Wei-Liang Zhu

List of Publications by Year
in descending order

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153	6,087	87723 38	88477 70
papers	citations	h-index	g-index

167	167	167	7691
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Halogen Bondingâ€"A Novel Interaction for Rational Drug Design?. Journal of Medicinal Chemistry, 2009, 52, 2854-2862.	2.9	524
2	Nonbonding interactions of organic halogens in biological systems: implications for drug discovery and biomolecular design. Physical Chemistry Chemical Physics, 2010, 12, 4543.	1.3	338
3	Halogen Bond: Its Role beyond Drugâ€"Target Binding Affinity for Drug Discovery and Development. Journal of Chemical Information and Modeling, 2014, 54, 69-78.	2.5	287
4	Halogen bonding for rational drug design and new drug discovery. Expert Opinion on Drug Discovery, 2012, 7, 375-383.	2.5	249
5	Conformational transition of amyloid Â-peptide. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 5403-5407.	3.3	238
6	Advances in the study of berberine and its derivatives: a focus on anti-inflammatory and anti-tumor effects in the digestive system. Acta Pharmacologica Sinica, 2017, 38, 157-167.	2.8	236
7	SARS-CoV-2 Omicron RBD shows weaker binding affinity than the currently dominant Delta variant to human ACE2. Signal Transduction and Targeted Therapy, 2022, 7, 8.	7.1	178
8	Redoxâ€Neutral Rhodiumâ€Catalyzed Cï£¿H Functionalization of Arylamine Nâ€Oxides with Diazo Compounds: Primary C(sp³)ï£¿H/C(sp²)ï£¿H Activation and Oxygenâ€Atom Transfer. Angewandte Chemie - International Edition, 2015, 54, 12121-12126.	7.2	126
9	Rh(III)-Catalyzed Redox-Neutral Unsymmetrical Câ€"H Alkylation and Amidation Reactions of N-Phenoxyacetamides. Journal of the American Chemical Society, 2018, 140, 42-45.	6.6	120
10	How Does Halogen Bonding Behave in Solution? A Theoretical Study Using Implicit Solvation Model. Journal of Physical Chemistry A, 2011, 115, 4467-4475.	1.1	116
11	Utilization of Halogen Bond in Lead Optimization: A Case Study of Rational Design of Potent Phosphodiesterase Type 5 (PDE5) Inhibitors. Journal of Medicinal Chemistry, 2011, 54, 5607-5611.	2.9	108
12	Differentiation of Cationâ^Ï€ Bonding from Cationâ^Ï€ Intermolecular Interactions:Â A Quantum Chemistry Study Using Density-Functional Theory and Morokuma Decomposition Methods. Journal of Physical Chemistry A, 2003, 107, 2296-2303.	1.1	82
13	The Multiplicity, Strength, and Nature of the Interaction of Nucleobases with Alkaline and Alkaline Earth Metal Cations:Â A Density Functional Theory Investigation. Journal of Physical Chemistry A, 2004, 108, 4008-4018.	1.1	82
14	Energetic Effects between Halogen Bonds and Anion-Ï€ or Lone Pair-Ï€ Interactions: A Theoretical Study. Journal of Physical Chemistry A, 2012, 116, 2591-2597.	1.1	77
15	A computational analysis of binding modes and conformation changes of MDM2 induced by p53 and inhibitor bindings. Journal of Computer-Aided Molecular Design, 2013, 27, 965-974.	1.3	70
16	Quantum/Classical Mechanical Comparison of Cationâ^Ï€ Interactions between Tetramethylammonium and Benzene. Journal of Physical Chemistry A, 2001, 105, 1326-1333.	1.1	69
17	How Does Ammonium Interact with Aromatic Groups? A Density Functional Theory (DFT/B3LYP) Investigation. Journal of Physical Chemistry A, 2000, 104, 9573-9580.	1.1	68
18	Molecular Mechanism of Binding Selectivity of Inhibitors toward BACE1 and BACE2 Revealed by Multiple Short Molecular Dynamics Simulations and Free-Energy Predictions. ACS Chemical Neuroscience, 2019, 10, 4303-4318.	1.7	68

