Chihae Yang

List of Publications by Year in Descending Order

51 papers	3,140 citations	24 h-index	56 g-index
65 ext. papers	3,774 ext. citations	4.8 avg, IF	4.47 L-index

#	Paper	IF	Citations
51	A review of in silico toxicology approaches to support the safety assessment of cosmetics-related materials. *Computational Toxicology*, **2022**, 21, 100213	3.1	1
50	Development of a Battery of Prediction Tools for Drug-Induced Liver Injury from the Vantage Point of Translational Safety Assessment. *Chemical Research in Toxicology*, **2021**, 34, 601-615	4	3
49	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	4
48	Integration of evidence to evaluate the potential for neurobehavioral effects following exposure to USFDA-approved food colors. *Food and Chemical Toxicology*, **2021**, 151, 112097	4.7	2
47	Safer chemicals using less animals: kick-off of the European ONTOX project. *Toxicology*, **2021**, 458, 152846	4.1	10
46	Threshold of Toxicological Concern-An Update for Non-Genotoxic Carcinogens.. *Frontiers in Toxicology*, **2021**, 3, 688321	1.6	0
45	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	4.7	
44	The Tox21 10K Compound Library: Collaborative Chemistry Advancing Toxicology. *Chemical Research in Toxicology*, **2021**, 34, 189-216	4	40
43	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	4	6
42	A Robust, Mechanistically Based Structural Profiler for Hepatic Cholestasis. *Chemical Research in Toxicology*, **2021**, 34, 641-655	4	3
41	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	4.7	13
40	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	3.4	16
39	Unlocking the potential of chemical safety assessment - A report on a cross-sector symposium on current opportunities and future challenges. *Computational Toxicology*, **2019**, 10, 38-43	3.1	16
38	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	1.1	11
37	Improvement of quantitative structure-activity relationship (QSAR) tools for predicting Ames mutagenicity: outcomes of the Ames/QSAR International Challenge Project. *Mutagenesis*, **2019**, 34, 3-16	2.8	53
36	Chemoinformatics in Modern Regulatory Science **2018**, 439-470		
35	Dempster-Shafer theory for combining in silico evidence and estimating uncertainty in chemical risk assessment. *Computational Toxicology*, **2018**, 6, 16-31	3.1	16

34	The application of molecular modelling in the safety assessment of chemicals: A case study on ligand-dependent PPAR dysregulation. *Toxicology*, **2017**, 392, 140-154	4.4	18
33	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, 705-727	5.7	27
32	Legacy data sharing to improve drug safety assessment: the eTOX project. *Nature Reviews Drug Discovery*, **2017**, 16, 811-812	64.1	37
31	Thresholds of Toxicological Concern for cosmetics-related substances: New database, thresholds, and enrichment of chemical space. *Food and Chemical Toxicology*, **2017**, 109, 170-193	4.7	64
30	Quantitative structure-skin permeability relationships. *Toxicology*, **2017**, 387, 27-42	4.4	45
29	The Consultancy Activity on In Silico Models for Genotoxic Prediction of Pharmaceutical Impurities. *Methods in Molecular Biology*, **2016**, 1425, 511-29	1.4	2
28	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, 174-86	3.4	40
27	ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology. *Chemical Research in Toxicology*, **2016**, 29, 1225-51	4	301
26	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, 510-28	6.1	114
25	QSAR modeling: where have you been? Where are you going to?. *Journal of Medicinal Chemistry*, **2014**, 57, 4977-5010	8.3	996
24	Toward better understanding of liver steatosis MoA: Molecular modelling study of PPAR gamma receptor. *Toxicology Letters*, **2013**, 221, S85	4.4	2
23	Threshold of toxicological concern (TTC) task force: a strategy to support application of TTC to dermally applied cosmetic ingredients. *Toxicology Letters*, **2013**, 221, S35	4.4	2
22	A toxicology ontology roadmap. *ALTEX: Alternatives To Animal Experimentation*, **2012**, 29, 129-37	4.3	14
21	Toxicology ontology perspectives. *ALTEX: Alternatives To Animal Experimentation*, **2012**, 29, 139-56	4.3	27
20	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, 373-88	4.3	35
19	Use of computational tools in the field of food safety. *Regulatory Toxicology and Pharmacology*, **2011**, 60, 354-62	3.4	11
18	A structural feature-based computational approach for toxicology predictions. *Expert Opinion on Drug Metabolism and Toxicology*, **2010**, 6, 505-18	5.5	25
17	Computational toxicology approaches at the US Food and Drug Administration. *ATLA Alternatives To Laboratory Animals*, **2009**, 37, 523-31	2.1	28

16	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	3.4	61
15	Evaluation of high-throughput genotoxicity assays used in profiling the US EPA ToxCast chemicals. *Regulatory Toxicology and Pharmacology*, **2009**, 55, 188-99	3.4	89
14	Combined Use of MC4PC, MDL-QSAR, BioEpisteme, Leadscope PDM, and Derek for Windows Software to Achieve High-Performance, High-Confidence, Mode of Action-Based Predictions of Chemical Carcinogenesis in Rodents. *Toxicology Mechanisms and Methods*, **2008**, 18, 189-206	3.6	73
13	Toxicity data informatics: supporting a new paradigm for toxicity prediction. *Toxicology Mechanisms and Methods*, **2008**, 18, 103-18	3.6	63
12	Toward a checklist for exchange and interpretation of data from a toxicology study. *Toxicological Sciences*, **2007**, 99, 26-34	4.4	22
11	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	4.5	92
10	Comparison of methods for sequential screening of large compound sets. *Combinatorial Chemistry and High Throughput Screening*, **2006**, 9, 115-22	1.3	10
9	The Art of Data Mining the Minefields of Toxicity Databases to Link Chemistry to Biology. *Current Computer-Aided Drug Design*, **2006**, 2, 135-150	1.4	30
8	Chemical effects in biological systems--data dictionary (CEBS-DD): a compendium of terms for the capture and integration of biological study design description, conventional phenotypes, and Tomics data. *Toxicological Sciences*, **2005**, 88, 585-601	4.4	35
7	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, 5984-94	8.3	37
6	Systematic analysis of large screening sets in drug discovery. *Current Drug Discovery Technologies*, **2004**, 1, 37-47	1.5	21
5	Finding discriminating structural features by reassembling common building blocks. *Journal of Medicinal Chemistry*, **2003**, 46, 4770-5	8.3	38
4	Confocal Microscopy Analysis of Supercritical Fluid Impregnation of Polypropylene. *Industrial & Engineering Chemistry Research*, **2002**, 41, 1780-1786	3.9	23
3	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	1.8	1
2	Adsorption-solution structure relationships of PET/POET polymeric surfactants in aqueous solutions. *Polymer*, **1996**, 37, 4621-4627	3.9	10
1	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	2.7	15