# Nicole C Kleinstreuer

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | High-Throughput Chemical Screening and Structure-Based Models to Predict hERG Inhibition. Biology, 2022, 11, 209. | 2.8 | 8 |
| 2 | STopTox: An in Silico Alternative to Animal Testing for Acute Systemic and Topical Toxicity. Environmental Health Perspectives, 2022, 130, 27012. | 6.0 | 38 |
| 3 | Evaluation of Variability Across Rat Acute Oral Systemic Toxicity Studies. Toxicological Sciences, 2022, 188, 34-47. | 3.1 | 22 |
| 4 | Application of an Accessible Interface for Pharmacokinetic Modeling and In Vitro to In Vivo Extrapolation. Frontiers in Pharmacology, 2022, 13, 864742. | 3.5 | 8 |
| 5 | 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 |
| 6 | Application of Defined Approaches for Skin Sensitization to Agrochemical Products. Frontiers in Toxicology, 2022, 4, 852856. | 3.1 | 7 |
| 7 | IVIVE: Facilitating the Use of In Vitro Toxicity Data in Risk Assessment and Decision Making. Toxics, 2022, 10, 232. | 3.7 | 35 |
| 8 | 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 |
| 9 | Mixtures-Inclusive In Silico Models of Ocular Toxicity Based on United States and International Hazard Categories. Chemical Research in Toxicology, 2022, 35, 992-1000. | 3.3 | 1 |
| 10 | Current ecotoxicity testing needs among selected U.S. federal agencies. Regulatory Toxicology and Pharmacology, 2022, 133, 105195. | 2.7 | 5 |
| 11 | 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 |
| 12 | Pred-Skin: A Web Portal for Accurate Prediction of Human Skin Sensitizers. Chemical Research in Toxicology, 2021, 34, 258-267. | 3.3 | 32 |
| 13 | High-Throughput Screening to Identify Chemical Cardiotoxic Potential. Chemical Research in Toxicology, 2021, 34, 566-583. | 3.3 | 20 |
| 14 | Retrospective analysis of dermal absorption triple pack data. ALTEX: Alternatives To Animal Experimentation, 2021, 38, 463-476. | 1.5 | 6 |
| 15 | Introduction to Special Issue: Computational Toxicology. Chemical Research in Toxicology, 2021, 34, 171-175. | 3.3 | 10 |
| 16 | FutureTox IV Workshop Summary: Predictive Toxicology for Healthy Children. Toxicological Sciences, 2021, 180, 198-211. | 3.1 | 15 |
| 17 | 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 |
| 18 | CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013. | 6.0 | 63 |

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|---|---|---|---|
| 19 | Human-relevant approaches to assess eye corrosion/irritation potential of agrochemical formulations. Cutaneous and Ocular Toxicology, 2021, 40, 145-167. | 1.3 | 21 |
| 20 | Curated Data In â€" Trustworthy In Silico 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 |
| 21 | Analysis of variability in the rabbit skin irritation assay. Regulatory Toxicology and Pharmacology, 2021, 122, 104920. | 2.7 | 18 |
| 22 | 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 |
| 23 | Usefulness and Applicability of Integrated Strategy Approaches in Toxicology. Applied in Vitro Toxicology, 2021, 7, 89-90. | 1.1 | 0 |
| 24 | Performance of the GHS Mixtures Equation for Predicting Acute Oral Toxicity. Regulatory Toxicology and Pharmacology, 2021, 125, 105007. | 2.7 | 6 |
| 25 | Application of new approach methodologies: ICE tools to support chemical evaluations. Computational Toxicology, 2021, 20, 100184. | 3.3 | 31 |
| 26 | 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 |
| 27 | Saagarâ€"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 |
| 28 | 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 |
| 29 | Opportunities and challenges related to saturation of toxicokinetic processes: Implications for risk assessment. Regulatory Toxicology and Pharmacology, 2021, 127, 105070. | 2.7 | 10 |
| 30 | U.S. Federal Agency interests and key considerations for new approach methodologies for nanomaterials. ALTEX: Alternatives To Animal Experimentation, 2021, , . | 1.5 | 5 |
| 31 | 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 |
| 32 | Selecting a minimal set of androgen receptor assays for screening chemicals. Regulatory Toxicology and Pharmacology, 2020, 117, 104764. | 2.7 | 15 |
| 33 | InterPred: a webtool to predict chemical autofluorescence and luminescence interference. Nucleic Acids Research, 2020, 48, W586-W590. | 14.5 | 11 |
| 34 | Tox21BodyMap: a webtool to map chemical effects on the human body. Nucleic Acids Research, 2020, 48, W472-W476. | 14.5 | 4 |
| 35 | Computational Toxicology. Chemical Research in Toxicology, 2020, 33, 687-688. | 3.3 | 12 |
| 36 | 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 |

