Hao Zhu

List of Publications by Year
in descending order

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93 papers	5,600 citations	66343 42 h-index	82547 72 g-index
97 all docs	97 docs citations	97 times ranked	5967 citing authors

#	Article	IF	Citations
1	Automatic Quantitative Structureâ€“Activity Relationship Modeling to Fill Data Gaps in High-Throughput Screening. Methods in Molecular Biology, 2022, 2474, 169-187.	0.9	1
2	High-Throughput Screening Assay Profiling for Large Chemical Databases. Methods in Molecular Biology, 2022, 2474, 125-132.	0.9	1
3	Replacement per- and polyfluoroalkyl substances (PFAS) are potent modulators of lipogenic and drug metabolizing gene expression signatures in primary human hepatocytes. Toxicology and Applied Pharmacology, 2022, 442, 115991.	2.8	21
4	Predicting Prenatal Developmental Toxicity Based On the Combination of Chemical Structures and Biological Data. Environmental Science & Technology, 2022, 56, 5984-5998.	10.0	11
5	Metal Azolate Coordination Polymer-Enabled High Payload and Non-Destructive Enzyme Immobilization for Biocatalysis and Biosensing. Analytical Chemistry, 2022, 94, 6827-6832.	6.5	9
6	Comparison of Linear Response Theory, Projected Initial Maximum Overlap Method, and Molecular Dynamics-Based Vibronic Spectra: The Case of Methylene Blue. Journal of Chemical Theory and Computation, 2022, 18, 3039-3051.	5.3	2
7	Mechanism-driven modeling of chemical hepatotoxicity using structural alerts and an in vitro screening assay. Journal of Hazardous Materials, 2022, 436, 129193.	12.4	18
8	Predictive modeling of estrogen receptor agonism, antagonism, and binding activities using machine- and deep-learning approaches. Laboratory Investigation, 2021, 101, 490-502.	3.7	29
9	Construction of a Virtual Opioid Bioprofile: A Data-Driven QSAR Modeling Study to Identify New Analgesic Opioids. ACS Sustainable Chemistry and Engineering, 2021, 9, 3909-3919.	6.7	17
10	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	6.0	63
11	Revealing Adverse Outcome Pathways from Public High-Throughput Screening Data to Evaluate New Toxicants by a Knowledge-Based Deep Neural Network Approach. Environmental Science & Technology, 2021, 55, 10875-10887.	10.0	29
12	Sustainable Management of Synthetic Chemicals. ACS Sustainable Chemistry and Engineering, 2021, 9, 13703-13704.	6.7	3
13	Comprehensive Interrogation on Acetylcholinesterase Inhibition by Ionic Liquids Using Machine Learning and Molecular Modeling. Environmental Science & Technology, 2021, 55, 14720-14731.	10.0	24
14	Big Data and Artificial Intelligence Modeling for Drug Discovery. Annual Review of Pharmacology and Toxicology, 2020, 60, 573-589.	9.4	209
15	FTIR spectroscopy coupled with machine learning approaches as a rapid tool for identification and quantification of artificial sweeteners. Food Chemistry, 2020, 303, 125404.	8.2	39
16	Regulation of Cell Uptake and Cytotoxicity by Nanoparticle Core under the Controlled Shape, Size, and Surface Chemistries. ACS Nano, 2020, 14, 289-302.	14.6	83
17	Regulation of Aryl Hydrocarbon Receptor Signaling Pathway and Dioxin Toxicity by Novel Agonists and Antagonists. Chemical Research in Toxicology, 2020, 33, 614-624.	3.3	6
18	Virtual Molecular Projections and Convolutional Neural Networks for the End-to-End Modeling of Nanoparticle Activities and Properties. Analytical Chemistry, 2020, 92, 13971-13979.	6.5	15

