development of Environmental Quality Standards for biota. Ecotoxicology and Environmental Safety, 2011, 74, 244-252.	2.9	13
141	Assessing Herbal Products with Health Claims. Critical Reviews in Food Science and Nutrition, 2015, 55, 1918-1928.	5.4	13
142	Validation of Computational Methods. Advances in Experimental Medicine and Biology, 2016, 856, 165-187.	0.8	13
143	Capturing the applicability of in vitro-in silico membrane transporter data in chemical risk assessment and biomedical research. Science of the Total Environment, 2018, 645, 97-108.	3.9	13
144	QSARs for toxicity to the bacteriumSinorhizobium meliloti. SAR and QSAR in Environmental Research, 2004, 15, 169-190.	1.0	12

#	Article	IF	CITATIONS
145	Mode of action-based classification and prediction of activity of uncouplers for the screening of chemical inventories. SAR and QSAR in Environmental Research, 2008, 19, 433-463.	1.0	12
146	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
147	The use of genetically engineered cells for assessing CYP2D6-related polymorphic effects. Toxicology in Vitro, 2001, 15, 553-556.	1.1	11
148	Structural motifs modulating the carcinogenic risk of aromatic amines. Environmental and Molecular Mutagenesis, 2009, 50, 152-161.	0.9	11
149	Applicability of QSAR analysis in the evaluation of developmental and neurotoxicity effects for the assessment of the toxicological relevance of metabolites and degradates of pesticide active substances for dietary risk assessment. EFSA Supporting Publications, 2011, 8, 169E.	0.3	11
150	A Tutorial for Analysing the Cost-effectiveness of Alternative Methods for Assessing Chemical Toxicity: The Case of Acute Oral Toxicity Prediction. ATLA Alternatives To Laboratory Animals, 2014, 42, 115-127.	0.7	11
151	The acute effects of daily nicotine intake on heart rate – A toxicokinetic and toxicodynamic modelling study. Regulatory Toxicology and Pharmacology, 2014, 70, 312-324.	1.3	11
152	Waiving chronic fish tests: possible use of acute-to-chronic relationships and interspecies correlations. Toxicological and Environmental Chemistry, 2016, , 1-23.	0.6	11
153	Computational modelling for the sustainable management of chemicals. Computational Toxicology, 2020, 14, 100122.	1.8	11
154	The Principles of Validation and the ECVAM Validation Process. ATLA Alternatives To Laboratory Animals, 2002, 30, 15-21.	0.7	10
155	Accelerated In Vivo Proliferation of Memory Phenotype CD4+ T-cells in Human HIV-1 Infection Irrespective of Viral Chemokine Co-receptor Tropism. PLoS Pathogens, 2013, 9, e1003310.	2.1	10
156	The virtual cell based assay: Current status and future perspectives. Toxicology in Vitro, 2017, 45, 258-267.	1.1	10
157	Recent Advances in the Molecular Modeling of Estrogen Receptor-Mediated Toxicity. Advances in Protein Chemistry and Structural Biology, 2011, 85, 217-251.	1.0	9
158	Automated workflows for modelling chemical fate, kinetics and toxicity. Toxicology in Vitro, 2017, 45, 249-257.	1.1	9
159	Practical use of the Virtual Cell Based Assay: Simulation of repeated exposure experiments in liver cell lines. Toxicology in Vitro, 2017, 45, 233-240.	1.1	9
160	The future of in silico chemical safety $\hat{a} \in \$ and beyond. Computational Toxicology, 2019, 10, 60-62.	1.8	9
161	Computational Tools for Regulatory Needs. , 0, , 751-775.		8
162	Virtual Cell Based Assay simulations of intra-mitochondrial concentrations in hepatocytes and cardiomyocytes. Toxicology in Vitro, 2017, 45, 222-232.	1.1	7