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|---|---|---|---|
| 37 | High-Throughput Screening to Predict Chemical-Assay Interference. Scientific Reports, 2020, 10, 3986. | 3.3 | 28 |
| 38 | An integrated chemical environment with tools for chemical safety testing. Toxicology in Vitro, 2020, 67, 104916. | 2.4 | 37 |
| 39 | CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002. | 6.0 | 120 |
| 40 | 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 |
| 41 | An evaluation framework for new approach methodologies (NAMs) for human health safety assessment. Regulatory Toxicology and Pharmacology, 2020, 112, 104592. | 2.7 | 108 |
| 42 | 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 |
| 43 | 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 |
| 44 | Bringing Big Data to Bear in Environmental Public Health: Challenges and Recommendations. Frontiers in Artificial Intelligence, 2020, 3, . | 3.4 | 5 |
| 45 | Identification of potential endocrine disrupting chemicals using gene expression biomarkers. Toxicology and Applied Pharmacology, 2019, 380, 114683. | 2.8 | 29 |
| 46 | Identification and Profiling of Environmental Chemicals That Inhibit the TGFÎ²/SMAD Signaling Pathway. Chemical Research in Toxicology, 2019, 32, 2433-2444. | 3.3 | 4 |
| 47 | SAR and QSAR modeling of a large collection of LD50 rat acute oral toxicity data. Journal of Cheminformatics, 2019, 11, 58. | 6.1 | 71 |
| 48 | Open-source QSAR models for pKa prediction using multiple machine learning approaches. Journal of Cheminformatics, 2019, 11, 60. | 6.1 | 90 |
| 49 | Systems modeling of developmental vascular toxicity. Current Opinion in Toxicology, 2019, 15, 55-63. | 5.0 | 25 |
| 50 | Exploring current read-across applications and needs among selected U.S. Federal Agencies. Regulatory Toxicology and Pharmacology, 2019, 106, 197-209. | 2.7 | 23 |
| 51 | 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 |
| 52 | 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 |
| 53 | Chronic inflammation in the etiology of disease across the life span. Nature Medicine, 2019, 25, 1822-1832. | 30.7 | 2,195 |
| 54 | Skin sensitization testing needs and data uses by US regulatory and research agencies. Archives of Toxicology, 2019, 93, 273-291. | 4.2 | 16 |