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19	Xishacorenes Aâ€“C, Diterpenes with Bicyclo[3.3.1]nonane Nucleus from the Xisha Soft Coral Sinularia polydactyla. Organic Letters, 2017, 19, 4183-4186.	2.4	67
20	D3Targets-2019-nCoV: a webserver for predicting drug targets and for multi-target and multi-site based virtual screening against COVID-19. Acta Pharmaceutica Sinica B, 2020, 10, 1239-1248.	5.7	65
21	Molecular docking and 3-D-QSAR studies on the possible antimalarial mechanism of artemisinin analogues. Bioorganic and Medicinal Chemistry, 2002, 10, 2883-2891.	1.4	64
22	Interplay between halogen bonds and Ï€â€“Ï€ stacking interactions: CSD search and theoretical study. Physical Chemistry Chemical Physics, 2012, 14, 9948.	1.3	61
23	Exploring Transition Pathway and Free-Energy Profile of Large-Scale Protein Conformational Change by Combining Normal Mode Analysis and Umbrella Sampling Molecular Dynamics. Journal of Physical Chemistry B, 2014, 118, 134-143.	1.2	58
24	Pterostilbene induces apoptosis and cell cycle arrest in diffuse large B-cell lymphoma cells. Scientific Reports, 2016, 6, 37417.	1.6	54
25	D3Pockets: A Method and Web Server for Systematic Analysis of Protein Pocket Dynamics. Journal of Chemical Information and Modeling, 2019, 59, 3353-3358.	2.5	54
26	Substitution Effect of the Trifluoromethyl Group on the Bioactivity in Medicinal Chemistry: Statistical Analysis and Energy Calculations. Journal of Chemical Information and Modeling, 2020, 60, 6242-6250.	2.5	54
27	Structure-Based Design and Synthesis of C-1- and C-4-Modified Analogs of Zanamivir as Neuraminidase Inhibitors. Journal of Medicinal Chemistry, 2013, 56, 671-684.	2.9	50
28	Force fields and scoring functions for carbohydrate simulation. Carbohydrate Research, 2015, 401, 73-81.	1.1	49
29	Inhibition of GPR40 protects MIN6 Î² cells from palmitateâ€induced ER stress and apoptosis. Journal of Cellular Biochemistry, 2012, 113, 1152-1158.	1.2	48
30	Transgelin-2 as a therapeutic target for asthmatic pulmonary resistance. Science Translational Medicine, 2018, 10, .	5.8	47
31	Influence of the Water Molecule on Cationâ^Ï€ Interaction:Â Ab Initio Second Order MÃ¸llerâ^Plesset Perturbation Theory (MP2) Calculations. Journal of Physical Chemistry B, 2005, 109, 5945-5949.	1.2	46
32	Theoretical Insight into the Interactions of TMA-Benzene and TMA-Pyrrole with B3LYP Density-Functional Theory (DFT) and ab Initio Second Order MÃ¸llerâ^Plesset Perturbation Theory (MP2) Calculations. Journal of Physical Chemistry A, 2001, 105, 5431-5437.	1.1	45
33	Mutual Influence between Halogen Bonds and Cationâ€“Ï€ Interactions: A Theoretical Study. ChemPhysChem, 2012, 13, 2154-2161.	1.0	45
34	Mutation L1196M-induced conformational changes and the drug resistant mechanism of anaplastic lymphoma kinase studied by free energy perturbation and umbrella sampling. Physical Chemistry Chemical Physics, 2017, 19, 30239-30248.	1.3	45
35	Effect of cationâ€“Ï€ interaction on NMR: A theoretical investigation on complexes of Li+, Na+, Be2+, and Mg2+ with aromatics. Chemical Physics Letters, 2006, 422, 455-460.	1.2	44
36	Stability and Characteristics of the Halogen Bonding Interaction in an Anionâ€“Anion Complex: A Computational Chemistry Study. Journal of Physical Chemistry B, 2016, 120, 610-620.	1.2	44

