

Li-Jiao Zhao

List of Publications by Year in descending order

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64
papers

1,106
citations

430874

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434195

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64
docs citations

64
times ranked

1209
citing authors

#	ARTICLE	IF	CITATIONS
1	Identification of Pharmacophoric Fragments of DYRK1A Inhibitors Using Machine Learning Classification Models. <i>Molecules</i> , 2022, 27, 1753.	3.8	0
2	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. <i>Biochemical Pharmacology</i> , 2022, 199, 115029.	4.4	9
3	Systematic QSAR and iQCCR modelling of fused/non-fused aromatic hydrocarbons (FNFAHs) carcinogenicity to rodents: reducing unnecessary chemical synthesis and animal testing. <i>Green Chemistry</i> , 2022, 24, 5304-5319.	9.0	17
4	Development of the C12Im-Cl-assisted method for rapid sample preparation in proteomic application. <i>Analytical Methods</i> , 2021, 13, 776-781.	2.7	5
5	Quantitative Structure-Activity Relationship (QSAR) Studies on the Toxic Effects of Nitroaromatic Compounds (NACs): A Systematic Review. <i>International Journal of Molecular Sciences</i> , 2021, 22, 8557.	4.1	37
6	Chemometric QSAR modeling of acute oral toxicity of Polycyclic Aromatic Hydrocarbons (PAHs) to rat using simple 2D descriptors and interspecies toxicity modeling with mouse. <i>Ecotoxicology and Environmental Safety</i> , 2021, 222, 112525.	6.0	31
7	Development and biological evaluation of AzoBCNU: A novel hypoxia-activated DNA crosslinking prodrug with AGT-inhibitory activity. <i>Biomedicine and Pharmacotherapy</i> , 2021, 144, 112338.	5.6	5
8	Machine Learning Models for the Classification of CK2 Natural Products Inhibitors with Molecular Fingerprint Descriptors. <i>Processes</i> , 2021, 9, 2074.	2.8	5
9	The Potential of Lonidamine in Combination with Chemotherapy and Physical Therapy in Cancer Treatment. <i>Cancers</i> , 2020, 12, 3332.	3.7	53
10	Chemopreventive Role of Apigenin against the Synergistic Carcinogenesis of Human Papillomavirus and 4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanone. <i>Biomedicines</i> , 2020, 8, 472.	3.2	2
11	In vivo toxicity of nitroaromatic compounds to rats: QSTR modelling and interspecies toxicity relationship with mouse. <i>Journal of Hazardous Materials</i> , 2020, 399, 122981.	12.4	31
12	Glycolytic inhibition by 3-bromopyruvate increases the cytotoxic effects of chloroethylnitrosoureas to human glioma cells and the DNA interstrand cross-links formation. <i>Toxicology</i> , 2020, 435, 152413.	4.2	13
13	Synergistic Effect between Human Papillomavirus 18 and 4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanone on Malignant Transformation of Immortalized SHEE Cells. <i>Chemical Research in Toxicology</i> , 2020, 33, 470-481.	3.3	3
14	Identification and Biological Evaluation of CK2 Allosteric Fragments through Structure-Based Virtual Screening. <i>Molecules</i> , 2020, 25, 237.	3.8	8
15	3-Bromopyruvate regulates the status of glycolysis and BCNU sensitivity in human hepatocellular carcinoma cells. <i>Biochemical Pharmacology</i> , 2020, 177, 113988.	4.4	26
16	Prediction on the mutagenicity of nitroaromatic compounds using quantum chemistry descriptors based QSAR and machine learning derived classification methods. <i>Ecotoxicology and Environmental Safety</i> , 2019, 186, 109822.	6.0	39
17	Tumor Energy Metabolism and Potential of 3-Bromopyruvate as an Inhibitor of Aerobic Glycolysis: Implications in Tumor Treatment. <i>Cancers</i> , 2019, 11, 317.	3.7	119
18	Structure-based identification of novel CK2 inhibitors with a linear 2-propenone scaffold as anti-cancer agents. <i>Biochemical and Biophysical Research Communications</i> , 2019, 512, 208-212.	2.1	4

