Chihae Yang

List of Publications by Year
in descending order

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55	4,372	218592	175177
papers	citations	26 h-index	52 g-index

65	65	65	4535
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010.	2.9	1,401
2	ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology. Chemical Research in Toxicology, 2016, 29, 1225-1251.	1.7	456
3	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
4	The Tox21 10K Compound Library: Collaborative Chemistry Advancing Toxicology. Chemical Research in Toxicology, 2021, 34, 189-216.	1.7	145
5	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
6	Evaluation of high-throughput genotoxicity assays used in profiling the US EPA ToxCastâ„¢ chemicals. Regulatory Toxicology and Pharmacology, 2009, 55, 188-199.	1.3	105
7	The Expanding Role of Predictive Toxicology: An Update on the (Q)SAR Models for Mutagens and Carcinogens. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2007, 25, 53-97.	2.9	103
8	Improvement of quantitative structureâ€“activity relationship (QSAR) tools for predicting Ames mutagenicity: outcomes of the Ames/QSAR International Challenge Project. Mutagenesis, 2019, 34, 3-16.	1.0	93
9	Combined Use of MC4PC, MDL-QSAR, BioEpisteme, Leadscope PDM, and Derek for Windows Software to Achieve High-Performance, High-Confidence, Mode of Actionâ€“Based Predictions of Chemical Carcinogenesis in Rodents. Toxicology Mechanisms and Methods, 2008, 18, 189-206.	1.3	77
10	Quantitative structure-skin permeability relationships. Toxicology, 2017, 387, 27-42.	2.0	69
11	Toxicity Data Informatics: Supporting a New Paradigm for Toxicity Prediction. Toxicology Mechanisms and Methods, 2008, 18, 103-118.	1.3	68
12	Identification of structure-activity relationships for adverse effects of pharmaceuticals in humans: Part B. Use of (Q)SAR systems for early detection of drug-induced hepatobiliary and urinary tract toxicities. Regulatory Toxicology and Pharmacology, 2009, 54, 23-42.	1.3	65
13	Legacy data sharing to improve drug safety assessment: the eTOX project. Nature Reviews Drug Discovery, 2017, 16, 811-812.	21.5	56
14	Novel technologies and an overall strategy to allow hazard assessment and risk prediction of chemicals, cosmetics, and drugs with animal-free methods. ALTEX: Alternatives To Animal Experimentation, 2012, 29, 373-388.	0.9	54
15	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
16	Chemical Effects in Biological Systemsâ€”Data Dictionary (CEBS-DD): A Compendium of Terms for the Capture and Integration of Biological Study Design Description, Conventional Phenotypes, and â€˜Omics Data. Toxicological Sciences, 2005, 88, 585-601.	1.4	43
17	Finding Discriminating Structural Features by Reassembling Common Building Blocks. Journal of Medicinal Chemistry, 2003, 46, 4770-4775.	2.9	38
18	Building Predictive Models for Protein Tyrosine Phosphatase 1B Inhibitors Based on Discriminating Structural Features by Reassembling Medicinal Chemistry Building Blocks. Journal of Medicinal Chemistry, 2004, 47, 5984-5994.	2.9	38