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37	Computational Insights into the Conformational Accessibility and Binding Strength of SARS-CoV-2 Spike Protein to Human Angiotensin-Converting Enzyme 2. Journal of Physical Chemistry Letters, 2020, 11, 10482-10488.	2.1	42
38	Advances in studying of the pharmacological activities and structureâ€“activity relationships of natural C-glycosylflavonoids. Acta Pharmaceutica Sinica B, 2013, 3, 154-162.	5.7	41
39	Structural basis for the Mg ²⁺ recognition and regulation of the CorC Mg ²⁺ transporter. Science Advances, 2021, 7, .	4.7	41
40	Enhanced sampling molecular dynamics simulation captures experimentally suggested intermediate and unfolded states in the folding pathway of Trp-cage miniprotein. Journal of Chemical Physics, 2012, 137, 125103.	1.2	40
41	Probing Origin of Binding Difference of inhibitors to MDM2 and MDMX by Polarizable Molecular Dynamics Simulation and QM/MM-GBSA Calculation. Scientific Reports, 2015, 5, 17421.	1.6	39
42	Pterostilbene Inhibits Human Multiple Myeloma Cells via ERK1/2 and JNK Pathway In Vitro and In Vivo. International Journal of Molecular Sciences, 2016, 17, 1927.	1.8	39
43	Interaction Nature and Computational Methods for Halogen Bonding: A Perspective. Journal of Chemical Information and Modeling, 2020, 60, 2683-2696.	2.5	39
44	DC260126, a small-molecule antagonist of GPR40, improves insulin tolerance but not glucose tolerance in obese Zucker rats. Biomedicine and Pharmacotherapy, 2010, 64, 647-651.	2.5	38
45	Inhibition of hepatitis B virus replication by targeting ribonucleotide reductase M2 protein. Biochemical Pharmacology, 2016, 103, 118-128.	2.0	38
46	Thermodynamic and Structural Characterization of Halogen Bonding in Proteinâ€“Ligand Interactions: A Case Study of PDE5 and Its Inhibitors. Journal of Medicinal Chemistry, 2014, 57, 3588-3593.	2.9	37
47	Halogen bonding in differently charged complexes: basic profile, essential interaction terms and intrinsic Ïƒ-hole. Physical Chemistry Chemical Physics, 2019, 21, 15106-15119.	1.3	37
48	DC260126: A Small-Molecule Antagonist of GPR40 that Protects against Pancreatic Î²-Cells Dysfunction in db/db Mice. PLoS ONE, 2013, 8, e66744.	1.1	36
49	A knowledge-based halogen bonding scoring function for predicting protein-ligand interactions. Journal of Molecular Modeling, 2013, 19, 5015-5030.	0.8	35
50	A comparative study of trypsin specificity based on QM/MM molecular dynamics simulation and QM/MM GBSA calculation. Journal of Biomolecular Structure and Dynamics, 2015, 33, 2606-2618.	2.0	35
51	Discovery of New and Potent InhA Inhibitors as Antituberculosis Agents: Structure-Based Virtual Screening Validated by Biological Assays and X-ray Crystallography. Journal of Chemical Information and Modeling, 2020, 60, 226-234.	2.5	34
52	Unveiling conformational dynamics changes of H-Ras induced by mutations based on accelerated molecular dynamics. Physical Chemistry Chemical Physics, 2020, 22, 21238-21250.	1.3	34
53	Binding Modes of Three Inhibitors 8CA, F8A and I4A to A-FABP Studied Based on Molecular Dynamics Simulation. PLoS ONE, 2014, 9, e99862.	1.1	33
54	How Does Ammonium Dynamically Interact with Benzene in Aqueous Media? A First Principle Study Using the Carâ€“Parrinello Molecular Dynamics Method. Journal of Physical Chemistry B, 2006, 110, 5094-5098.	1.2	31

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55	N-Methylformamideâ˜Benzene Complex as a Prototypical Peptide Nâ˜HÂ·Â·Â·Ï€ Hydrogen-Bonded System:Â Density Functional Theory and MP2 Studies. Journal of Organic Chemistry, 2003, 68, 7490-7495.	1.7	30
