

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
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97
all docs

97
docs citations

97
times ranked

5967
citing authors

#	ARTICLE	IF	CITATIONS
1	From machine learning to deep learning: progress in machine intelligence for rational drug discovery. <i>Drug Discovery Today</i> , 2017, 22, 1680-1685.	6.4	468
2	Critical Assessment of QSAR Models of Environmental Toxicity against <i>Tetrahymena pyriformis</i> : Focusing on Applicability Domain and Overfitting by Variable Selection. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 1733-1746.	5.4	350
3	Combinatorial QSAR Modeling of Chemical Toxicants Tested against <i>Tetrahymena pyriformis</i> . <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 766-784.	5.4	258
4	Does Rational Selection of Training and Test Sets Improve the Outcome of QSAR Modeling?. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 2570-2578.	5.4	232
5	Quantitative Structure-Activity Relationship Modeling of Rat Acute Toxicity by Oral Exposure. <i>Chemical Research in Toxicology</i> , 2009, 22, 1913-1921.	3.3	210
6	Big Data and Artificial Intelligence Modeling for Drug Discovery. <i>Annual Review of Pharmacology and Toxicology</i> , 2020, 60, 573-589.	9.4	209
7	Predicting Drug-Induced Hepatotoxicity Using QSAR and Toxicogenomics Approaches. <i>Chemical Research in Toxicology</i> , 2011, 24, 1251-1262.	3.3	190
8	QSAR Modeling of the Blood-Brain Barrier Permeability for Diverse Organic Compounds. <i>Pharmaceutical Research</i> , 2008, 25, 1902-1914.	3.5	163
9	Toward Good Read-Across Practice (GRAP) guidance. <i>ALTEX: Alternatives To Animal Experimentation</i> , 2016, 33, 149-166.	1.5	134
10	Comparing Multiple Machine Learning Algorithms and Metrics for Estrogen Receptor Binding Prediction. <i>Molecular Pharmaceutics</i> , 2018, 15, 4361-4370.	4.6	120
11	Advancing Computational Toxicology in the Big Data Era by Artificial Intelligence: Data-Driven and Mechanism-Driven Modeling for Chemical Toxicity. <i>Chemical Research in Toxicology</i> , 2019, 32, 536-547.	3.3	120
12	Big Data in Chemical Toxicity Research: The Use of High-Throughput Screening Assays To Identify Potential Toxicants. <i>Chemical Research in Toxicology</i> , 2014, 27, 1643-1651.	3.3	119
13	Tuning Cell Autophagy by Diversifying Carbon Nanotube Surface Chemistry. <i>ACS Nano</i> , 2014, 8, 2087-2099.	14.6	113
14	Modeling Liver-Related Adverse Effects of Drugs Using k-Nearest Neighbor Quantitative Structure-Activity Relationship Method. <i>Chemical Research in Toxicology</i> , 2010, 23, 724-732.	3.3	104
15	Use of <i>in Vitro</i> HTS-Derived Concentration-Response Data as Biological Descriptors Improves the Accuracy of QSAR Models of <i>in Vivo</i> Toxicity. <i>Environmental Health Perspectives</i> , 2011, 119, 364-370.	6.0	103
16	Advancing computer-aided drug discovery (CADD) by big data and data-driven machine learning modeling. <i>Drug Discovery Today</i> , 2020, 25, 1624-1638.	6.4	103
17	A new NIR-triggered doxorubicin and photosensitizer indocyanine green co-delivery system for enhanced multidrug resistant cancer treatment through simultaneous chemo/photothermal/photodynamic therapy. <i>Acta Biomaterialia</i> , 2017, 59, 170-180.	8.3	88
18	Regulation of Cell Uptake and Cytotoxicity by Nanoparticle Core under the Controlled Shape, Size, and Surface Chemistries. <i>ACS Nano</i> , 2020, 14, 289-302.	14.6	83