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|---|---|---|---|
| 55 | Mice-to-men comparison of inhaled drug-aerosol deposition and clearance. Respiratory Physiology and Neurobiology, 2019, 260, 82-94. | 1.6 | 28 |
| 56 | Workflow for Defining Reference Chemicals for Assessing Performance of In Vitro Assays. ALTEX: Alternatives To Animal Experimentation, 2019, 36, 261-276. | 1.5 | 11 |
| 57 | International regulatory requirements for skin sensitization testing. Regulatory Toxicology and Pharmacology, 2018, 95, 52-65. | 2.7 | 59 |
| 58 | Non-animal methods to predict skin sensitization (I): the Cosmetics Europe database. Critical Reviews in Toxicology, 2018, 48, 344-358. | 3.9 | 122 |
| 59 | Non-animal methods to predict skin sensitization (II): an assessment of defined approaches. Critical Reviews in Toxicology, 2018, 48, 359-374. | 3.9 | 157 |
| 60 | 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 |
| 61 | 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 |
| 62 | In vitro to in vivo extrapolation for high throughput prioritization and decision making. Toxicology in Vitro, 2018, 47, 213-227. | 2.4 | 162 |
| 63 | 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 |
| 64 | New approach methods for testing chemicals for endocrine disruption potential. Current Opinion in Toxicology, 2018, 9, 40-47. | 5.0 | 14 |
| 65 | Evaluation and Optimization of Pharmacokinetic Models for in Vitro to in Vivo Extrapolation of Estrogenic Activity for Environmental Chemicals. Environmental Health Perspectives, 2018, 126, 97001. | 6.0 | 31 |
| 66 | Development of a curated Hershberger database. Reproductive Toxicology, 2018, 81, 259-271. | 2.9 | 22 |
| 67 | Evaluation of androgen assay results using a curated Hershberger database. Reproductive Toxicology, 2018, 81, 272-280. | 2.9 | 25 |
| 68 | Exploring drug space with ChemMaps.com. Bioinformatics, 2018, 34, 3773-3775. | 4.1 | 15 |
| 69 | Identification of Androgen Receptor Modulators in a Prostate Cancer Cell Line Microarray Compendium. Toxicological Sciences, 2018, 166, 146-162. | 3.1 | 16 |
| 70 | 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 |
| 71 | 3S - Systematic, systemic, and systems biology and toxicology. ALTEX: Alternatives To Animal Experimentation, 2018, 35, 139-162. | 1.5 | 50 |
| 72 | Prediction of skin sensitization potency using machine learning approaches. Journal of Applied Toxicology, 2017, 37, 792-805. | 2.8 | 52 |

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|---|---|---|---|
| 73 | Embryonic vascular disruption adverse outcomes: Linking high throughput signaling signatures with functional consequences. Reproductive Toxicology, 2017, 71, 16-31. | 2.9 | 3 |
| 74 | 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 |
| 75 | 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 |
| 76 | Embryonic vascular disruption adverse outcomes: Linking high throughput signaling signatures with functional consequences. Reproductive Toxicology, 2017, 70, 82-96. | 2.9 | 13 |
| 77 | Development and Validation of a Computational Model for Androgen Receptor Activity. Chemical Research in Toxicology, 2017, 30, 946-964. | 3.3 | 163 |
| 78 | 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 |
| 79 | Screening for angiogenic inhibitors in zebrafish to evaluate a predictive model for developmental vascular toxicity. Reproductive Toxicology, 2017, 70, 70-81. | 2.9 | 36 |
| 80 | Identification of vascular disruptor compounds by analysis in zebrafish embryos and mouse embryonic endothelial cells. Reproductive Toxicology, 2017, 70, 60-69. | 2.9 | 17 |
| 81 | Multivariate models for prediction of human skin sensitization hazard. Journal of Applied Toxicology, 2017, 37, 347-360. | 2.8 | 58 |
| 82 | Cosmetics Europe assessment of non-animal approaches for predicting skin sensitization. Toxicology Letters, 2017, 280, S129. | 0.8 | 1 |
| 83 | Low-Dose Mixture Hypothesis of Carcinogenesis Workshop: Scientific Underpinnings and Research Recommendations. Environmental Health Perspectives, 2017, 125, 163-169. | 6.0 | 35 |
| 84 | An Integrated Chemical Environment to Support 21st-Century Toxicology. Environmental Health Perspectives, 2017, 125, 054501. | 6.0 | 41 |
| 85 | A design thinking approach to primary ovarian insufficiency. Panminerva Medica, 2017, 59, 15-32. | 0.8 | 13 |
| 86 | A Curated Database of Rodent Uterotrophic Bioactivity. Environmental Health Perspectives, 2016, 124, 556-562. | 6.0 | 85 |
| 87 | Editor's Highlight: Analysis of the Effects of Cell Stress and Cytotoxicity onIn VitroAssay Activity Across a Diverse Chemical and Assay Space. Toxicological Sciences, 2016, 152, 323-339. | 3.1 | 171 |
| 88 | 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 |
| 89 | QSAR models of human data can enrich or replace LLNA testing for human skin sensitization. Green Chemistry, 2016, 18, 6501-6515. | 9.0 | 42 |
| 90 | Integrated decision strategies for skin sensitization hazard. Journal of Applied Toxicology, 2016, 36, 1150-1162. | 2.8 | 87 |