56	Applying high-performance computing in drug discovery and molecular simulation. National Science Review, 2016, 3, 49-63.	4.6	30
57	Additivity of Cationâ˜Ï€ Interactions:Â An ab Initio Computational Study on Ï€â˜Cationâ˜Ï€ Sandwich Complexes. Journal of Physical Chemistry A, 2004, 108, 9400-9405.	1.1	29
58	Discovery of highly selective inhibitors of human fatty acid binding protein 4 (FABP4) by virtual screening. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 3675-3679.	1.0	27
59	Repositioning organohalogen drugs: a case study for identification of potent B-Raf V600E inhibitors via docking and bioassay. Scientific Reports, 2016, 6, 31074.	1.6	27
60	Different structures of berberine and five other protoberberine alkaloids that affect P-glycoprotein-mediated efflux capacity. Acta Pharmacologica Sinica, 2019, 40, 133-142.	2.8	27
61	Ligand-based approach for predicting drug targets and for virtual screening against COVID-19. Briefings in Bioinformatics, 2021, 22, 1053-1064.	3.2	27
62	Benzbromarone, an old uricosuric drug, inhibits human fatty acid binding protein 4 in vitro and lowers the blood glucose level in db/db mice. Acta Pharmacologica Sinica, 2013, 34, 1397-1402.	2.8	26
63	Thermodynamics calculation of proteinâ€“ligand interactions by QM/MM polarizable charge parameters. Journal of Biomolecular Structure and Dynamics, 2016, 34, 163-176.	2.0	26
64	Inhibition of Calcium Influx Reduces Dysfunction and Apoptosis in Lipotoxic Pancreatic Î²-Cells via Regulation of Endoplasmic Reticulum Stress. PLoS ONE, 2015, 10, e0132411.	1.1	25
65	Novel fatty acid binding protein 4 (FABP4) inhibitors: Virtual screening, synthesis and crystal structure determination. European Journal of Medicinal Chemistry, 2015, 90, 241-250.	2.6	25
66	Underestimated Noncovalent Interactions in Protein Data Bank. Journal of Chemical Information and Modeling, 2019, 59, 3389-3399.	2.5	25
67	Pharmacokinetics-Driven Optimization of 4(3H)-Pyrimidinones as Phosphodiesterase Type 5 Inhibitors Leading to TPN171, a Clinical Candidate for the Treatment of Pulmonary Arterial Hypertension. Journal of Medicinal Chemistry, 2019, 62, 4979-4990.	2.9	25
68	Research progress in cation-Ï€ interactions. Science in China Series B: Chemistry, 2008, 51, 709-717.	0.8	24
69	A quantum mechanics-based halogen bonding scoring function for protein-ligand interactions. Journal of Molecular Modeling, 2015, 21, 138.	0.8	22
70	QSAR analyses on avian influenza virus neuraminidase inhibitors using CoMFA, CoMSIA, and HQSAR. Journal of Computer-Aided Molecular Design, 2006, 20, 549-566.	1.3	21
71	Understanding the regulation mechanisms of PAF receptor by agonists and antagonists: Molecular modeling and molecular dynamics simulation studies. Proteins: Structure, Function and Bioinformatics, 2007, 67, 41-52.	1.5	21
72	Cationâ€“Ï€ complexes formed between cyclooctatetraene and alkaline earth metals: Predicted and recorded NMR features. Chemical Physics Letters, 2008, 462, 45-48.	1.2	21

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73	Noncovalent interactions in halogenated ionic liquids: theoretical study and crystallographic implications. Physical Chemistry Chemical Physics, 2013, 15, 4405.	1.3	21
74	The Underestimated Halogen Bonds Forming with Protein Side Chains in Drug Discovery and Design. Journal of Chemical Information and Modeling, 2017, 57, 22-26.	2.5	21
