Nicole C Kleinstreuer

List of Publications by Year
in descending order

118 papers	8,450 citations	57758 44 h-index	49909 87 g-index
126 all docs	126 docs citations	126 times ranked	8873 citing authors

#	Article	IF	Citations
1	Chronic inflammation in the etiology of disease across the life span. Nature Medicine, 2019, 25, 1822-1832.	30.7	2,195
2	Update on EPAâ€™s ToxCast Program: Providing High Throughput Decision Support Tools for Chemical Risk Management. Chemical Research in Toxicology, 2012, 25, 1287-1302.	3.3	410
3	Zebrafish developmental screening of the ToxCastâ„¢ Phase I chemical library. Reproductive Toxicology, 2012, 33, 174-187.	2.9	267
4	Assessing the carcinogenic potential of low-dose exposures to chemical mixtures in the environment: the challenge ahead. Carcinogenesis, 2015, 36, S254-S296.	2.8	239
5	Screening Chemicals for Estrogen Receptor Bioactivity Using a Computational Model. Environmental Science & Technology, 2015, 49, 8804-8814.	10.0	224
6	Predictive Models of Prenatal Developmental Toxicity from ToxCast High-Throughput Screening Data. Toxicological Sciences, 2011, 124, 109-127.	3.1	186
7	Phenotypic screening of the ToxCast chemical library to classify toxic and therapeutic mechanisms. Nature Biotechnology, 2014, 32, 583-591.	17.5	175
8	Editor's Highlight: Analysis of the Effects of Cell Stress and Cytotoxicity on<i>In Vitro</i>Assay Activity Across a Diverse Chemical and Assay Space. Toxicological Sciences, 2016, 152, 323-339.	3.1	171
9	Development and Validation of a Computational Model for Androgen Receptor Activity. Chemical Research in Toxicology, 2017, 30, 946-964.	3.3	163
10	In vitro to in vivo extrapolation for high throughput prioritization and decision making. Toxicology in Vitro, 2018, 47, 213-227.	2.4	162
11	Non-animal methods to predict skin sensitization (II): an assessment of defined approaches. Critical Reviews in Toxicology, 2018, 48, 359-374.	3.9	157
12	Toward Good Read-Across Practice (GRAP) guidance. ALTEX: Alternatives To Animal Experimentation, 2016, 33, 149-166.	1.5	134
13	Activity profiles of 309 ToxCastâ„¢ chemicals evaluated across 292 biochemical targets. Toxicology, 2011, 282, 1-15.	4.2	124
14	Non-animal methods to predict skin sensitization (I): the Cosmetics Europe database. Critical Reviews in Toxicology, 2018, 48, 344-358.	3.9	122
15	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
16	Environmental Impact on Vascular Development Predicted by High-Throughput Screening. Environmental Health Perspectives, 2011, 119, 1596-1603.	6.0	112
17	An evaluation framework for new approach methodologies (NAMs) for human health safety assessment. Regulatory Toxicology and Pharmacology, 2020, 112, 104592.	2.7	108
18	In Silico Prediction of Physicochemical Properties of Environmental Chemicals Using Molecular Fingerprints and Machine Learning. Journal of Chemical Information and Modeling, 2017, 57, 36-49.	5.4	106