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19	Use of Cell Viability Assay Data Improves the Prediction Accuracy of Conventional Quantitative Structure–Activity Relationship Models of Animal Carcinogenicity. <i>Environmental Health Perspectives</i> , 2008, 116, 506-513.	6.0	82
20	Predicting Nano–Bio Interactions by Integrating Nanoparticle Libraries and Quantitative Nanostructure Activity Relationship Modeling. <i>ACS Nano</i> , 2017, 11, 12641-12649.	14.6	80
21	Identification of putative estrogen receptor-mediated endocrine disrupting chemicals using QSAR- and structure-based virtual screening approaches. <i>Toxicology and Applied Pharmacology</i> , 2013, 272, 67-76.	2.8	78
22	Supporting read-across using biological data. <i>ALTEX: Alternatives To Animal Experimentation</i> , 2016, 33, 167-182.	1.5	78
23	Discovery of Novel Antimalarial Compounds Enabled by QSAR-Based Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 475-492.	5.4	77
24	Construction of a web-based nanomaterial database by big data curation and modeling friendly nanostructure annotations. <i>Nature Communications</i> , 2020, 11, 2519.	12.8	77
25	Human Intestinal Transporter Database: QSAR Modeling and Virtual Profiling of Drug Uptake, Efflux and Interactions. <i>Pharmaceutical Research</i> , 2013, 30, 996-1007.	3.5	76
26	Critical Evaluation of Human Oral Bioavailability for Pharmaceutical Drugs by Using Various Cheminformatics Approaches. <i>Pharmaceutical Research</i> , 2014, 31, 1002-1014.	3.5	76
27	Recent Methodologies for the Estimation of N-Octanol / Water Partition Coefficients and their Use in the Prediction of Membrane Transport Properties of Drugs. <i>Mini-Reviews in Medicinal Chemistry</i> , 2005, 5, 127-133.	2.4	73
28	Developing Enhanced Blood–Brain Barrier Permeability Models: Integrating External Bio-Assay Data in QSAR Modeling. <i>Pharmaceutical Research</i> , 2015, 32, 3055-3065.	3.5	70
29	Analysis of Draize eye irritation testing and its prediction by mining publicly available 2008-2014 REACH data. <i>ALTEX: Alternatives To Animal Experimentation</i> , 2016, 33, 123-34.	1.5	67
30	<i>In silico</i> profiling nanoparticles: predictive nanomodeling using universal nanodescriptors and various machine learning approaches. <i>Nanoscale</i> , 2019, 11, 8352-8362.	5.6	64
31	CATMoS: Collaborative Acute Toxicity Modeling Suite. <i>Environmental Health Perspectives</i> , 2021, 129, 47013.	6.0	63
32	A Novel Two-Step Hierarchical Quantitative Structure–Activity Relationship Modeling Work Flow for Predicting Acute Toxicity of Chemicals in Rodents. <i>Environmental Health Perspectives</i> , 2009, 117, 1257-1264.	6.0	59
33	Mechanism Profiling of Hepatotoxicity Caused by Oxidative Stress Using Antioxidant Response Element Reporter Gene Assay Models and Big Data. <i>Environmental Health Perspectives</i> , 2016, 124, 634-641.	6.0	56
34	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. <i>Journal of Colloid and Interface Science</i> , 2018, 509, 47-57.	9.4	56
35	Nonanimal Models for Acute Toxicity Evaluations: Applying Data-Driven Profiling and Read-Across. <i>Environmental Health Perspectives</i> , 2019, 127, 47001.	6.0	56
36	Anti-AIDS agents 79. Design, synthesis, molecular modeling and structure–activity relationships of novel dicamphanoyl-2,2-dimethyldihydropyranochromone (DCP) analogs as potent anti-HIV agents. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 6678-6689.	3.0	54