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19	Predictive Modeling of Angiotensin I-Converting Enzyme Inhibitory Peptides Using Various Machine Learning Approaches. Journal of Agricultural and Food Chemistry, 2020, 68, 12132-12140.	5.2	16
20	Prediction of Nanoâ€“Bio Interactions through Convolutional Neural Network Analysis of Nanostructure Images. ACS Sustainable Chemistry and Engineering, 2020, 8, 19096-19104.	6.7	28
21	Construction of a web-based nanomaterial database by big data curation and modeling friendly nanostructure annotations. Nature Communications, 2020, 11, 2519.	12.8	77
22	Predicting plant cuticle-water partition coefficients for organic pollutants using pp-LFER model. Science of the Total Environment, 2020, 725, 138455.	8.0	12
23	Read-across: Principle, case study and its potential regulatory application in China. Regulatory Toxicology and Pharmacology, 2020, 116, 104728.	2.7	1
24	Advancing computer-aided drug discovery (CADD) by big data and data-driven machine learning modeling. Drug Discovery Today, 2020, 25, 1624-1638.	6.4	103
25	Mechanism-Driven Read-Across of Chemical Hepatotoxicants Based on Chemical Structures and Biological Data. Toxicological Sciences, 2020, 174, 178-188.	3.1	20
26	Analysis of model PM2.5-induced inflammation and cytotoxicity by the combination of a virtual carbon nanoparticle library and computational modeling. Ecotoxicology and Environmental Safety, 2020, 191, 110216.	6.0	20
27	Mechanistic in silico modeling of bisphenols to predict estrogen and glucocorticoid disrupting potentials. Science of the Total Environment, 2020, 728, 138854.	8.0	11
28	Universal nanohydrophobicity predictions using virtual nanoparticle library. Journal of Cheminformatics, 2019, 11, 6.	6.1	14
29	Using a hybrid read-across method to evaluate chemical toxicity based on chemical structure and biological data. Ecotoxicology and Environmental Safety, 2019, 178, 178-187.	6.0	16
30	Advancing Computational Toxicology in the Big Data Era by Artificial Intelligence: Data-Driven and Mechanism-Driven Modeling for Chemical Toxicity. Chemical Research in Toxicology, 2019, 32, 536-547.	3.3	120
31	In silico profiling nanoparticles: predictive nanomodeling using universal nanodescriptors and various machine learning approaches. Nanoscale, 2019, 11, 8352-8362.	5.6	64
32	Nonanimal Models for Acute Toxicity Evaluations: Applying Data-Driven Profiling and Read-Across. Environmental Health Perspectives, 2019, 127, 47001.	6.0	56
33	Near-infrared triggered co-delivery of doxorubicin and quercetin by using gold nanocages with tetradecanol to maximize anti-tumor effects on MCF-7/ADR cells. Journal of Colloid and Interface Science, 2018, 509, 47-57.	9.4	56
34	Comparing Multiple Machine Learning Algorithms and Metrics for Estrogen Receptor Binding Prediction. Molecular Pharmaceutics, 2018, 15, 4361-4370.	4.6	120
35	CIIPro: a new read-across portal to fill data gaps using public large-scale chemical and biological data. Bioinformatics, 2017, 33, 464-466.	4.1	27
36	Alternative approaches for identifying acute systemic toxicity: Moving from research to regulatory testing. Toxicology in Vitro, 2017, 41, 245-259.	2.4	54

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37	Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment. , 2017, , 2303-2340.		13
38	Nanodiamond mediated co-delivery of doxorubicin and malaridine to maximize synergistic anti-tumor effects on multi-drug resistant MCF-7/ADR cells. Journal of Materials Chemistry B, 2017, 5, 3531-3540.	5.8	29
39	A new NIR-triggered doxorubicin and photosensitizer indocyanine green co-delivery system for enhanced multidrug resistant cancer treatment through simultaneous chemo/photothermal/photodynamic therapy. Acta Biomaterialia, 2017, 59, 170-180.	8.3	88
40	Experimental Errors in QSAR Modeling Sets: What We Can Do and What We Cannot Do. ACS Omega, 2017, 2, 2805-2812.	3.5	47
41	Elucidation of the Molecular Determinants for Optimal Perfluorooctanesulfonate Adsorption Using a Combinatorial Nanoparticle Library Approach. Environmental Science & Technology, 2017, 51, 7120-7127.	10.0	8
42	PEGylated Doxorubicin Micelles Loaded with Curcumin Exerting Synergic Effects on Multidrug Resistant Tumor Cells. Journal of Nanoscience and Nanotechnology, 2017, 17, 2873-2880.	0.9	9
43	Toward a systematic exploration of nano-bio interactions. Toxicology and Applied Pharmacology, 2017, 323, 66-73.	2.8	48
44	Predicting Nanoâ€“Bio Interactions by Integrating Nanoparticle Libraries and Quantitative Nanostructure Activity Relationship Modeling. ACS Nano, 2017, 11, 12641-12649.	14.6	80
45	From machine learning to deep learning: progress in machine intelligence for rational drug discovery. Drug Discovery Today, 2017, 22, 1680-1685.	6.4	468
46	Mechanism Profiling of Hepatotoxicity Caused by Oxidative Stress Using Antioxidant Response Element Reporter Gene Assay Models and Big Data. Environmental Health Perspectives, 2016, 124, 634-641.	6.0	56
47	Analysis of Draize eye irritation testing and its prediction by mining publicly available 2008-2014 REACH data. ALTEX: Alternatives To Animal Experimentation, 2016, 33, 123-34.	1.5	67
48	Global analysis of publicly available safety data for 9,801 substances registered under REACH from 2008-2014. ALTEX: Alternatives To Animal Experimentation, 2016, 33, 95-109.	1.5	49
49	Analysis of public oral toxicity data from REACH registrations 2008-2014. ALTEX: Alternatives To Animal Experimentation, 2016, 33, 111-22.	1.5	32
50	Predictive Modeling of Estrogen Receptor Binding Agents Using Advanced Cheminformatics Tools and Massive Public Data. Frontiers in Environmental Science, 2016, 4, .	3.3	49
51	Modulation of Carbon Nanotubes' Perturbation to the Metabolic Activity of CYP3A4 in the Liver. Advanced Functional Materials, 2016, 26, 841-850.	14.9	19
52	Carbon Nanotubes: Modulation of Carbon Nanotube's Perturbation to the Metabolic Activity of CYP3A4 in the Liver (Adv. Funct. Mater. 6/2016). Advanced Functional Materials, 2016, 26, 980-980.	14.9	0
53	Discovery of Novel Tricyclic Thiazepine Derivatives as Anti-Drug-Resistant Cancer Agents by Combining Diversity-Oriented Synthesis and Converging Screening Approach. ACS Combinatorial Science, 2016, 18, 230-235.	3.8	18
54	Accessing the High-Throughput Screening Data Landscape. Methods in Molecular Biology, 2016, 1473, 153-159.	0.9	1