75	Exploring the Ligand Binding/Unbinding Pathway by Selectively Enhanced Sampling of Ligand in a Proteinâ€“Ligand Complex. Journal of Physical Chemistry B, 2019, 123, 7974-7983.	1.2	21
76	Exploring Conformational Change of Adenylate Kinase by Replica Exchange Molecular Dynamic Simulation. Biophysical Journal, 2020, 118, 1009-1018.	0.2	21
77	Density functional theory (DFT) study on the interaction of ammonium (NH4+) and aromatic nitrogen heterocyclics. Journal of the Chemical Society Perkin Transactions II, 1999, , 2615-2622.	0.9	20
78	Determining Protein Folding Pathway and Associated Energetics through Partitioned Integrated-Tempering-Sampling Simulation. Journal of Chemical Theory and Computation, 2017, 13, 1229-1243.	2.3	20
79	The Relationship between Binding Models of TMA with Furan and Imidazole and the Molecular Electrostatic Potentials:â€‰ DFT and MP2 Computational Studies. Journal of Physical Chemistry A, 2002, 106, 157-164.	1.1	19
80	Molecular Dynamics Simulations on the Mechanism of Transporting Methylamine and Ammonia by Ammonium Transporter AmtB. Journal of Physical Chemistry B, 2010, 114, 15172-15179.	1.2	19
81	How Do Distance and Solvent Affect Halogen Bonding Involving Negatively Charged Donors?. Journal of Physical Chemistry B, 2016, 120, 8784-8793.	1.2	19
82	Underestimated Halogen Bonds Forming with Protein Backbone in Protein Data Bank. Journal of Chemical Information and Modeling, 2017, 57, 1529-1534.	2.5	19
83	From hit to lead: Structure-based discovery of naphthalene-1-sulfonamide derivatives as potent and selective inhibitors of fatty acid binding protein 4. European Journal of Medicinal Chemistry, 2018, 154, 44-59.	2.6	19
84	Exploring the immune evasion of SARS-CoV-2 variant harboring E484K by molecular dynamics simulations. Briefings in Bioinformatics, 2022, 23, .	3.2	19
85	DCZ5248, a novel dual inhibitor of Hsp90 and autophagy, exerts antitumor activity against colon cancer. Acta Pharmacologica Sinica, 2021, 42, 132-141.	2.8	18
86	Knowledge-Based Scoring Functions in Drug Design: 3. A Two-Dimensional Knowledge-Based Hydrogen-Bonding Potential for the Prediction of Proteinâ€“Ligand Interactions. Journal of Chemical Information and Modeling, 2011, 51, 2994-3004.	2.5	17
87	Energetics and structural characterization of the â€œDFG-flipâ€•conformational transition of B-RAF kinase: a SITS molecular dynamics study. Physical Chemistry Chemical Physics, 2017, 19, 1257-1267.	1.3	17
88	Structural insights into HIV-1 protease flap opening processes and key intermediates. RSC Advances, 2017, 7, 45121-45128.	1.7	16
89	How Well Can Implicit Solvent Simulations Explore Folding Pathways? A Quantitative Analysis of Î±-Helix Bundle Proteins. Journal of Chemical Theory and Computation, 2017, 13, 6177-6190.	2.3	15
90	Pterostilbene Induces Cell Apoptosis and Cell Cycle Arrest in T-Cell Leukemia/Lymphoma by Suppressing the ERK1/2 Pathway. BioMed Research International, 2017, 2017, 1-11.	0.9	15

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91	Exploring binding mechanisms of VEGFR2 with three drugs lenvatinib, sorafenib, and sunitinib by molecular dynamics simulation and free energy calculation. Chemical Biology and Drug Design, 2019, 93, 934-948.	1.5	15
92	Towards discovering dual functional inhibitors against both wild type and K103N mutant HIV-1 reverse transcriptases: molecular docking and QSAR studies on 4,1-benzoxazepinone analogues. Journal of Computer-Aided Molecular Design, 2006, 20, 281-293.	1.3	14
