Li-Jiao Zhao

List of Publications by Year in descending order

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430874 434195 1,106 64 18 31 citations h-index g-index papers 64 64 64 1209 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	Determination of Pb (Lead), Cd (Cadmium), Cr (Chromium), Cu (Copper), and Ni (Nickel) in Chinese tea with high-resolution continuum source graphite furnace atomic absorption spectrometry. Journal of Food and Drug Analysis, 2016, 24, 46-55.	1.9	186
2	Tumor Energy Metabolism and Potential of 3-Bromopyruvate as an Inhibitor of Aerobic Glycolysis: Implications in Tumor Treatment. Cancers, 2019, 11, 317.	3.7	119
3	The Potential of Lonidamine in Combination with Chemotherapy and Physical Therapy in Cancer Treatment. Cancers, 2020, 12, 3332.	3.7	53
4	QSAR and Classification Study on Prediction of Acute Oral Toxicity of N-Nitroso Compounds. International Journal of Molecular Sciences, 2018, 19, 3015.	4.1	42
5	Prediction on the mutagenicity of nitroaromatic compounds using quantum chemistry descriptors based QSAR and machine learning derived classification methods. Ecotoxicology and Environmental Safety, 2019, 186, 109822.	6.0	39
6	Quantitation of Pyridyloxobutyl-DNA Adducts in Tissues of Rats Treated Chronically with $(\langle i\rangle R\langle i\rangle)$ -or $(\langle i\rangle S\langle i\rangle)$ - $\langle i\rangle R\langle i\rangle$ Research in Toxicology, 2013, 26, 1526-1535.	3.3	38
7	Quantitative Structure-Activity Relationship (QSAR) Studies on the Toxic Effects of Nitroaromatic Compounds (NACs): A Systematic Review. International Journal of Molecular Sciences, 2021, 22, 8557.	4.1	37
8	Facile access to novel 1,2,4-oxadiazinan-5-ones via [3 + 3] cycloaddition of in situ generated azaoxyallyl cations with nitrones. RSC Advances, 2017, 7, 12916-12922.	3.6	36
9	The specific role of O ⁶ -methylguanine-DNA methyltransferase inhibitors in cancer chemotherapy. Future Medicinal Chemistry, 2018, 10, 1971-1996.	2.3	33
10	In vivo toxicity of nitroaromatic compounds to rats: QSTR modelling and interspecies toxicity relationship with mouse. Journal of Hazardous Materials, 2020, 399, 122981.	12.4	31
11	Chemometric QSAR modeling of acute oral toxicity of Polycyclic Aromatic Hydrocarbons (PAHs) to rat using simple 2D descriptors and interspecies toxicity modeling with mouse. Ecotoxicology and Environmental Safety, 2021, 222, 112525.	6.0	31
12	Determination of Lead in Human Hair by High Resolution Continuum Source Graphite Furnace Atomic Absorption Spectrometry with Microwave Digestion and Solid Sampling. Analytical Letters, 2012, 45, 2467-2481.	1.8	26
13	In Silico Prediction of O6-Methylguanine-DNA Methyltransferase Inhibitory Potency of Base Analogs with QSAR and Machine Learning Methods. Molecules, 2018, 23, 2892.	3.8	26
14	3-Bromopyruvate regulates the status of glycolysis and BCNU sensitivity in human hepatocellular carcinoma cells. Biochemical Pharmacology, 2020, 177, 113988.	4.4	26
15	Underlying mechanisms of cyclic peptide inhibitors interrupting the interaction of CK2α/CK2β: comparative molecular dynamics simulation studies. Physical Chemistry Chemical Physics, 2016, 18, 9202-9210.	2.8	25
16	The potential of combi-molecules with DNA-damaging function as anticancer agents. Future Medicinal Chemistry, 2017, 9, 403-435.	2.3	24
17	Investigations on the Effect of O ⁶ -Benzylguanine on the Formation of dG-dC Interstrand Cross-Links Induced by Chloroethylnitrosoureas in Human Glioma Cells Using Stable Isotope Dilution High-Performance Liquid Chromatography Electrospray Ionization Tandem Mass Spectrometry. Chemical Research in Toxicology, 2014, 27, 1253-1262.	3.3	20
18	Synthesis and antitumor activity evaluation of a novel combi-nitrosourea prodrug: Designed to release a DNA cross-linking agent and an inhibitor of O6-alkylguanine-DNA alkyltransferase. Bioorganic and Medicinal Chemistry, 2016, 24, 2097-2107.	3.0	20