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19	A Computational Model Predicting Disruption of Blood Vessel Development. PLoS Computational Biology, 2013, 9, e1002996.	3.2	104
20	Identifying developmental toxicity pathways for a subset of ToxCast chemicals using human embryonic stem cells and metabolomics. Toxicology and Applied Pharmacology, 2011, 257, 111-121.	2.8	102
21	Open-source QSAR models for pKa prediction using multiple machine learning approaches. Journal of Cheminformatics, 2019, 11, 60.	6.1	90
22	Integrated decision strategies for skin sensitization hazard. Journal of Applied Toxicology, 2016, 36, 1150-1162.	2.8	87
23	A Curated Database of Rodent Uterotrophic Bioactivity. Environmental Health Perspectives, 2016, 124, 556-562.	6.0	85
24	Pred-Skin: A Fast and Reliable Web Application to Assess Skin Sensitization Effect of Chemicals. Journal of Chemical Information and Modeling, 2017, 57, 1013-1017.	5.4	79
25	Supporting read-across using biological data. ALTEX: Alternatives To Animal Experimentation, 2016, 33, 167-182.	1.5	78
26	Disruption of embryonic vascular development in predictive toxicology. Birth Defects Research Part C: Embryo Today Reviews, 2011, 93, 312-323.	3.6	74
27	Predicting chemically-induced skin reactions. Part I: QSAR models of skin sensitization and their application to identify potentially hazardous compounds. Toxicology and Applied Pharmacology, 2015, 284, 262-272.	2.8	72
28	SAR and QSAR modeling of a large collection of LD50 rat acute oral toxicity data. Journal of Cheminformatics, 2019, 11, 58.	6.1	71
29	A <i>C. elegans</i> Screening Platform for the Rapid Assessment of Chemical Disruption of Germline Function. Environmental Health Perspectives, 2013, 121, 717-724.	6.0	68
30	In Vitro Perturbations of Targets in Cancer Hallmark Processes Predict Rodent Chemical Carcinogenesis. Toxicological Sciences, 2013, 131, 40-55.	3.1	67
31	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	6.0	63
32	Predictive models for acute oral systemic toxicity: A workshop to bridge the gap from research to regulation. Computational Toxicology, 2018, 8, 21-24.	3.3	62
33	International regulatory requirements for skin sensitization testing. Regulatory Toxicology and Pharmacology, 2018, 95, 52-65.	2.7	59
34	Multivariate models for prediction of human skin sensitization hazard. Journal of Applied Toxicology, 2017, 37, 347-360.	2.8	58
35	Status of acute systemic toxicity testing requirements and data uses by U.S. regulatory agencies. Regulatory Toxicology and Pharmacology, 2018, 94, 183-196.	2.7	58
36	Evaluation of 309 Environmental Chemicals Using a Mouse Embryonic Stem Cell Adherent Cell Differentiation and Cytotoxicity Assay. PLoS ONE, 2011, 6, e18540.	2.5	57

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37	Predicting chemically-induced skin reactions. Part II: QSAR models of skin permeability and the relationships between skin permeability and skin sensitization. Toxicology and Applied Pharmacology, 2015, 284, 273-280.	2.8	53
38	Standardisation of defined approaches for skin sensitisation testing to support regulatory use and international adoption: position of the International Cooperation on Alternative Test Methods. Archives of Toxicology, 2018, 92, 611-617.	4.2	53
39	Prediction of skin sensitization potency using machine learning approaches. Journal of Applied Toxicology, 2017, 37, 792-805.	2.8	52
40	The Key Characteristics of Carcinogens: Relationship to the Hallmarks of Cancer, Relevant Biomarkers, and Assays to Measure Them. Cancer Epidemiology Biomarkers and Prevention, 2020, 29, 1887-1903.	2.5	52
41	3S - Systematic, systemic, and systems biology and toxicology. ALTEX: Alternatives To Animal Experimentation, 2018, 35, 139-162.	1.5	50
42	Internationalization of read-across as a validated new approach method (NAM) for regulatory toxicology. ALTEX: Alternatives To Animal Experimentation, 2020, 37, 579-606.	1.5	48
43	Dosimetric Anchoring of In Vivo and In Vitro Studies for Perfluorooctanoate and Perfluorooctanesulfonate. Toxicological Sciences, 2013, 136, 308-327.	3.1	44
44	QSAR models of human data can enrich or replace LLNA testing for human skin sensitization. Green Chemistry, 2016, 18, 6501-6515.	9.0	42
45	Assessing the carcinogenic potential of low-dose exposures to chemical mixtures in the environment: focus on the cancer hallmark of tumor angiogenesis. Carcinogenesis, 2015, 36, S184-S202.	2.8	41
46	An Integrated Chemical Environment to Support 21st-Century Toxicology. Environmental Health Perspectives, 2017, 125, 054501.	6.0	41
47	Predictive Models and Computational Toxicology. Methods in Molecular Biology, 2013, 947, 343-374.	0.9	40
48	STopTox: An <i>in Silico</i> Alternative to Animal Testing for Acute Systemic and Topical Toxicity. Environmental Health Perspectives, 2022, 130, 27012.	6.0	38
49	An integrated chemical environment with tools for chemical safety testing. Toxicology in Vitro, 2020, 67, 104916.	2.4	37
50	Screening for angiogenic inhibitors in zebrafish to evaluate a predictive model for developmental vascular toxicity. Reproductive Toxicology, 2017, 70, 70-81.	2.9	36
51	Integration of Life-Stage Physiologically Based Pharmacokinetic Models with Adverse Outcome Pathways and Environmental Exposure Models to Screen for Environmental Hazards. Toxicological Sciences, 2016, 152, 230-243.	3.1	35
52	Low-Dose Mixture Hypothesis of Carcinogenesis Workshop: Scientific Underpinnings and Research Recommendations. Environmental Health Perspectives, 2017, 125, 163-169.	6.0	35
53	Large-Scale Modeling of Multispecies Acute Toxicity End Points Using Consensus of Multitask Deep Learning Methods. Journal of Chemical Information and Modeling, 2021, 61, 653-663.	5.4	35
54	IVIVE: Facilitating the Use of In Vitro Toxicity Data in Risk Assessment and Decision Making. Toxics, 2022, 10, 232.	3.7	35