93	Dynamics revelation of conformational changes and binding modes of heat shock protein 90 induced by inhibitor associations. RSC Advances, 2018, 8, 25456-25467.	1.7	14
94	Induction of an Aromatic Six-Membered Nitrogen Ring via Cationâ˜Ï€ Interaction. Journal of Physical Chemistry A, 2006, 110, 12236-12240.	1.1	13
95	Improving the accuracy of predicting proteinâ€“ligand binding-free energy with semiempirical quantum chemistry charge. Future Medicinal Chemistry, 2019, 11, 303-321.	1.1	13
96	Conformation of the Macrocyclic Drug Lorlatinib in Polar and Nonpolar Environments: A MD Simulation and NMR Study. ACS Omega, 2019, 4, 22245-22250.	1.6	13
97	D3AI-CoV: a deep learning platform for predicting drug targets and for virtual screening against COVID-19. Briefings in Bioinformatics, 2022, 23, .	3.2	13
98	Pharmacophore-directed Homology Modeling and Molecular Dynamics Simulation of G Protein-coupled Receptor: Study of Possible Binding Modes of 5-HT2CReceptor Agonists. Acta Biochimica Et Biophysica Sinica, 2007, 39, 413-422.	0.9	12
99	Regioselectivity and Mechanism of Synthesizing N-Substituted 2-Pyridones and 2-Substituted Pyridines via Metal-Free C-O and C-N Bond-Cleaving of Oxazoline[3,2-a]pyridiniums. Scientific Reports, 2017, 7, 41287.	1.6	12
100	DCZ3301, a novel cytotoxic agent, inhibits proliferation in diffuse large B-cell lymphoma via the STAT3 pathway. Cell Death and Disease, 2017, 8, e3111-e3111.	2.7	12
101	Preclinical activity of DCZ3301, a novel aryl-guanidino compound in the therapy of multiple myeloma. Theranostics, 2017, 7, 3690-3699.	4.6	12
102	CoVac501, a self-adjuvanting peptide vaccine conjugated with TLR7 agonists, against SARS-CoV-2 induces protective immunity. Cell Discovery, 2022, 8, 9.	3.1	12
103	Robustness in Protein Folding Revealed by Thermodynamics Calculations. Journal of Physical Chemistry B, 2012, 116, 13848-13856.	1.2	11
104	Discovery of N-substituted 3-arylisoquinolone derivatives as antitumor agents originating from O-substituted 3-arylisoquinolines via [2,3] or [3,3] rearrangement. European Journal of Medicinal Chemistry, 2014, 77, 204-210.	2.6	11
105	Mass Spectrometry and Theoretical Investigation of VN_n⁺ (n = 8,) Tj ETQq1 1 0.784314 rgBT	1.1	11
106	A novel silicone derivative of natural osalmid (DCZ0858) induces apoptosis and cell cycle arrest in diffuse large B-cell lymphoma via the JAK2/STAT3 pathway. Signal Transduction and Targeted Therapy, 2020, 5, 31.	7.1	11
107	D3DistalMutation: a Database to Explore the Effect of Distal Mutations on Enzyme Activity. Journal of Chemical Information and Modeling, 2021, 61, 2499-2508.	2.5	11
108	X66, a novel N-terminal heat shock protein 90 inhibitor, exerts antitumor effects without induction of heat shock response. Oncotarget, 2016, 7, 29648-29663.	0.8	11

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109	Halogen Bonds Exist between Noncovalent Ligands and Natural Nucleic Acids. Journal of Medicinal Chemistry, 2022, 65, 4424-4435.	2.9	11
110	A computational study on electron transfer mechanism between alkaline earth metal atoms and cyclooctatetraene to form cationâ€“Ï€ bonded complexes. Chemical Physics Letters, 2006, 423, 339-343.	1.2	10
111	Cation sitting in aromatic cages:ab initio computational studies on tetramethylammoniumâ€“(benzene)n (n=3â€“4) complexes. Journal of Physical Organic Chemistry, 2007, 20, 448-453.	0.9	10