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37	Alternative approaches for identifying acute systemic toxicity: Moving from research to regulatory testing. <i>Toxicology in Vitro</i> , 2017, 41, 245-259.	2.4	54
38	Global analysis of publicly available safety data for 9,801 substances registered under REACH from 2008-2014. <i>ALTEX: Alternatives To Animal Experimentation</i> , 2016, 33, 95-109.	1.5	49
39	Predictive Modeling of Estrogen Receptor Binding Agents Using Advanced Cheminformatics Tools and Massive Public Data. <i>Frontiers in Environmental Science</i> , 2016, 4, .	3.3	49
40	Toward a systematic exploration of nano-bio interactions. <i>Toxicology and Applied Pharmacology</i> , 2017, 323, 66-73.	2.8	48
41	Experimental Errors in QSAR Modeling Sets: What We Can Do and What We Cannot Do. <i>ACS Omega</i> , 2017, 2, 2805-2812.	3.5	47
42	ESP: A Method To Predict Toxicity and Pharmacological Properties of Chemicals Using Multiple MCASE Databases. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 704-715.	2.8	44
43	The Use of Pseudo-Equilibrium Constant Affords Improved QSAR Models of Human Plasma Protein Binding. <i>Pharmaceutical Research</i> , 2013, 30, 1790-1798.	3.5	43
44	Analysis of publicly available skin sensitization data from REACH registrations 2008-2014. <i>ALTEX: Alternatives To Animal Experimentation</i> , 2016, 33, 135-48.	1.5	43
45	Predicting Chemical Ocular Toxicity Using a Combinatorial QSAR Approach. <i>Chemical Research in Toxicology</i> , 2012, 25, 2763-2769.	3.3	42
46	FTIR spectroscopy coupled with machine learning approaches as a rapid tool for identification and quantification of artificial sweeteners. <i>Food Chemistry</i> , 2020, 303, 125404.	8.2	39
47	Experimental modulation and computational model of nano-hydrophobicity. <i>Biomaterials</i> , 2015, 52, 312-317.	11.4	37
48	Profiling Animal Toxicants by Automatically Mining Public Bioassay Data: A Big Data Approach for Computational Toxicology. <i>PLoS ONE</i> , 2014, 9, e99863.	2.5	34
49	Analysis of public oral toxicity data from REACH registrations 2008-2014. <i>ALTEX: Alternatives To Animal Experimentation</i> , 2016, 33, 111-22.	1.5	32
50	Nanodiamond mediated co-delivery of doxorubicin and malaridine to maximize synergistic anti-tumor effects on multi-drug resistant MCF-7/ADR cells. <i>Journal of Materials Chemistry B</i> , 2017, 5, 3531-3540.	5.8	29
51	Predictive modeling of estrogen receptor agonism, antagonism, and binding activities using machine- and deep-learning approaches. <i>Laboratory Investigation</i> , 2021, 101, 490-502.	3.7	29
52	Revealing Adverse Outcome Pathways from Public High-Throughput Screening Data to Evaluate New Toxicants by a Knowledge-Based Deep Neural Network Approach. <i>Environmental Science & Technology</i> , 2021, 55, 10875-10887.	10.0	29
53	Prediction of Nano-Bio Interactions through Convolutional Neural Network Analysis of Nanostructure Images. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 19096-19104.	6.7	28
54	ClIPro: a new read-across portal to fill data gaps using public large-scale chemical and biological data. <i>Bioinformatics</i> , 2017, 33, 464-466.	4.1	27