#	Article	IF	CITATIONS
163	Chapter 11. Development and Evaluation of Structure–Reactivity Models for Predicting the In Vitro Oxidative Stress of Metal Oxide Nanoparticles. RSC Nanoscience and Nanotechnology, 2012, , 257-283.	0.2	6
164	Training Needs for Toxicity Testing in the 21st Century: A Survey-informed Analysis. ATLA Alternatives To Laboratory Animals, 2012, 40, 313-320.	0.7	6
165	In Silico Models for Acute Systemic Toxicity. Methods in Molecular Biology, 2016, 1425, 177-200.	0.4	6
166	Alternative Toxicity Test Methods. , 2019, , 317-323.		6
167	Insights into in vitro biokinetics using Virtual Cell Based Assay simulations. ALTEX: Alternatives To Animal Experimentation, 2019, 36, 447-461.	0.9	6
168	3D QSAR investigation of the blood–brain barrier penetration of chemical compounds. SAR and QSAR in Environmental Research, 2005, 16, 79-91.	1.0	5
169	Evaluation of Non-animal Methods for Assessing Skin Sensitisation Hazard: A Bayesian Value-of-Information Analysis. ATLA Alternatives To Laboratory Animals, 2016, 44, 255-269.	0.7	5
170	The Validation of Alternative Test Methods. , 2019, , 307-314.		5
171	Settling dynamics of nanoparticles in simple and biological media. Royal Society Open Science, 2021, 8, 210068.	1.1	5
172	Exploring Waiving Opportunities for Mammalian Acute Systemic Toxicity Tests. ATLA Alternatives To Laboratory Animals, 2016, 44, 271-279.	0.7	4
173	A matter of trust: Learning lessons about causality will make qAOPs credible. Computational Toxicology, 2022, 21, 100205.	1.8	4
174	In Silico Models for Predicting Acute Systemic Toxicity. Methods in Molecular Biology, 2022, 2425, 259-289.	0.4	4
175	Linear and nonlinear QSAR models of acute intravenous toxicity of organic chemicals for mice. Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry, 2011, 5, 213-225.	0.2	3
176	A Framework for Promoting the Acceptance and Regulatory Use of ( Quantitative) Structure- Activity Relationships. , 2004, , .		3
177	ECVAM News & amp; Views. ATLA Alternatives To Laboratory Animals, 2001, 29, 391-392.	0.7	2
178	Toward better understanding of liver steatosis MoA: Molecular modelling study of PPAR gamma receptor. Toxicology Letters, 2013, 221, S85.	0.4	2
179	Toxicity Testing, Modeling. , 2005, , 288-293.		2
180	Making better use of toxicity studies for human health by extrapolating across endpoints. ALTEX: Alternatives To Animal Experimentation, 2020, 37, 519-531.	0.9	2

#	Article	IF	CITATIONS
181	Extension of the Virtual Cell Based Assay from a 2-D to a 3-D Cell Culture Model. ATLA Alternatives To Laboratory Animals, 2022, 50, 45-56.	0.7	2
182	ECVAM's Activities on Computer Modelling and Integrated Testing. ATLA Alternatives To Laboratory Animals, 2002, 30, 133-137.	0.7	1
183	The Role of ECVAM. , 2019, , 95-107.		1
184	Involvement of the Organisation for Economic Cooperation and Development. , 2019, , 147-154.		1
185	Integrated Approaches to Testing and Assessment. , 2019, , 301-306.		1
186	Alternative Approaches for the Assessment of Chemicals in Food. , 2019, , 185-195.		1
187	Optimising testing strategies for classification of human health and environmental hazards – A proof-of-concept study. Toxicology Letters, 2020, 335, 64-70.	0.4	1
188	The Tiered Approach to Toxicity Assessment Based on the Integrated Use of Alternative (Non-Animal) Tests. , 2004, , .		1
189	Editorial: Advances and Refinements in the Development and Application of Threshold of Toxicological Concern. Frontiers in Toxicology, 2022, 4, 882321.	1.6	1
190	Environmental Modelling Based on a Structural Fragments Approach. Indoor and Built Environment, 1996, 5, 334-340.	1.5	0
191	Improving the application of quantitative methods in validation work. Toxicology in Vitro, 2001, 15, 601-604.	1.1	Ο
192	Reply to the Comment by Hoffmann <i>et al.</i> . ATLA Alternatives To Laboratory Animals, 2002, 30, 555-557.	0.7	0
193	The Use of Computer Models as Alternatives to Animal Experiments in Chemical Risk Assessment. ATLA Alternatives To Laboratory Animals, 2003, 31, 67-73.	0.7	0
194	Calculations of acute intravenous toxicity in mice based on local regression models in superoverlapping clusters (LRMSC). Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry, 2011, 5, 346-356.	0.2	0
195	Development of integrated in silico models for toxicity prediction focussing on cosmetic ingredients. Toxicology Letters, 2013, 221, S81.	0.4	0
196	Applicability of in silico models for the prediction of the sensitization potential of industrial chemicals. Toxicology Letters, 2013, 221, S204.	0.4	0
197	Dedication to Dr J.M. ZaldÃvar Comenges (1958–2012). Toxicology in Vitro, 2017, 45, 207-208.	1.1	0
198	Advancing risk assessment of cosmetics using COSMOS in silico modelling and database. Toxicology Letters, 2018, 295, S28.	0.4	0

#	Article	IF	CITATIONS
199	Types of Toxicity and Applications of Toxicity Testing. , 2019, , 7-10.		0
200	Chapter 4. Towards a Common Regulatory Framework for Computational Toxicology: Current Status and Future Perspectives. RSC Drug Discovery Series, 2011, , 38-69.	0.2	0
201	The challenge of combined exposure to multiple chemicals: scientific and regulatory approaches to protect human health. European Journal of Public Health, 2020, 30, .	0.1	0