112	The universality of Î²-hairpin misfolding indicated by molecular dynamics simulations. Journal of Chemical Physics, 2013, 139, 165103.	1.2	9
113	Unstable, Metastable, or Stable Halogen Bonding Interaction Involving Negatively Charged Donors? A Statistical and Computational Chemistry Study. Journal of Physical Chemistry B, 2014, 118, 14223-14233.	1.2	9
114	Why does Î²-secretase zymogen possess catalytic activity? Molecular modeling and molecular dynamics simulation studies. Computational Biology and Chemistry, 2007, 31, 186-195.	1.1	8
115	The nature and magnitude of specific halogen bonds between iodoâ€perfluorobenzene and heterocyclic systems. International Journal of Quantum Chemistry, 2011, 111, 2352-2358.	1.0	8
116	Overman rearrangement and Pomeranzâ€“Fritsch reaction for the synthesis of benzoazepinoisoquinolones to discover novel antitumor agents. European Journal of Medicinal Chemistry, 2013, 70, 677-684.	2.6	8
117	Dual inhibition of mTORC1/2 by DCZ0358 induces cytotoxicity in multiple myeloma and overcomes the protective effect of the bone marrow microenvironment. Cancer Letters, 2018, 421, 135-144.	3.2	7
118	Nonnative contact effects in protein folding. Physical Chemistry Chemical Physics, 2019, 21, 11924-11936.	1.3	7
119	Discovery of dihydrooxazolo[2,3-a]isoquinoliniums as highly specific inhibitors of hCE2. RSC Advances, 2019, 9, 35904-35912.	1.7	7
120	Increasing the Sampling Efficiency of Protein Conformational Change by Combining a Modified Replica Exchange Molecular Dynamics and Normal Mode Analysis. Journal of Chemical Theory and Computation, 2021, 17, 13-28.	2.3	7
121	Theoretical studies on cation-Ï€ interactions (I)â€”Densityfunctional theory investigation on the configurations and interaction for ammonium cation-benzene complex. Science in China Series B: Chemistry, 1998, 41, 535-542.	0.8	6
122	The open-close mechanism of M2 channel protein in influenza A virus: A computational study on the hydrogen bonds and cation-Ï€ interactions among His37 and Trp41. Science in China Series B: Chemistry, 2008, 51, 768-775.	0.8	6
123	The Conserved Lys-95 Charged Residue Cluster Is Critical for the Homodimerization and Enzyme Activity of Human Ribonucleotide Reductase Small Subunit M2. Journal of Biological Chemistry, 2014, 289, 909-920.	1.6	6
124	DCZ3301, a novel aryl-guanidino inhibitor, induces cell apoptosis and cell cycle arrest via suppressing the PI3K/AKT pathway in T-cell leukemia/lymphoma. Acta Biochimica Et Biophysica Sinica, 2018, 50, 643-650.	0.9	6
125	Inhibiting mechanism of small molecule toward the p53â€<scp>MDM</scp>2 interaction: A molecular dynamic exploration. Chemical Biology and Drug Design, 2018, 92, 1763-1777.	1.5	6
126	Preclinical validation and phase I trial of 4-hydroxysalicylanilide, targeting ribonucleotide reductase mediated dNTP synthesis in multiple myeloma. Journal of Biomedical Science, 2022, 29, 32.	2.6	6

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127	Is Free Cyclooctatetraene Dianion an Aromatic System? A Quantum Chemistry Study. Chinese Journal of Chemistry, 2009, 27, 1914-1918.	2.6	5
128	Facile Synthesis of Substituted 4-Alkoxy-2-oxazolines and Exploration of the Reaction Mechanism. Synthesis, 2016, 48, 1331-1343.	1.2	5
129	Combined Virtual Screening and Substructure Search for Discovery of Novel FABP4 Inhibitors. Journal of Chemical Information and Modeling, 2017, 57, 2329-2335.	2.5	5
130	mD3DOCKxb: An Ultra-Scalable CPU-MIC Coordinated Virtual Screening Framework. , 2017, , .		5