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55	Pred-Skin: A Web Portal for Accurate Prediction of Human Skin Sensitizers. Chemical Research in Toxicology, 2021, 34, 258-267.	3.3	32
56	Evaluation and Optimization of Pharmacokinetic Models for <i>in Vitro</i> to <i>in Vivo</i> Extrapolation of Estrogenic Activity for Environmental Chemicals. Environmental Health Perspectives, 2018, 126, 97001.	6.0	31
57	Application of new approach methodologies: ICE tools to support chemical evaluations. Computational Toxicology, 2021, 20, 100184.	3.3	31
58	Identification of potential endocrine disrupting chemicals using gene expression biomarkers. Toxicology and Applied Pharmacology, 2019, 380, 114683.	2.8	29
59	Mice-to-men comparison of inhaled drug-aerosol deposition and clearance. Respiratory Physiology and Neurobiology, 2019, 260, 82-94.	1.6	28
60	High-Throughput Screening to Predict Chemical-Assay Interference. Scientific Reports, 2020, 10, 3986.	3.3	28
61	Workshop on the validation and regulatory acceptance of innovative 3R approaches in regulatory toxicology â€“ Evolution versus revolution. Toxicology in Vitro, 2019, 59, 1-11.	2.4	27
62	Two-Dimensional Cellular and Three-Dimensional Bio-Printed Skin Models to Screen Topical-Use Compounds for Irritation Potential. Frontiers in Bioengineering and Biotechnology, 2020, 8, 109.	4.1	26
63	Evaluation of androgen assay results using a curated Hershberger database. Reproductive Toxicology, 2018, 81, 272-280.	2.9	25
64	Systems modeling of developmental vascular toxicity. Current Opinion in Toxicology, 2019, 15, 55-63.	5.0	25
65	Immediate and long-term consequences of vascular toxicity during zebrafish development. Reproductive Toxicology, 2014, 48, 51-61.	2.9	24
66	Identifying environmental chemicals as agonists of the androgen receptor by using a quantitative high-throughput screening platform. Toxicology, 2017, 385, 48-58.	4.2	24
67	Dynamic myogenic autoregulation in the rat kidney: a whole-organ model. American Journal of Physiology - Renal Physiology, 2008, 294, F1453-F1464.	2.7	23
68	Exploring current read-across applications and needs among selected U.S. Federal Agencies. Regulatory Toxicology and Pharmacology, 2019, 106, 197-209.	2.7	23
69	Development of a curated Hershberger database. Reproductive Toxicology, 2018, 81, 259-271.	2.9	22
70	Yale School of Public Health Symposium: An overview of the challenges and opportunities associated with per- and polyfluoroalkyl substances (PFAS). Science of the Total Environment, 2021, 778, 146192.	8.0	22
71	Evaluation of Variability Across Rat Acute Oral Systemic Toxicity Studies. Toxicological Sciences, 2022, 188, 34-47.	3.1	22
72	Incorporating Biological, Chemical, and Toxicological Knowledge Into Predictive Models of Toxicity. Toxicological Sciences, 2012, 130, 440-441.	3.1	21

