Hong Lin Zhai

List of Publications by Year
in descending order

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109	1,127	394286	552653
papers	citations	19 h-index	26 g-index

112	112	112	1370
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	QSAR Model Study of 2,3,4,5-tetrahydro-1H-pyrido[4,3-b]indole of Cystic- brosis-transmembrane Conductance-regulator Gene Potentiators. Letters in Drug Design and Discovery, 2022, 19, 269-278.	0.4	3
2	Rhenium nanoparticles for the delivery of HSP 90 inhibitors: A new drug delivery platform designed by molecular dynamics simulation. Journal of Molecular Liquids, 2022, 347, 117995.	2.3	4
3	Rapid Determination in the Quality Control of Chinese Patent Medicine. Journal of Pharmaceutical Innovation, 2022, 17, 1305-1313.	1.1	1
4	DNA-Templated Gold Nanoclusters for Fluorescence Resonance Energy Transfer-Based Human Serum Albumin Detection. Journal of Analytical Chemistry, 2022, 77, 216-223.	0.4	3
5	Rapid determination of trace homogeneous catalyst in chemical production. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 279, 121413.	2.0	1
6	An effective approach to the early diagnosis of colorectal cancer based on three-dimensional fluorescence spectra of human blood plasma. Journal of Pharmaceutical and Biomedical Analysis, 2021, 193, 113757.	1.4	5
7	Exploring the effect of silicene monolayer on the structure and function of villin headpiece and amyloid fibrils by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2021, 89, 107-115.	1.5	2
8	A simple approach to the determination of three curcuminoids with similar chemical structures in different substrates. Journal of Food Science and Technology, 2021, 58, 2170-2177.	1.4	0
9	Novel quantitative structureâ€“activity relationship model to predict activities of natural products against COVIDâ€19. Chemical Biology and Drug Design, 2021, 97, 978-983.	1.5	7
10	Adsorption Behaviors of Typical Proteins on BP, GR, and C2N Surfaces. Journal of Chemical Information and Modeling, 2021, 61, 1300-1306.	2.5	4
11	Selective inhibition mechanism of nitroxoline to the BET family: Insight from molecular simulations. Life Sciences, 2021, 270, 119141.	2.0	2
12	QSAR Studies on the IC50 of a Class of Thiazolidinone/Thiazolide Based Hybrids as Antitrypanosomal Agents. Letters in Drug Design and Discovery, 2021, 18, 406-415.	0.4	3
13	Study on novel PtNPâ€“sorafenib and its interaction with VEGFR2. Journal of Biochemistry, 2021, 170, 411-417.	0.9	2
14	Chemometrics-assisted simultaneous voltammetric determination of multiple neurotransmitters in human serum. Bioelectrochemistry, 2021, 139, 107739.	2.4	14
15	A simple approach to the prediction of soil sorption of organophosphorus pesticides. Journal of Environmental Science and Health - Part B Pesticides, Food Contaminants, and Agricultural Wastes, 2021, 56, 1-7.	0.7	1
16	Gold nanoclusters reversible switches based on aluminum ions-triggered for detection of pyrophosphate and acid phosphatase activity. Journal of Molecular Structure, 2021, 1242, 130755.	1.8	10
17	The activity prediction of indole inhibitors against HCV NS5B polymerase. Chemical Biology and Drug Design, 2020, 95, 240-247.	1.5	3
18	A Simple Approach to the Toxicity Prediction of Anilines and Phenols Towards Aquatic Organisms. Archives of Environmental Contamination and Toxicology, 2020, 78, 545-554.	2.1	1