131	Structural evolution of LiNn+ (n = 2, 4, 6, 8, and 10) clusters: mass spectrometry and theoretical calculations. RSC Advances, 2019, 9, 6762-6769.	1.7	5
132	Celamonols Aâ€“D, four triterpenoid and catechin conjugates with immunosuppressive activities from the stems of Celastrus monospermus. Organic Chemistry Frontiers, 2019, 6, 3786-3792.	2.3	5
133	Computational study of the substituent effect of halogenated fused-ring heteroaromatics on halogen bonding. Journal of Molecular Modeling, 2020, 26, 270.	0.8	5
134	Novel cyclophosphamide of natural products osalmide and pterostilbene induces cytotoxicity and cell cycle arrest in diffuse large B-cell lymphoma cells. Acta Biochimica Et Biophysica Sinica, 2020, 52, 401-410.	0.9	5
135	Anti-DLBCL efficacy of DCZ0825 and : involvement of the PI3Kâ€'AKTâ€'mTOR/JNK pathway. Acta Biochimica Et Biophysica Sinica, 2021, 53, 575-583.	0.9	5
136	Identification and mechanistic analysis of an inhibitor of the CorC Mg2+ transporter. IScience, 2021, 24, 102370.	1.9	5
137	Halogen Bonding: From Fundamentals to Applications. ChemPlusChem, 2021, 86, 1229-1230.	1.3	5
138	Design, Synthesis and Pharmacological Evaluation of Novel Hsp90Nâ€terminal Inhibitors Without Induction of Heat Shock Response. ChemistryOpen, 2019, 8, 344-353.	0.9	4
139	Mass spectrometry detection of LiN12+ cluster and theoretical investigation of its structures and stability. Chemical Physics Letters, 2020, 747, 137310.	1.2	4
140	Glycolysis is suppressed by DCZ0801-induced inactivation of the Akt/mTOR pathway in Multiple Myeloma. Journal of Cancer, 2020, 11, 4907-4916.	1.2	4
141	The effects of implicit modeling of nonpolar solvation on protein folding simulations. Physical Chemistry Chemical Physics, 2018, 20, 18410-18419.	1.3	3
142	Metal-free quinolylation of the primary amino groups of amino acid derivatives and peptides with dihydrooxazolo[3,2-a]quinoliniums. Green Chemistry, 2019, 21, 4231-4237.	4.6	3
143	Accurate prediction of relative binding affinities of a series of HIVâ€1 protease inhibitors using semiâ€empirical quantum mechanical charge. Journal of Computational Chemistry, 2020, 41, 1773-1780.	1.5	3
144	Conserved protein targets for developing pan-coronavirus drugs based on sequence and 3D structure similarity analyses. Computers in Biology and Medicine, 2022, 145, 105455.	3.9	3

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145	DCZ0814 induces apoptosis and G0/G1 phase cell cycle arrest in myeloma by dual inhibition of mTORC1/2 . Cancer Management and Research, 2019, Volume 11, 4797-4808.	0.9	2
146	Synthesis and Structureâ€Activity Relationships of 3â€Arylisoquinolone Analogues as Highly Specific hCES2A Inhibitors. ChemMedChem, 2021, 16, 388-398.	1.6	2
147	Predicting spike protein NTD mutations of SARS-CoV-2 causing immune evasion by molecular dynamics simulations. Physical Chemistry Chemical Physics, 2022, 24, 3410-3419.	1.3	2
148	D3PM: a comprehensive database for protein motions ranging from residue to domain. BMC Bioinformatics, 2022, 23, 70.	1.2	2
149	The Effects of a Transgelin-2 Agonist Administered at Different Times in a Mouse Model of Airway Hyperresponsiveness. Frontiers in Pharmacology, 0, 13, .	1.6	2
150	DCZ3301, an aryl-guanidino agent, inhibits ocular neovascularization via PI3K/AKT and ERK1/2 signaling pathways. Experimental Eye Research, 2020, 201, 108267.	1.2	1
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