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73	Human-relevant approaches to assess eye corrosion/irritation potential of agrochemical formulations. Cutaneous and Ocular Toxicology, 2021, 40, 145-167.	1.3	21
74	Hierarchical Quantitative Structureâ€“Activity Relationship Modeling Approach for Integrating Binary, Multiclass, and Regression Models of Acute Oral Systemic Toxicity. Chemical Research in Toxicology, 2020, 33, 353-366.	3.3	20
75	High-Throughput Screening to Identify Chemical Cardiotoxic Potential. Chemical Research in Toxicology, 2021, 34, 566-583.	3.3	20
76	Curated Data In â€” Trustworthy <i>In Silico</i> Models Out: The Impact of Data Quality on the Reliability of Artificial Intelligence Models as Alternatives to Animal Testing. ATLA Alternatives To Laboratory Animals, 2021, 49, 73-82.	1.0	20
77	Application of Reverse Dosimetry to Compare <i>In Vitro</i> and <i>In Vivo</i> Estrogen Receptor Activity. Applied in Vitro Toxicology, 2015, 1, 33-44.	1.1	19
78	Analysis of variability in the rabbit skin irritation assay. Regulatory Toxicology and Pharmacology, 2021, 122, 104920.	2.7	18
79	Identification of vascular disruptor compounds by analysis in zebrafish embryos and mouse embryonic endothelial cells. Reproductive Toxicology, 2017, 70, 60-69.	2.9	17
80	Identification of Androgen Receptor Modulators in a Prostate Cancer Cell Line Microarray Compendium. Toxicological Sciences, 2018, 166, 146-162.	3.1	16
81	Skin sensitization testing needs and data uses by US regulatory and research agencies. Archives of Toxicology, 2019, 93, 273-291.	4.2	16
82	Exploring drug space with <i>ChemMaps.com</i>. Bioinformatics, 2018, 34, 3773-3775.	4.1	15
83	Selecting a minimal set of androgen receptor assays for screening chemicals. Regulatory Toxicology and Pharmacology, 2020, 117, 104764.	2.7	15
84	FutureTox IV Workshop Summary: <i>Predictive Toxicology for Healthy Children</i>. Toxicological Sciences, 2021, 180, 198-211.	3.1	15
85	Open source software implementation of an integrated testing strategy for skin sensitization potency based on a Bayesian network. ALTEX: Alternatives To Animal Experimentation, 2014, 31, 336-340.	1.5	15
86	New approach methods for testing chemicals for endocrine disruption potential. Current Opinion in Toxicology, 2018, 9, 40-47.	5.0	14
87	Embryonic vascular disruption adverse outcomes: Linking high throughput signaling signatures with functional consequences. Reproductive Toxicology, 2017, 70, 82-96.	2.9	13
88	A design thinking approach to primary ovarian insufficiency. Panminerva Medica, 2017, 59, 15-32.	0.8	13
89	Computational Toxicology. Chemical Research in Toxicology, 2020, 33, 687-688.	3.3	12
90	InterPred: a webtool to predict chemical autofluorescence and luminescence interference. Nucleic Acids Research, 2020, 48, W586-W590.	14.5	11