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|---|---|---|---|
| 91 | Toward Good Read-Across Practice (GRAP) guidance. ALTEX: Alternatives To Animal Experimentation, 2016, 33, 149-166. | 1.5 | 134 |
| 92 | Supporting read-across using biological data. ALTEX: Alternatives To Animal Experimentation, 2016, 33, 167-182. | 1.5 | 78 |
| 93 | A Vision of Toxicity Testing in the 21st Century. Applied in Vitro Toxicology, 2015, 1, 10-15. | 1.1 | 3 |
| 94 | Application of Reverse Dosimetry to Compare In Vitro and In Vivo Estrogen Receptor Activity. Applied in Vitro Toxicology, 2015, 1, 33-44. | 1.1 | 19 |
| 95 | 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 |
| 96 | 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 |
| 97 | Screening Chemicals for Estrogen Receptor Bioactivity Using a Computational Model. Environmental Science & Technology, 2015, 49, 8804-8814. | 10.0 | 224 |
| 98 | 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 |
| 99 | 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 |
| 100 | Phenotypic screening of the ToxCast chemical library to classify toxic and therapeutic mechanisms. Nature Biotechnology, 2014, 32, 583-591. | 17.5 | 175 |
| 101 | Immediate and long-term consequences of vascular toxicity during zebrafish development. Reproductive Toxicology, 2014, 48, 51-61. | 2.9 | 24 |
| 102 | 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 |
| 103 | Predictive Models and Computational Toxicology. Methods in Molecular Biology, 2013, 947, 343-374. | 0.9 | 40 |
| 104 | A Computational Model Predicting Disruption of Blood Vessel Development. PLoS Computational Biology, 2013, 9, e1002996. | 3.2 | 104 |
| 105 | Dosimetric Anchoring of In Vivo and In Vitro Studies for Perfluorooctanoate and Perfluorooctanesulfonate. Toxicological Sciences, 2013, 136, 308-327. | 3.1 | 44 |
| 106 | In Vitro Perturbations of Targets in Cancer Hallmark Processes Predict Rodent Chemical Carcinogenesis. Toxicological Sciences, 2013, 131, 40-55. | 3.1 | 67 |
| 107 | A C. elegans Screening Platform for the Rapid Assessment of Chemical Disruption of Germline Function. Environmental Health Perspectives, 2013, 121, 717-724. | 6.0 | 68 |
| 108 | Incorporating Biological, Chemical, and Toxicological Knowledge Into Predictive Models of Toxicity. Toxicological Sciences, 2012, 130, 440-441. | 3.1 | 21 |

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| 109 | 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 |
| 110 | Zebrafish developmental screening of the ToxCastâ„¢ Phase I chemical library. Reproductive Toxicology, 2012, 33, 174-187. | 2.9 | 267 |
| 111 | Predictive Models of Prenatal Developmental Toxicity from ToxCast High-Throughput Screening Data. Toxicological Sciences, 2011, 124, 109-127. | 3.1 | 186 |
| 112 | Environmental Impact on Vascular Development Predicted by High-Throughput Screening. Environmental Health Perspectives, 2011, 119, 1596-1603. | 6.0 | 112 |
| 113 | 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 |
| 114 | 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 |
| 115 | Disruption of embryonic vascular development in predictive toxicology. Birth Defects Research Part C: Embryo Today Reviews, 2011, 93, 312-323. | 3.6 | 74 |
| 116 | Activity profiles of 309 ToxCastâ„¢ chemicals evaluated across 292 biochemical targets. Toxicology, 2011, 282, 1-15. | 4.2 | 124 |
| 117 | Predictive modeling and computational toxicology. , 2011, , 578-591. | | 1 |
| 118 | Dynamic myogenic autoregulation in the rat kidney: a whole-organ model. American Journal of Physiology - Renal Physiology, 2008, 294, F1453-F1464. | 2.7 | 23 |