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55	Curating and Preparing High-Throughput Screening Data for Quantitative Structure-Activity Relationship Modeling. Methods in Molecular Biology, 2016, 1473, 161-172.	0.9	11
56	From fighting depression to conquering tumors: a novel tricyclic thiazepine compound as a tubulin polymerization inhibitor. Cell Death and Disease, 2016, 7, e2143-e2143.	6.3	5
57	Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment. , 2016, , 1-48.		4
58	Analysis of publically available skin sensitization data from REACH registrations 2008-2014. ALTEX: Alternatives To Animal Experimentation, 2016, 33, 135-48.	1.5	43
59	Toward Good Read-Across Practice (GRAP) guidance. ALTEX: Alternatives To Animal Experimentation, 2016, 33, 149-166.	1.5	134
60	Supporting read-across using biological data. ALTEX: Alternatives To Animal Experimentation, 2016, 33, 167-182.	1.5	78
61	Experimental modulation and computational model of nano-hydrophobicity. Biomaterials, 2015, 52, 312-317.	11.4	37
62	Developing Enhanced Bloodâ€“Brain Barrier Permeability Models: Integrating External Bio-Assay Data in QSAR Modeling. Pharmaceutical Research, 2015, 32, 3055-3065.	3.5	70
63	Improving both aqueous solubility and anti-cancer activity by assessing progressive lead optimization libraries. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 1971-1975.	2.2	7
64	Profiling Animal Toxicants by Automatically Mining Public Bioassay Data: A Big Data Approach for Computational Toxicology. PLoS ONE, 2014, 9, e99863.	2.5	34
65	Tuning Cell Autophagy by Diversifying Carbon Nanotube Surface Chemistry. ACS Nano, 2014, 8, 2087-2099.	14.6	113
66	Design, synthesis and experimental validation of novel potential chemopreventive agents using random forest and support vector machine binary classifiers. Journal of Computer-Aided Molecular Design, 2014, 28, 631-646.	2.9	25
67	Critical Evaluation of Human Oral Bioavailability for Pharmaceutical Drugs by Using Various Cheminformatics Approaches. Pharmaceutical Research, 2014, 31, 1002-1014.	3.5	76
68	Big Data in Chemical Toxicity Research: The Use of High-Throughput Screening Assays To Identify Potential Toxicants. Chemical Research in Toxicology, 2014, 27, 1643-1651.	3.3	119
69	Identification of putative estrogen receptor-mediated endocrine disrupting chemicals using QSAR- and structure-based virtual screening approaches. Toxicology and Applied Pharmacology, 2013, 272, 67-76.	2.8	78
70	Human Intestinal Transporter Database: QSAR Modeling and Virtual Profiling of Drug Uptake, Efflux and Interactions. Pharmaceutical Research, 2013, 30, 996-1007.	3.5	76
71	Discovery of Novel Antimalarial Compounds Enabled by QSAR-Based Virtual Screening. Journal of Chemical Information and Modeling, 2013, 53, 475-492.	5.4	77
72	The Use of Pseudo-Equilibrium Constant Affords Improved QSAR Models of Human Plasma Protein Binding. Pharmaceutical Research, 2013, 30, 1790-1798.	3.5	43