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19	Study of the controversial resveratrol that interact with the endogenous glutathione thiyl radical in cancer cells. Free Radical Research, 2020, 54, 687-693.	1.5	1
20	Exploring the interactions between flawed materials and YAP65 to reveal the role of vacancy defects in MoS2 sheet nanotoxicity. Journal of Nanoparticle Research, 2020, 22, 1.	0.8	2
21	Investigating the interaction between DNA-templated gold nanoclusters and HSA via spectroscopy. New Journal of Chemistry, 2020, 44, 14060-14066.	1.4	10
22	Potential toxicity mechanism of MoS2 nanotube in the interaction between YAP65 WW domain and PRM. Colloids and Surfaces B: Biointerfaces, 2020, 196, 111317.	2.5	2
23	Novel Approach to the Analysis of Chemical Third-Order Data. Journal of Chemical Information and Modeling, 2020, 60, 4750-4756.	2.5	5
24	An effective and rapid approach to predict molecular composition of naphtha based on raw NIR spectra. Vibrational Spectroscopy, 2020, 109, 103071.	1.2	12
25	Rational design of a near-infrared fluorescence probe for highly selective sensing butyrylcholinesterase (BChE) and its bioimaging applications in living cell. Talanta, 2020, 219, 121278.	2.9	19
26	Simple and fast spectrophotometric method based on chemometrics for the measurement of multicomponent adsorption kinetics. Journal of Chemometrics, 2020, 34, e3249.	0.7	6
27	The binding mechanism of nitroreductase fluorescent probe: Active pocket deformation and intramolecular hydrogen bonds. International Journal of Biological Macromolecules, 2020, 150, 509-518.	3.6	6
28	One-pot facile synthesis of CuNCs/RGO nanocomposite for the sensitive detection of heparin in human serum samples. Talanta, 2020, 213, 120838.	2.9	10
29	Development of a facile and sensitive method for detecting alkaline phosphatase activity in serum with fluorescent gold nanoclusters based on the inner filter effect. Analyst, The, 2020, 145, 3871-3877.	1.7	19
30	Quantitative Structure-activity Relationships; Studying the Toxicity of Metal Nanoparticles. Current Topics in Medicinal Chemistry, 2020, 20, 2506-2517.	1.0	4
31	3D-QSAR and Molecular Docking Studies on Design Anti-Prostate Cancer Curcumin Analogues. Current Computer-Aided Drug Design, 2020, 16, 245-256.	0.8	9
32	Studies on the pIC50 of 4,5-Diarylisoxazole as HSP90 Inhibitors. Letters in Drug Design and Discovery, 2020, 17, 467-478.	0.4	0
33	Multi-omics integrative analysis and survival risk model construction of non-small cell lung cancer based on The Cancer Genome Atlas datasets. Oncology Letters, 2020, 20, 58.	0.8	2
34	A fast chemometrics approach to quantitative analysis of metformin hydrochloride, enalapril maleate, and captopril in tablets based on HPLC-PAD spectra. Acta Chromatographica, 2019, 31, 228-234.	0.7	4
35	Molecular mechanism study of several inhibitors binding to BRD9 bromodomain based on molecular simulations. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2970-2979.	2.0	8
36	Design of novel quinoline-aminopiperidine derivatives as Mycobacterium tuberculosis (MTB) GyrB inhibitors: an in silico study. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2913-2925.	2.0	7