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19	Mass Spectrometric Quantitation of Pyridyloxobutyl DNA Phosphate Adducts in Rats Chronically Treated with <i>N</i> -Nitrosornicotine. <i>Chemical Research in Toxicology</i> , 2019, 32, 773-783.	3.3	11
20	Reductive Activity and Mechanism of Hypoxia- Targeted AGT Inhibitors: An Experimental and Theoretical Investigation. <i>International Journal of Molecular Sciences</i> , 2019, 20, 6308.	4.1	5
21	NBGNU: a hypoxia-activated tripartite combi-nitrosourea prodrug overcoming AGT-mediated chemoresistance. <i>Future Medicinal Chemistry</i> , 2019, 11, 269-284.	2.3	8
22	Metabolic Activation and Carcinogenesis of Tobacco-Specific Nitrosamine <i>N</i> -Nitrosornicotine (NNN): A Density Function Theory and Molecular Docking Study. <i>International Journal of Environmental Research and Public Health</i> , 2019, 16, 178.	2.6	9
23	Structure-based Discovery of Novel CK2-binding Cyclic Peptides with Anti-cancer Activity. <i>Molecular Informatics</i> , 2019, 38, e1800089.	2.5	5
24	In Silico Prediction of O6-Methylguanine-DNA Methyltransferase Inhibitory Potency of Base Analogs with QSAR and Machine Learning Methods. <i>Molecules</i> , 2018, 23, 2892.	3.8	26
25	QSAR and Classification Study on Prediction of Acute Oral Toxicity of N-Nitroso Compounds. <i>International Journal of Molecular Sciences</i> , 2018, 19, 3015.	4.1	42
26	Water Carcinogenicity and Prevalence of HPV Infection in Esophageal Cancer Patients in Huaihe River Basin, China. <i>Gastroenterology Research and Practice</i> , 2018, 2018, 1-8.	1.5	10
27	Insights into the Impact of Linker Flexibility and Fragment Ionization on the Design of CK2 Allosteric Inhibitors: Comparative Molecular Dynamics Simulation Studies. <i>International Journal of Molecular Sciences</i> , 2018, 19, 111.	4.1	2
28	The specific role of O ⁶ -methylguanine-DNA methyltransferase inhibitors in cancer chemotherapy. <i>Future Medicinal Chemistry</i> , 2018, 10, 1971-1996.	2.3	33
29	Synthesis and Antitumor Activity Evaluation of a Novel Combi-nitrosourea Prodrug: BGCNU. <i>ACS Medicinal Chemistry Letters</i> , 2017, 8, 174-178.	2.8	11
30	Facile access to novel 1,2,4-oxadiazinan-5-ones via [3 + 3] cycloaddition of in situ generated azaoxyallyl cations with nitrones. <i>RSC Advances</i> , 2017, 7, 12916-12922.	3.6	36
31	Construction of 2,3,4,5-tetrahydro-1,2,4-triazines via [4 + 2] cycloaddition of α -halogeno hydrazones to imines. <i>RSC Advances</i> , 2017, 7, 9264-9271.	3.6	11
32	The potential of combi-molecules with DNA-damaging function as anticancer agents. <i>Future Medicinal Chemistry</i> , 2017, 9, 403-435.	2.3	24
33	Determination of heavy metals in cigarettes using high-resolution continuum source graphite furnace atomic absorption spectrometry. <i>Analytical Methods</i> , 2017, 9, 4033-4043.	2.7	12
34	1,3-Dipolar [3 + 3] cycloaddition of α -halohydroxamate-based azaoxyallyl cations with hydrazoneyl chloride-derived nitrile imines. <i>RSC Advances</i> , 2017, 7, 55106-55109.	3.6	20
35	Exploring the Pivotal Role of the CK2 Hinge Region Sub-Pocket in Binding with Tricyclic Quinolone Analogues by Computational Analysis. <i>Molecules</i> , 2017, 22, 840.	3.8	3
36	Identification of the Structural Features of Guanine Derivatives as MGMT Inhibitors Using 3D-QSAR Modeling Combined with Molecular Docking. <i>Molecules</i> , 2016, 21, 823.	3.8	18