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91	Workflow for Defining Reference Chemicals for Assessing Performance of In Vitro Assays. ALTEX: Alternatives To Animal Experimentation, 2019, 36, 261-276.	1.5	11
92	Highlight report: â€˜Big data in the 3Râ€™s: outlook and recommendationsâ€™, a roundtable summary. Archives of Toxicology, 2018, 92, 1015-1020.	4.2	10
93	Introduction to Special Issue: Computational Toxicology. Chemical Research in Toxicology, 2021, 34, 171-175.	3.3	10
94	Characteristics to consider when selecting a positive control material for an in vitro assay. ALTEX: Alternatives To Animal Experimentation, 2021, 38, 365-376.	1.5	10
95	Opportunities and challenges related to saturation of toxicokinetic processes: Implications for risk assessment. Regulatory Toxicology and Pharmacology, 2021, 127, 105070.	2.7	10
96	<i>Saagar</i>â€"A New, Extensible Set of Molecular Substructures for QSAR/QSPR and Read-Across Predictions. Chemical Research in Toxicology, 2021, 34, 634-640.	3.3	8
97	High-Throughput Chemical Screening and Structure-Based Models to Predict hERG Inhibition. Biology, 2022, 11, 209.	2.8	8
98	Application of an Accessible Interface for Pharmacokinetic Modeling and In Vitro to In Vivo Extrapolation. Frontiers in Pharmacology, 2022, 13, 864742.	3.5	8
99	Novel computational models offer alternatives to animal testing for assessing eye irritation and corrosion potential of chemicals. Artificial Intelligence in the Life Sciences, 2021, 1, 100028.	2.2	7
100	Application of Defined Approaches for Skin Sensitization to Agrochemical Products. Frontiers in Toxicology, 2022, 4, 852856.	3.1	7
101	Retrospective analysis of dermal absorption triple pack data. ALTEX: Alternatives To Animal Experimentation, 2021, 38, 463-476.	1.5	6
102	Performance of the GHS Mixtures Equation for Predicting Acute Oral Toxicity. Regulatory Toxicology and Pharmacology, 2021, 125, 105007.	2.7	6
103	COVID-19 â€" prime time for microphysiological systems, as illustrated for the brain. ALTEX: Alternatives To Animal Experimentation, 2021, 38, 535-549.	1.5	6
104	Multi-laboratory Validation Study of the Vitrigel-Eye Irritancy Test Method as an Alternative to In Vivo Eye Irritation Testing. ATLA Alternatives To Laboratory Animals, 2019, 47, 140-157.	1.0	5
105	Bringing Big Data to Bear in Environmental Public Health: Challenges and Recommendations. Frontiers in Artificial Intelligence, 2020, 3, .	3.4	5
106	U.S. Federal Agency interests and key considerations for new approach methodologies for nanomaterials. ALTEX: Alternatives To Animal Experimentation, 2021, , .	1.5	5
107	Impact of High-Throughput Model Parameterization and Data Uncertainty on Thyroid-Based Toxicological Estimates for Pesticide Chemicals. Environmental Science & Technology, 2022, 56, 5620-5631.	10.0	5
108	Current ecotoxicity testing needs among selected U.S. federal agencies. Regulatory Toxicology and Pharmacology, 2022, 133, 105195.	2.7	5

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109	Identification and Profiling of Environmental Chemicals That Inhibit the TGFÎ²/SMAD Signaling Pathway. Chemical Research in Toxicology, 2019, 32, 2433-2444.	3.3	4
110	Tox21BodyMap: a webtool to map chemical effects on the human body. Nucleic Acids Research, 2020, 48, W472-W476.	14.5	4
111	Quantitative in vitro to in vivo extrapolation for developmental toxicity potency of valproic acid analogues. Birth Defects Research, 2022, 114, 1037-1055.	1.5	4
112	Towards replacement of animal tests with in vitro assays: a gene expression biomarker predicts in vitro and in vivo estrogen receptor activity. Chemico-Biological Interactions, 2022, 363, 109995.	4.0	4
113	A Vision of Toxicity Testing in the 21st Century. Applied in Vitro Toxicology, 2015, 1, 10-15.	1.1	3
114	Embryonic vascular disruption adverse outcomes: Linking high throughput signaling signatures with functional consequences. Reproductive Toxicology, 2017, 71, 16-31.	2.9	3
115	Cosmetics Europe assessment of non-animal approaches for predicting skin sensitization. Toxicology Letters, 2017, 280, S129.	0.8	1
116	Predictive modeling and computational toxicology. , 2011, , 578-591.		1
117	Mixtures-Inclusive <i>In Silico</i> Models of Ocular Toxicity Based on United States and International Hazard Categories. Chemical Research in Toxicology, 2022, 35, 992-1000.	3.3	1
118	Usefulness and Applicability of Integrated Strategy Approaches in Toxicology. Applied in Vitro Toxicology, 2021, 7, 89-90.	1.1	0