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19	1,3-Dipolar $[3 + 3]$ cycloaddition of \hat{l} ±-halohydroxamate-based azaoxyallyl cations with hydrazonoyl chloride-derived nitrile imines. RSC Advances, 2017, 7, 55106-55109.	3.6	20
20	Identification of the Structural Features of Guanine Derivatives as MGMT Inhibitors Using 3D-QSAR Modeling Combined with Molecular Docking. Molecules, 2016, 21, 823.	3.8	18
21	Systematic QSAR and iQCCR modelling of fused/non-fused aromatic hydrocarbons (FNFAHs) carcinogenicity to rodents: reducing unnecessary chemical synthesis and animal testing. Green Chemistry, 2022, 24, 5304-5319.	9.0	17
22	A density functional theory investigation on the formation mechanisms of DNA interstrand crosslinks induced by chloroethylnitrosoureas. International Journal of Quantum Chemistry, 2013, 113, 1299-1306.	2.0	15
23	Quantification of <scp>meCCNU</scp> â€induced <scp>dGâ€dC</scp> crosslinks in oligonucleotide duplexes by liquid chromatography/electrospray ionization tandem mass spectrometry. Rapid Communications in Mass Spectrometry, 2011, 25, 2027-2034.	1.5	13
24	Comparative theoretical investigation of the formation of DNA interstrand crosslinks induced by two kinds of <i>N</i> â€nitroso compounds: nitrosoureas and nitrosamines. Journal of Physical Organic Chemistry, 2012, 25, 1153-1167.	1.9	13
25	Determination of Lead, Cadmium, Copper, and Nickel in the Tonghui River of Beijing, China, by Cloud Point Extraction-High Resolution Continuum Source Graphite Furnace Atomic Absorption Spectrometry. Journal of Environmental Quality, 2013, 42, 1752-1762.	2.0	13
26	Glycolytic inhibition by 3-bromopyruvate increases the cytotoxic effects of chloroethylnitrosoureas to human glioma cells and the DNA interstrand cross-links formation. Toxicology, 2020, 435, 152413.	4.2	13
27	Determination of heavy metals in cigarettes using high-resolution continuum source graphite furnace atomic absorption spectrometry. Analytical Methods, 2017, 9, 4033-4043.	2.7	12
28	Quantification of DNA interstrand crosslinks induced by ACNU in NIH/3T3 and L1210 cells using high-performance liquid chromatography/electrospray ionization tandem mass spectrometry. Rapid Communications in Mass Spectrometry, 2014, 28, 439-447.	1.5	11
29	Synthesis and Antitumor Activity Evaluation of a Novel Combi-nitrosourea Prodrug: BGCNU. ACS Medicinal Chemistry Letters, 2017, 8, 174-178.	2.8	11
30	Construction of 2,3,4,5-tetrahydro-1,2,4-triazines via $[4+2]$ cycloaddition of \hat{l} ±-halogeno hydrazones to imines. RSC Advances, 2017, 7, 9264-9271.	3.6	11
31	Mass Spectrometric Quantitation of Pyridyloxobutyl DNA Phosphate Adducts in Rats Chronically Treated with <i>N</i> à€²-Nitrosonornicotine. Chemical Research in Toxicology, 2019, 32, 773-783.	3.3	11
32	Water Carcinogenicity and Prevalence of HPV Infection in Esophageal Cancer Patients in Huaihe River Basin, China. Gastroenterology Research and Practice, 2018, 2018, 1-8.	1.5	10
33	Metabolic Activation and Carcinogenesis of Tobacco-Specific Nitrosamine N'-Nitrosonornicotine (NNN): A Density Function Theory and Molecular Docking Study. International Journal of Environmental Research and Public Health, 2019, 16, 178.	2.6	9
34	2-Deoxy-D-glucose increases the sensitivity of glioblastoma cells to BCNU through the regulation of glycolysis, ROS and ERS pathways: In vitro and in vivo validation. Biochemical Pharmacology, 2022, 199, 115029.	4.4	9
35	AN ONIOM STUDY ON THE CROSSLINKED BASE PAIRS IN DNA REACTED WITH CHLOROETHYLNITROSOUREAS. Journal of Theoretical and Computational Chemistry, 2007, 06, 631-639.	1.8	8
36	NBGNU: a hypoxia-activated tripartite combi-nitrosourea prodrug overcoming AGT-mediated chemoresistance. Future Medicinal Chemistry, 2019, 11, 269-284.	2.3	8