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73	From QSAR to QSIIR: Searching for Enhanced Computational Toxicology Models. Methods in Molecular Biology, 2013, 930, 53-65.	0.9	14
74	Computers Instead of Cells: Computational Modeling of Chemical Toxicity. Issues in Toxicology, 2013, , 163-182.	0.1	1
75	Predicting Chemical Ocular Toxicity Using a Combinatorial QSAR Approach. Chemical Research in Toxicology, 2012, 25, 2763-2769.	3.3	42
76	Does Rational Selection of Training and Test Sets Improve the Outcome of QSAR Modeling?. Journal of Chemical Information and Modeling, 2012, 52, 2570-2578.	5.4	232
77	Antitumor agents 294. Novel E-ring-modified camptothecinâ€“4Î²-anilino-4â€²-O-demethyl-epipodophyllotoxin conjugates as DNA topoisomerase I inhibitors and cytotoxic agents. Bioorganic and Medicinal Chemistry, 2012, 20, 4489-4494.	3.0	9
78	Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment. , 2012, , 1309-1342.		17
79	Antitumor Agents. 284. New Desmosdumotin B Analogues with Bicyclic B-Ring as Cytotoxic and Antitubulin Agents. Journal of Medicinal Chemistry, 2011, 54, 1244-1255.	6.4	25
80	Predicting Drug-Induced Hepatotoxicity Using QSAR and Toxicogenomics Approaches. Chemical Research in Toxicology, 2011, 24, 1251-1262.	3.3	190
81	Use of in Vitro HTS-Derived Concentrationâ€“Response Data as Biological Descriptors Improves the Accuracy of QSAR Models of in Vivo Toxicity. Environmental Health Perspectives, 2011, 119, 364-370.	6.0	103
82	Anti-AIDS agents 79. Design, synthesis, molecular modeling and structureâ€“activity relationships of novel dicamphanoyl-2â€²,2â€²-dimethyldihydropyranochromone (DCP) analogs as potent anti-HIV agents. Bioorganic and Medicinal Chemistry, 2010, 18, 6678-6689.	3.0	54
83	Antitumor Agents. 280. Multidrug Resistance-Selective Desmosdumotin B Analogues. Journal of Medicinal Chemistry, 2010, 53, 6699-6705.	6.4	21
84	Modeling Liver-Related Adverse Effects of Drugs Using kNearest Neighbor Quantitative Structureâ^'Activity Relationship Method. Chemical Research in Toxicology, 2010, 23, 724-732.	3.3	104
85	A Novel Two-Step Hierarchical Quantitative Structureâ€“Activity Relationship Modeling Work Flow for Predicting Acute Toxicity of Chemicals in Rodents. Environmental Health Perspectives, 2009, 117, 1257-1264.	6.0	59
86	Quantitative Structureâ^'Activity Relationship Modeling of Rat Acute Toxicity by Oral Exposure. Chemical Research in Toxicology, 2009, 22, 1913-1921.	3.3	210
87	QSAR Modeling of the Bloodâ€“Brain Barrier Permeability for Diverse Organic Compounds. Pharmaceutical Research, 2008, 25, 1902-1914.	3.5	163
88	Combinatorial QSAR Modeling of Chemical Toxicants Tested against Tetrahymena pyriformis. Journal of Chemical Information and Modeling, 2008, 48, 766-784.	5.4	258
89	Critical Assessment of QSAR Models of Environmental Toxicity against Tetrahymena pyriformis: Focusing on Applicability Domain and Overfitting by Variable Selection. Journal of Chemical Information and Modeling, 2008, 48, 1733-1746.	5.4	350
90	Use of Cell Viability Assay Data Improves the Prediction Accuracy of Conventional Quantitative Structureâ€“Activity Relationship Models of Animal Carcinogenicity. Environmental Health Perspectives, 2008, 116, 506-513.	6.0	82

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91	Recent Methodologies for the Estimation of N-Octanol / Water Partition Coefficients and their Use in the Prediction of Membrane Transport Properties of Drugs. Mini-Reviews in Medicinal Chemistry, 2005, 5, 127-133.	2.4	73
92	ESP:â€‰ A Method To Predict Toxicity and Pharmacological Properties of Chemicals Using Multiple MCASE Databases. Journal of Chemical Information and Computer Sciences, 2004, 44, 704-715.	2.8	44
93	MCASE study of the multidrug resistance reversal activity of propafenone analogs. Journal of Computer-Aided Molecular Design, 2003, 17, 291-297.	2.9	17