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19	A new paradigm in threshold of toxicological concern based on chemoinformatics analysis of a highly curated database enriched with antimicrobials. Food and Chemical Toxicology, 2020, 143, 111561.	1.8	38
20	The Art of Data Mining the Minefields of Toxicity Databases to Link Chemistry to Biology. Current Computer-Aided Drug Design, 2006, 2, 135-150.	0.8	34
21	Origin of the TTC values for compounds that are genotoxic and/or carcinogenic and an approach for their re-evaluation. Critical Reviews in Toxicology, 2017, 47, 710-732.	1.9	33
22	Safer chemicals using less animals: kick-off of the European ONTOX project. Toxicology, 2021, 458, 152846.	2.0	33
23	Toxicology ontology perspectives. ALTEX: Alternatives To Animal Experimentation, 2012, 29, 139-156.	0.9	33
24	Computational Toxicology Approaches at the US Food and Drug Administration. ATLA Alternatives To Laboratory Animals, 2009, 37, 523-531.	0.7	32
25	Confocal Microscopy Analysis of Supercritical Fluid Impregnation of Polypropylene. Industrial & Engineering Chemistry Research, 2002, 41, 1780-1786.	1.8	27
26	A structural feature-based computational approach for toxicology predictions. Expert Opinion on Drug Metabolism and Toxicology, 2010, 6, 505-518.	1.5	27
27	Toward a Checklist for Exchange and Interpretation of Data from a Toxicology Study. Toxicological Sciences, 2007, 99, 26-34.	1.4	24
28	Dempster-Shafer theory for combining in silico evidence and estimating uncertainty in chemical risk assessment. Computational Toxicology, 2018, 6, 16-31.	1.8	23
29	Systematic Analysis of Large Screening Sets in Drug Discovery. Current Drug Discovery Technologies, 2004, 1, 37-47.	0.6	22
30	A toxicology ontology roadmap. ALTEX: Alternatives To Animal Experimentation, 2012, 29, 129-137.	0.9	22
31	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
32	Evaluation of the applicability of existing (Q)SAR models for predicting the genotoxicity of pesticides and similarity analysis related with genotoxicity of pesticides for facilitating of grouping and read across: An EFSA funded project. Regulatory Toxicology and Pharmacology, 2020, 114, 104658.	1.3	21
33	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
34	Evaluation of the applicability of existing (Q)SAR models for predicting the genotoxicity of pesticides and similarity analysis related with genotoxicity of pesticides for facilitating of grouping and read across. EFSA Supporting Publications, 2019, 16, 1598E.	0.3	20
35	A review of in silico toxicology approaches to support the safety assessment of cosmetics-related materials. Computational Toxicology, 2022, 21, 100213.	1.8	20
36	Structural and stereochemical studies on reactive iridium(III) dihydride complexes of the triphosphine ligand C6H5P[CH2CH2CH2P(C6H11)2]2. Inorganica Chimica Acta, 1986, 114, 119-122.	1.2	16

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37	Do Similar Structures Have Similar No Observed Adverse Effect Level (NOAEL) Values? Exploring Chemoinformatics Approaches for Estimating NOAEL Bounds and Uncertainties. Chemical Research in Toxicology, 2021, 34, 616-633.	1.7	15
38	Use of computational tools in the field of food safety. Regulatory Toxicology and Pharmacology, 2011, 60, 354-362.	1.3	14
39	Comparison of Methods for Sequential Screening of Large Compound Sets. Combinatorial Chemistry and High Throughput Screening, 2006, 9, 115-122.	0.6	13
40	Adsorption-solution structure relationships of PET/POET polymeric surfactants in aqueous solutions. Polymer, 1996, 37, 4621-4627.	1.8	10
41	Development of a Battery of In Silico Prediction Tools for Drug-Induced Liver Injury from the Vantage Point of Translational Safety Assessment. Chemical Research in Toxicology, 2021, 34, 601-615.	1.7	9
42	The Consultancy Activity on In Silico Models for Genotoxic Prediction of Pharmaceutical Impurities. Methods in Molecular Biology, 2016, 1425, 511-529.	0.4	6
43	A Robust, Mechanistically Based In Silico Structural Profiler for Hepatic Cholestasis. Chemical Research in Toxicology, 2021, 34, 641-655.	1.7	6
44	Development of a New Threshold of Toxicological Concern Database of Non-cancer Toxicity Endpoints for Industrial Chemicals. Frontiers in Toxicology, 2021, 3, 626543.	1.6	6
45	Threshold of Toxicological Concernâ€"An Update for Non-Genotoxic Carcinogens. Frontiers in Toxicology, 2021, 3, 688321.	1.6	5
46	Integration of evidence to evaluate the potential for neurobehavioral effects following exposure to USFDA-approved food colors. Food and Chemical Toxicology, 2021, 151, 112097.	1.8	3
47	Mechanistic study of model monolayer membranes and their interactions with surfactants: correlation to effects on CHO cell cultures. Studies in Surface Science and Catalysis, 2001, , 435-438.	1.5	2
48	Toward better understanding of liver steatosis MoA: Molecular modelling study of PPAR gamma receptor. Toxicology Letters, 2013, 221, S85.	0.4	2
49	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
50	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
51	FDA's application of toxicological thresholds and structure activity analysis. Toxicology, 2007, 240, 130-131.	2.0	0
52	Development of integrated in silico models for toxicity prediction focussing on cosmetic ingredients. Toxicology Letters, 2013, 221, S81.	0.4	0
53	Description of the MoA/AOP linked with PPARgamma receptor dysregulation leading to liver fibrosis. Toxicology Letters, 2014, 229, S49.	0.4	0
54	Toward establishing a standardized process and tool within the read-across workflow: A case study of agrochemicals for reproductive toxicity. Toxicology Letters, 2017, 280, S285-S286.	0.4	0

#	Article	IF	Citations
55	RE: Response to the Office of Environmental Health Hazard Assessment on comments related to Gentry et al. (2021). Food and Chemical Toxicology, 2021, 152, 112202.	1.8	0