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37	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. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 2097-2107.	3.0	20
38	Measurement of O ⁶ -alkylguanine-DNA alkyltransferase activity in tumour cells using stable isotope dilution HPLC-ESI-MS/MS. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , 2016, 1033-1034, 138-146.	2.3	7
39	Underlying mechanisms of cyclic peptide inhibitors interrupting the interaction of CK2 [±] /CK2 ² : comparative molecular dynamics simulation studies. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 9202-9210.	2.8	25
40	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. <i>Journal of Food and Drug Analysis</i> , 2016, 24, 46-55.	1.9	186
41	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. <i>PLoS ONE</i> , 2015, 10, e0121225.	2.5	6
42	Quantification of DNA interstrand crosslinks induced by ACNU in NIH/3T3 and L1210 cells using high-performance liquid chromatography/electrospray ionization tandem mass spectrometry. <i>Rapid Communications in Mass Spectrometry</i> , 2014, 28, 439-447.	1.5	11
43	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. <i>International Journal of Mass Spectrometry</i> , 2014, 368, 30-36.	1.5	7
44	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. <i>Chemical Research in Toxicology</i> , 2014, 27, 1253-1262.	3.3	20
45	A density functional theory investigation on the formation mechanisms of DNA interstrand crosslinks induced by chloroethylnitrosoureas. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1299-1306.	2.0	15
46	Quantitation of Pyridyloxobutyl-DNA Adducts in Tissues of Rats Treated Chronically with (R)- or (S)-N-(2-chloroethyl)-N-cyclohexyl-N-nitrosourea (NNN) in a Carcinogenicity Study. <i>Chemical Research in Toxicology</i> , 2013, 26, 1526-1535.	3.3	38
47	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. <i>Journal of Environmental Quality</i> , 2013, 42, 1752-1762.	2.0	13
48	Determination of Lead in Human Hair by High Resolution Continuum Source Graphite Furnace Atomic Absorption Spectrometry with Microwave Digestion and Solid Sampling. <i>Analytical Letters</i> , 2012, 45, 2467-2481.	1.8	26
49	Relationship between the molecular structure and the anticancer activity of N-(2-chloroethyl)-N-cyclohexyl-N-nitrosoureas: A theoretical investigation. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 747-758.	2.0	4
50	Comparative theoretical investigation of the formation of DNA interstrand crosslinks induced by two kinds of N-nitroso compounds: nitrosoureas and nitrosamines. <i>Journal of Physical Organic Chemistry</i> , 2012, 25, 1153-1167.	1.9	13
51	Quantification of CCNU-induced dG-dC crosslinks in oligonucleotide duplexes by liquid chromatography/electrospray ionization tandem mass spectrometry. <i>Rapid Communications in Mass Spectrometry</i> , 2011, 25, 2027-2034.	1.5	13
52	Quantitative Analysis of DNA Interstrand Crosslink Induced by Chloroethylnitrosoureas with Real-Time Fluorometric Assay. <i>International Conference on Bioinformatics and Biomedical Engineering: [proceedings] International Conference on Bioinformatics and Biomedical Engineering, 2010, . . .</i>	0.0	0
53	Structural Characterization of the DNA Adducts Induced by 1,3-Bis-(2-Chloroethyl)-1-Nitrosourea Using Electrospray Ionization Tandem Mass Spectrometry. <i>International Conference on Bioinformatics and Biomedical Engineering: [proceedings] International Conference on Bioinformatics and Biomedical Engineering, 2010, . . .</i>	0.0	0
54	DFT studies on the quantitative structure-activity relationship of N-(2-chloroethyl)-N-cyclohexyl-N-nitrosoureas as anticancer agents. , 2010, , .		1

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55	HPLC-ESI-MS/MS Research on DNA Interstrand Cross-Links Formed by 1,3-Bis-(2-Chloroethyl)-1-Nitrosourea. , 2009, , .		0
56	A Theoretical Study on the Critical Difference between the Mechanism of DNA Alkylation by Nitrosamines and Nitrosoureas. , 2008, , .		0
57	Ab initio Studies on the Carcinogenic Mechanism of the Derivatives of 3,5-Dimethyl-Nitrosopiperazine. , 2008, , .		0
58	Study on N-Nitrosoureas by Electron Spray Ionization Mass Spectrometry. , 2008, , .		0
59	Agarose Gel Electrophoresis and Fluorometric Assays for the Determination of DNA Cross-Linking Induced by Semustine. , 2008, , .		0
60	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
61	The mechanism of DNA alkylation by the α -electrophilic center of nitrosamines and nitrosoureas: a theoretical study. , 2007, , .		0
62	Quantitative Structure-Activity Relationship Analysis of the Anticancer Activity of Chloroethylnitrosourea Derivatives. , 2007, , .		0
63	ONIOM Study on the DNA Interstrand Crosslinks by the Chloroethylnitrosoureas. , 2007, , .		0
64	Ab initio Researches on the Mechanism of DNA Alkylation by Nitrosamines. , 2007, , .		0