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37	Identification and Biological Evaluation of CK2 Allosteric Fragments through Structure-Based Virtual Screening. Molecules, 2020, 25, 237.	3.8	8
38	Comparative investigation of the DNA inter-strand crosslinks induced by ACNU, BCNU, CCNU and FTMS using high-performance liquid chromatography–electrospray ionization tandem mass spectrometry. International Journal of Mass Spectrometry, 2014, 368, 30-36.	1.5	7
39	Measurement of O 6 -alkylguanine-DNA alkyltransferase activity in tumour cells using stable isotope dilution HPLC-ESIâ¿¿MS/MS. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2016, 1033-1034, 138-146.	2.3	7
40	Influence of the Expression Level of O6-Alkylguanine-DNA Alkyltransferase on the Formation of DNA Interstrand Crosslinks Induced by Chloroethylnitrosoureas in Cells: A Quantitation Using High-Performance Liquid Chromatography-Mass Spectrometry. PLoS ONE, 2015, 10, e0121225.	2.5	6
41	Reductive Activity and Mechanism of Hypoxia-Targeted AGT Inhibitors: An Experimental and Theoretical Investigation. International Journal of Molecular Sciences, 2019, 20, 6308.	4.1	5
42	Structureâ€based Discovery of Novel CK2αâ€Binding Cyclic Peptides with Antiâ€cancer Activity. Molecular Informatics, 2019, 38, e1800089.	2.5	5
43	Development of the C12Im-Cl-assisted method for rapid sample preparation in proteomic application. Analytical Methods, 2021, 13, 776-781.	2.7	5
44	Development and biological evaluation of AzoBGNU: A novel hypoxia-activated DNA crosslinking prodrug with AGT-inhibitory activity. Biomedicine and Pharmacotherapy, 2021, 144, 112338.	5.6	5
45	Machine Learning Models for the Classification of CK2 Natural Products Inhibitors with Molecular Fingerprint Descriptors. Processes, 2021, 9, 2074.	2.8	5
46	Relationship between the molecular structure and the anticancer activity of ⟨i>N⟨ i>â€(2â€chloroethyl)â€ <i>N⟨ i>′â€cyclohexylâ€<i>N⟨ i>â€nitrosoureas: A theoretical investigation. International Journal of Quantum Chemistry, 2012, 112, 747-758.</i></i>	2.0	4
47	Structure-based identification of novel CK2 inhibitors with a linear 2-propenone scaffold as anti-cancer agents. Biochemical and Biophysical Research Communications, 2019, 512, 208-212.	2.1	4
48	Exploring the Pivotal Role of the CK2 Hinge Region Sub-Pocket in Binding with Tricyclic Quinolone Analogues by Computational Analysis. Molecules, 2017, 22, 840.	3.8	3
49	Synergistic Effect between Human Papillomavirus 18 and 4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanone on Malignant Transformation of Immortalized SHEE Cells. Chemical Research in Toxicology, 2020, 33, 470-481.	3.3	3
50	Insights into the Impact of Linker Flexibility and Fragment Ionization on the Design of CK2 Allosteric Inhibitors: Comparative Molecular Dynamics Simulation Studies. International Journal of Molecular Sciences, 2018, 19, 111.	4.1	2
51	Chemopreventive Role of Apigenin against the Synergistic Carcinogenesis of Human Papillomavirus and 4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanone. Biomedicines, 2020, 8, 472.	3.2	2
52	DFT studies on the quantitative structure-activity relationship of N-(2-chloroethyl)-N& $\#x2032$;-cyclohexyl-N-nitrosoureas as anticancer agents., 2010 ,,.		1
53	The mechanism of DNA alkylation by the β-electrophilic center of nitrosamines and nitrosoureas: a theoretical study., 2007,,.		0
54	Quantitative Structure-Activity Relationship Analysis of the Anticancer Activity of Chloroethylnitrosourea Derivatives., 2007,,.		0

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55	ONIOM Study on the DNA Interstrand Crosslinks by the Chloroethylnitrosoureas. , 2007, , .		0
56	Ab initio Researches on the Mechanism of DNA Alkylation by Nitrosamines. , 2007, , .		0
57	A Theoretical Study on the Critical Difference between the Mechanism of DNA Alkylation by Nitrosamines and Nitrosoureas. , 2008, , .		0
58	Ab initio Studies on the Carcinogenic Mechanism of the Derivatives of 3,5-Dimethyl-Nitrosopiperazine. , 2008, , .		0
59	Study on N-Nitrosoureas by Electron Spray Ionization Mass Spectrometry. , 2008, , .		0
60	Agarose Gel Electrophoresis and Fluorometric Assays for the Determination of DNA Cross-Linking Induced by Semustine. , 2008, , .		0
61	HPLC-ESI-MS/MS Research on DNA Interstrand Cross-Links Formed by 1,3-Bis-(2-Chloroethyl)-1-Nitrosourea. , 2009, , .		0
62	Quantitative Analysis of DNA Interstrand Crosslink Induced by Chloroethylnitrosoureas with Real-Time Fluorometric Assay. International Conference on Bioinformatics and Biomedical Engineering: [proceedings] International Conference on Bioinformatics and Biomedical Engineering, 2010, , .	0.0	0
63	Structural Characterization of the DNA Adducts Induced by 1,3-Bis-(2-Chloroethyl)-1-Nitrosourea Using Electrospray Ionization Tandem Mass Spectrometry. International Conference on Bioinformatics and Biomedical Engineering: [proceedings] International Conference on Bioinformatics and Biomedical Engineering, 2010	0.0	0
64	Identification of Pharmacophoric Fragments of DYRK1A Inhibitors Using Machine Learning Classification Models. Molecules, 2022, 27, 1753.	3.8	0