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37	Study on Biocompatibility of AuNPs and Theoretical Design of a Multi-CDR-Functional Nanobody. Journal of Physical Chemistry B, 2019, 123, 7570-7577.	1.2	7
38	Applications of Discrete Shmaliy Moments on the Quantitative Analysis of Multitarget Compounds Based on the Chemical Spectra. Journal of Chemical Information and Modeling, 2019, 59, 4159-4166.	2.5	2
39	Simultaneous quantification of multiple endogenous biothiols in cancer cells based on a multi-signal fluorescent probe. Analyst, The, 2019, 144, 4575-4581.	1.7	2
40	The rapid quantitative analysis of three pesticides in cherry tomatoes and red grape samples with Tchebichef image moments. Food Chemistry, 2019, 290, 72-78.	4.2	13
41	Investigation on Adsorption Mechanism of Peptides with Surface-Modified Super-Macroporous Resins. Langmuir, 2019, 35, 4471-4480.	1.6	17
42	An effective approach to the quantitative analysis of skin-whitening agents in cosmetics with different substrates based on conventional UV-Vis determination. Analytical Methods, 2019, 11, 1500-1507.	1.3	16
43	Molecular inhibitory mechanism study on the potent inhibitor brigatinib against four crizotinibâ€resistant ALK mutations. Journal of Cellular Biochemistry, 2019, 120, 562-574.	1.2	6
44	Molecular mechanisms of tetrahydropyrrolo[1,2-c]pyrimidines as HBV capsid assembly inhibitors. Archives of Biochemistry and Biophysics, 2019, 663, 1-10.	1.4	4
45	Applying Tchebichef image moments to quantitative analysis of the components in complex samples based on raw NIR spectra. Chemometrics and Intelligent Laboratory Systems, 2018, 173, 14-20.	1.8	8
46	Tchebichef image moment approach to the prediction of protein secondary structures based on circular dichroism. Proteins: Structure, Function and Bioinformatics, 2018, 86, 751-758.	1.5	6
47	Chemical image moments and their applications. TrAC - Trends in Analytical Chemistry, 2018, 103, 119-125.	5.8	21
48	Investigations of FAK inhibitors: a combination of 3D-QSAR, docking, and molecular dynamics simulations studies. Journal of Biomolecular Structure and Dynamics, 2018, 36, 1529-1549.	2.0	22
49	The multi-resolution capability of Tchebichef moments and its applications to the analysis of fluorescence excitation-emission spectra. Methods and Applications in Fluorescence, 2018, 6, 015008.	1.1	5
50	Molecular modeling study on resistance of WT/D473H SMO to antagonists LDE-225 and LEQ-506. Pharmacological Research, 2018, 129, 491-499.	3.1	18
51	Application of image moments in MIAâ€QSAR. Journal of Chemometrics, 2018, 32, e2958.	0.7	1
52	An effective approach to quantitative analysis of ternary amino acids in foxtail millet substrate based on terahertz spectroscopy. Food Chemistry, 2018, 246, 220-227.	4.2	24
53	The common quantitative model for the determination of multiple near infrared spectrometers. Chemometrics and Intelligent Laboratory Systems, 2018, 182, 117-123.	1.8	4
54	Selective mechanisms and molecular design of 2,4 Diarylaminopyrimidines as ALK inhibitors. International Journal of Biological Macromolecules, 2018, 118, 1149-1156.	3.6	3

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55	QSAR models for predicting the toxicity of halogenated phenols to Tetrahymena. Toxicological and Environmental Chemistry, 2017, 99, 273-284.	0.6	9
56	Quality assessment of Traditional Chinese Medicine using HPLC-PAD combined with Tchebichef image moments. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2017, 1040, 8-13.	1.2	11
57	Tchebichef-Hermite image moment method: A novel tool for chemometric analysis of three-dimensional spectra. Chemometrics and Intelligent Laboratory Systems, 2017, 167, 36-43.	1.8	5
58	Simultaneous quantitative analysis of three components in mixture samples based on NIR spectra with temperature effect. Analytical Methods, 2017, 9, 2076-2081.	1.3	10
59	Quantitative structureâ€“activity relationship and molecular docking studies on designing inhibitors of the perforin. Chemical Biology and Drug Design, 2017, 90, 535-544.	1.5	3
60	Exploring the binding mechanism of Heteroaryldihydropyrimidines and Hepatitis B Virus capsid combined 3D-QSAR and molecular dynamics. Antiviral Research, 2017, 137, 151-164.	1.9	22
61	Prediction of phosphorylation sites based on Krawtchouk image moments. Proteins: Structure, Function and Bioinformatics, 2017, 85, 2231-2238.	1.5	9
62	THMGUI: A user-friendly Matlab graphical user interface of Tchebichef-Hermite moment method for handing three-dimensional landscapes. Chemometrics and Intelligent Laboratory Systems, 2017, 171, 93-101.	1.8	4
63	An approach to the simultaneous quantitative analysis of metabolites in table wines by 1H NMR self-constructed three-dimensional spectra. Food Chemistry, 2017, 216, 52-59.	4.2	25
64	QSAR Study for Carcinogenic Potency of Aromatic Amines Based on GEP and MLPs. International Journal of Environmental Research and Public Health, 2016, 13, 1141.	1.2	7
65	Insights into mechanism of pyrido[2,3-d]pyrimidines as DYRK1A inhibitors based on molecular dynamic simulations. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1108-1123.	1.5	4
66	Quantitative analysis of multiple components based on liquid chromatography with mass spectrometry in full scan mode. Journal of Separation Science, 2016, 39, 3054-3061.	1.3	12
67	Insights into DFG-in and DFG-out JAK2 binding modes for a rational strategy of type II inhibitors combined computational study. RSC Advances, 2016, 6, 45540-45552.	1.7	6
68	Krawtchouk image moment method for the simultaneous determination of three drugs in human plasma based on fluorescence three-dimensional spectra. Talanta, 2016, 161, 99-104.	2.9	19
69	Longest distance shifting: A simple and efficient approach for the alignment of shifted chromatographic peaks. Journal of Separation Science, 2016, 39, 4549-4556.	1.3	1
70	The determination of multi-components utilizing 1H NMR three-dimensional spectra combined Tchebichef moments. Chemometrics and Intelligent Laboratory Systems, 2016, 156, 128-136.	1.8	11
71	Enhancing specificity in the Janus kinases: a study on the thienopyridine JAK2 selective mechanism combined molecular dynamics simulation. Molecular BioSystems, 2016, 12, 575-587.	2.9	10
72	An efficient approach to the quantitative analysis of humic acid in water. Food Chemistry, 2016, 190, 1033-1039.	4.2	20