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55	Antitumor Agents. 284. New Desmosdumotin B Analogues with Bicyclic B-Ring as Cytotoxic and Antitubulin Agents. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 1244-1255.	6.4	25
56	Design, synthesis and experimental validation of novel potential chemopreventive agents using random forest and support vector machine binary classifiers. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 631-646.	2.9	25
57	Comprehensive Interrogation on Acetylcholinesterase Inhibition by Ionic Liquids Using Machine Learning and Molecular Modeling. <i>Environmental Science & Technology</i> , 2021, 55, 14720-14731.	10.0	24
58	Antitumor Agents. 280. Multidrug Resistance-Selective Desmosdumotin B Analogues. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 6699-6705.	6.4	21
59	Replacement per- and polyfluoroalkyl substances (PFAS) are potent modulators of lipogenic and drug metabolizing gene expression signatures in primary human hepatocytes. <i>Toxicology and Applied Pharmacology</i> , 2022, 442, 115991.	2.8	21
60	Mechanism-Driven Read-Across of Chemical Hepatotoxicants Based on Chemical Structures and Biological Data. <i>Toxicological Sciences</i> , 2020, 174, 178-188.	3.1	20
61	Analysis of model PM2.5-induced inflammation and cytotoxicity by the combination of a virtual carbon nanoparticle library and computational modeling. <i>Ecotoxicology and Environmental Safety</i> , 2020, 191, 110216.	6.0	20
62	Modulation of Carbon Nanotubes' Perturbation to the Metabolic Activity of CYP3A4 in the Liver. <i>Advanced Functional Materials</i> , 2016, 26, 841-850.	14.9	19
63	Discovery of Novel Tricyclic Thiazepine Derivatives as Anti-Drug-Resistant Cancer Agents by Combining Diversity-Oriented Synthesis and Converging Screening Approach. <i>ACS Combinatorial Science</i> , 2016, 18, 230-235.	3.8	18
64	Mechanism-driven modeling of chemical hepatotoxicity using structural alerts and an in vitro screening assay. <i>Journal of Hazardous Materials</i> , 2022, 436, 129193.	12.4	18
65	MCASE study of the multidrug resistance reversal activity of propafenone analogs. <i>Journal of Computer-Aided Molecular Design</i> , 2003, 17, 291-297.	2.9	17
66	Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment. , 2012, , 1309-1342.		17
67	Construction of a Virtual Opioid Bioprofile: A Data-Driven QSAR Modeling Study to Identify New Analgesic Opioids. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 3909-3919.	6.7	17
68	Using a hybrid read-across method to evaluate chemical toxicity based on chemical structure and biological data. <i>Ecotoxicology and Environmental Safety</i> , 2019, 178, 178-187.	6.0	16
69	Predictive Modeling of Angiotensin I-Converting Enzyme Inhibitory Peptides Using Various Machine Learning Approaches. <i>Journal of Agricultural and Food Chemistry</i> , 2020, 68, 12132-12140.	5.2	16
70	Virtual Molecular Projections and Convolutional Neural Networks for the End-to-End Modeling of Nanoparticle Activities and Properties. <i>Analytical Chemistry</i> , 2020, 92, 13971-13979.	6.5	15
71	From QSAR to QSIR: Searching for Enhanced Computational Toxicology Models. <i>Methods in Molecular Biology</i> , 2013, 930, 53-65.	0.9	14
72	Universal nanohydrophobicity predictions using virtual nanoparticle library. <i>Journal of Cheminformatics</i> , 2019, 11, 6.	6.1	14

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73	Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment. , 2017, , 2303-2340.		13
74	Predicting plant cuticle-water partition coefficients for organic pollutants using pp-LFER model. Science of the Total Environment, 2020, 725, 138455.	8.0	12
75	Curating and Preparing High-Throughput Screening Data for Quantitative Structure-Activity Relationship Modeling. Methods in Molecular Biology, 2016, 1473, 161-172.	0.9	11
76	Mechanistic in silico modeling of bisphenols to predict estrogen and glucocorticoid disrupting potentials. Science of the Total Environment, 2020, 728, 138854.	8.0	11
77	Predicting Prenatal Developmental Toxicity Based On the Combination of Chemical Structures and Biological Data. Environmental Science & Technology, 2022, 56, 5984-5998.	10.0	11
78	Antitumor agents 294. Novel E-ring-modified camptothecin-4'-anilino-4-O-demethyl-epipodophyllotoxin conjugates as DNA topoisomerase I inhibitors and cytotoxic agents. Bioorganic and Medicinal Chemistry, 2012, 20, 4489-4494.	3.0	9
79	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
80	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
81	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
82	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
83	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
84	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
85	Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment. , 2016, , 1-48.		4
86	Sustainable Management of Synthetic Chemicals. ACS Sustainable Chemistry and Engineering, 2021, 9, 13703-13704.	6.7	3
87	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
88	Accessing the High-Throughput Screening Data Landscape. Methods in Molecular Biology, 2016, 1473, 153-159.	0.9	1
89	Read-across: Principle, case study and its potential regulatory application in China. Regulatory Toxicology and Pharmacology, 2020, 116, 104728.	2.7	1
90	Computers Instead of Cells: Computational Modeling of Chemical Toxicity. Issues in Toxicology, 2013, , 163-182.	0.1	1

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91	Automatic Quantitative Structure-Activity Relationship Modeling to Fill Data Gaps in High-Throughput Screening. <i>Methods in Molecular Biology</i> , 2022, 2474, 169-187.	0.9	1
92	High-Throughput Screening Assay Profiling for Large Chemical Databases. <i>Methods in Molecular Biology</i> , 2022, 2474, 125-132.	0.9	1
93	Carbon Nanotubes: Modulation of Carbon Nanotube's Perturbation to the Metabolic Activity of CYP3A4 in the Liver (<i>Adv. Funct. Mater.</i> 6/2016). <i>Advanced Functional Materials</i> , 2016, 26, 980-980.	14.9	0