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73	High-performance liquid chromatography with photodiode array detection and chemometrics method for the analysis of multiple components in the traditional Chinese medicine Shuanghuanglian oral liquid. Journal of Separation Science, 2015, 38, 4187-4195.	1.3	19
74	Fast determination of four active compounds in Sanqi Panax Notoginseng Injection samples by highâ€performance liquid chromatography with a chemometric method. Journal of Separation Science, 2015, 38, 1449-1457.	1.3	17
75	Structural insights into flavones as protein kinase CK2 inhibitors derived from a combined computational study. RSC Advances, 2015, 5, 462-476.	1.7	7
76	Study on the active mechanism of Î²-secretase inhibitors by molecular simulations. European Journal of Pharmaceutical Sciences, 2015, 76, 138-148.	1.9	6
77	The application of a Tchebichef moment method to the quantitative analysis of multiple compounds based on three-dimensional HPLC fingerprint spectra. Analyst, The, 2015, 140, 630-636.	1.7	26
78	Computational study of the effects of cations and anions to the cytotoxicity of diverse ionic liquids by supervised machine learning. Chemometrics and Intelligent Laboratory Systems, 2015, 144, 138-147.	1.8	12
79	A fast and effective method of quantitative analysis of VB 1 , VB 2 and VB 6 in B-vitamins complex tablets based on three-dimensional fluorescence spectra. Journal of Food Composition and Analysis, 2015, 41, 122-128.	1.9	33
80	Predicting the ecotoxicity of ionic liquids towards Vibrio fischeri using genetic function approximation and least squares support vector machine. Journal of Hazardous Materials, 2015, 283, 591-598.	6.5	61
81	Computational studies on the binding mechanism between triazolone inhibitors and Chk1 by molecular docking and molecular dynamics. Molecular BioSystems, 2015, 11, 275-286.	2.9	7
82	3D-QSAR modeling and molecular docking study on Mer kinase inhibitors of pyridine-substituted pyrimidines. Molecular Diversity, 2015, 19, 135-147.	2.1	17
83	Molecular modeling study on the structural basis of binding mechanism of C6-substituted phthalides with monoamine oxidases. Medicinal Chemistry Research, 2014, 23, 3624-3631.	1.1	0
84	Combined molecular docking, molecular dynamics simulation and quantitative structureâ€“activity relationship study of pyrimido[1,2-c][1,3]benzothiazin-6-imine derivatives as potent anti-HIV drugs. Journal of Molecular Structure, 2014, 1067, 1-13.	1.8	7
85	Study on the agonists for the human Toll-like receptor-8 by molecular modeling. Molecular BioSystems, 2014, 10, 2202.	2.9	4
86	Studies on the inhibitory models of pyrazoline derivatives as EGFR kinase inhibitors by 3D-QSAR and molecular docking. Medicinal Chemistry Research, 2014, 23, 2869-2879.	1.1	2
87	MLRMPA: An R package of multiple linear regression model population analysis based on a cluster sampling technique for variable selection of high dimensional data. Chemometrics and Intelligent Laboratory Systems, 2014, 132, 124-132.	1.8	4
88	Study on the antagonists for the orphan G protein-coupled receptor GPR55 by quantitative structureâ€“activity relationship. Chemometrics and Intelligent Laboratory Systems, 2014, 131, 51-60.	1.8	4
89	An application of wavelet moments to the similarity analysis of three-dimensional fingerprint spectra obtained by high-performance liquid chromatography coupled with diode array detector. Food Chemistry, 2014, 145, 625-631.	4.2	25
90	A practical application of wavelet moment method on the quantitative analysis of Shuanghuanglian oral liquid based on three-dimensional fingerprint spectra. Journal of Chromatography A, 2014, 1352, 55-61.	1.8	23

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91	Rapid separation and sensitive determination of banned aromatic amines with plastic microchip electrophoresis. Journal of Hazardous Materials, 2013, 248-249, 268-275.	6.5	23
92	Study on the activity of non-purine xanthine oxidase inhibitor by 3D-QSAR modeling and molecular docking. Journal of Molecular Structure, 2013, 1051, 56-65.	1.8	15
93	A simple approach to quantitative analysis using three-dimensional spectra based on selected Zernike moments. Analyst, The, 2013, 138, 683-687.	1.7	19
94	Molecular design of new aggrecanases-2 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 5339-5350.	1.0	3
95	Quantitative Structure Activity Relationship of New 7-Oxycoumarin Derivatives as Potent and Selective Monoamine Oxidase a Inhibitors. Advanced Materials Research, 2013, 798-799, 1109-1112.	0.3	1
96	Simultaneous Quantitative Analysis of Three Compounds Using Three-Dimensional Fluorescence Spectra Based on Digital Image Techniques. Journal of Fluorescence, 2012, 22, 1013-1019.	1.3	16
97	Simple and accurate approaches to predict the activity of benzothiadiazine derivatives as HCV inhibitors. Medicinal Chemistry Research, 2012, 21, 2079-2096.	1.1	5
98	Molecular Design of Anticancer Drug Leads Based on Three-Dimensional Quantitative Structureâ€“Activity Relationship. Journal of Chemical Information and Modeling, 2011, 51, 1999-2006.	2.5	21
99	Study on the Anticancer Activity of Coumarin Derivatives by Molecular Modeling. Chemical Biology and Drug Design, 2011, 78, 651-658.	1.5	75
100	Prediction of association constants of cesium chelates based on Uniform Design Optimized Support Vector Machine. Chemometrics and Intelligent Laboratory Systems, 2011, 105, 106-113.	1.8	9
101	The analysis of core promoter sequences based on their chemical features. Chemometrics and Intelligent Laboratory Systems, 2011, 107, 245-250.	1.8	1
102	The prediction of promoter sequences based on the chemical features. Expert Systems With Applications, 2011, 38, 7881-7885.	4.4	5
103	The application of digital image recognition to the analysis of two-dimensional fingerprints. Analytica Chimica Acta, 2010, 657, 131-135.	2.6	26
104	An approach to the elimination of inter-individual variability in tumor detection. Analyst, The, 2010, 135, 875.	1.7	1
105	A new approach for the identification of important variables. Chemometrics and Intelligent Laboratory Systems, 2006, 80, 130-135.	1.8	11
106	An assisted approach of the global optimization for the experimental conditions in capillary electrophoresis. Analytica Chimica Acta, 2005, 546, 112-118.	2.6	4
107	Determination of levodopa by capillary zone electrophoresis using an acidic phosphate buffer and its application in the analysis of beans. Food Chemistry, 2005, 92, 381-386.	4.2	33
108	Study on the relationship between intake of trace elements and breast cancer mortality with chemometric methods. Computational Biology and Chemistry, 2003, 27, 581-586.	1.1	26

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109	QSAR Study of the Anti-Cancer Activity of 38 Compounds in Different Cancer Cell Lines Based on Gene Expression Programming. Advanced Materials Research, 0, 850-851, 1291-1294.	0.3	0