

Tong Zhu

List of Publications by Year in descending order

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97
papers

3,170
citations

218592

26
h-index

168321

53
g-index

112
all docs

112
docs citations

112
times ranked

3936
citing authors

#	ARTICLE	IF	CITATIONS
1	Discovery of a Potent and Selective Inhibitor of Cyclin-Dependent Kinase 4/6. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 2388-2406.	2.9	438
2	Donor Engineering for NIR-II Molecular Fluorophores with Enhanced Fluorescent Performance. <i>Journal of the American Chemical Society</i> , 2018, 140, 1715-1724.	6.6	379
3	Fragment Quantum Mechanical Calculation of Proteins and Its Applications. <i>Accounts of Chemical Research</i> , 2014, 47, 2748-2757.	7.6	173
4	Enabling Light Work in Helical Self-Assembly for Dynamic Amplification of Chirality with Photoreversibility. <i>Journal of the American Chemical Society</i> , 2016, 138, 2219-2224.	6.6	142
5	Effect of mutations on binding of ligands to guanine riboswitch probed by free energy perturbation and molecular dynamics simulations. <i>Nucleic Acids Research</i> , 2019, 47, 6618-6631.	6.5	130
6	A Comparative Insight into Amprenavir Resistance of Mutations V32I, G48V, I50V, I54V, and I84V in HIV-1 Protease Based on Thermodynamic Integration and MM-PBSA Methods. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1903-1913.	2.5	118
7	Complex reaction processes in combustion unraveled by neural network-based molecular dynamics simulation. <i>Nature Communications</i> , 2020, 11, 5713.	5.8	111
8	Developing a Bright NIR-II Fluorophore with Fast Renal Excretion and Its Application in Molecular Imaging of Immune Checkpoint PD-L1. <i>Advanced Functional Materials</i> , 2018, 28, 1804956.	7.8	85
9	An Electrochemical Biosensor with Dual Signal Outputs: Toward Simultaneous Quantification of pH and O ₂ in the Brain upon Ischemia and in a Tumor during Cancer Starvation Therapy. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 10471-10475.	7.2	84
10	Fragment density functional theory calculation of NMR chemical shifts for proteins with implicit solvation. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 7837-7845.	1.3	74
11	Automated Fragmentation QM/MM Calculation of Amide Proton Chemical Shifts in Proteins with Explicit Solvent Model. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2104-2114.	2.3	73
12	Quantum Fragment Based <i>ab Initio</i> Molecular Dynamics for Proteins. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5897-5905.	2.3	59
13	CHARMM-GUI Supports Hydrogen Mass Repartitioning and Different Protonation States of Phosphates in Lipopolysaccharides. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 831-839.	2.5	59
14	AFNMR: automated fragmentation quantum mechanical calculation of NMR chemical shifts for biomolecules. <i>Journal of Biomolecular NMR</i> , 2015, 63, 125-139.	1.6	56
15	Self-Assembly of Metallo-Nucleoside Hydrogels for Injectable Materials That Promote Wound Closure. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 19743-19750.	4.0	55
16	ReacNetGenerator: an automatic reaction network generator for reactive molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 683-691.	1.3	54
17	Design, Synthesis, and Biological Evaluation of Imidazo[1,2- <i>a</i>]pyridine Derivatives as Novel PI3K/mTOR Dual Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 3028-3046.	2.9	50
18	Single Biosensor for Simultaneous Quantification of Glucose and pH in a Rat Brain of Diabetic Model Using Both Current and Potential Outputs. <i>Analytical Chemistry</i> , 2017, 89, 6656-6662.	3.2	45

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19	A New Quantum Calibrated Force Field for Zinc-Protein Complex. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1788-1798.	2.3	44
20	Structure-based design and synthesis of imidazo[1,2-a]pyridine derivatives as novel and potent Nek2 inhibitors with <i>in vitro</i> and <i>in vivo</i> antitumor activities. <i>European Journal of Medicinal Chemistry</i> , 2017, 126, 1083-1106.	2.6	41
21	Polarization of Intraprotein Hydrogen Bond Is Critical to Thermal Stability of Short Helix. <i>Journal of Physical Chemistry B</i> , 2012, 116, 549-554.	1.2	39
22	Ferrocene-Grafted Photochromic Triads Based on a Sterically Hindered Ethene Bridge: Redox-Switchable Fluorescence and Gated Photochromism. <i>Advanced Optical Materials</i> , 2016, 4, 1410-1416.	3.6	32
23	Some insights into mechanism for binding and drug resistance of wild type and I50V V82A and I84V mutations in HIV-1 protease with GRL-98065 inhibitor from molecular dynamic simulations. <i>European Journal of Medicinal Chemistry</i> , 2010, 45, 227-235.	2.6	30
24	Exploring drug-resistant mechanisms of I84V mutation in HIV-1 protease toward different inhibitors by thermodynamics integration and solvated interaction energy method. <i>Chemical Physics Letters</i> , 2018, 706, 400-408.	1.2	30
25	Decoding molecular mechanism of inhibitor bindings to CDK2 using molecular dynamics simulations and binding free energy calculations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 985-996.	2.0	29
26	Folding of a Helix Is Critically Stabilized by Polarization of Backbone Hydrogen Bonds: Study in Explicit Water. <i>Journal of Physical Chemistry B</i> , 2012, 116, 3430-3435.	1.2	27
27	Modeling and Simulation of Bacterial Outer Membranes with Lipopolysaccharides and Enterobacterial Common Antigen. <i>Journal of Physical Chemistry B</i> , 2020, 124, 5948-5956.	1.2	26
28	Molecular Dynamics Simulation of Zinc Ion in Water with an <i>ab Initio</i> Based Neural Network Potential. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6587-6595.	1.1	24
29	Invisible photochromism and optical anti-counterfeiting based on D-A type inverse diarylethene. <i>Journal of Materials Chemistry C</i> , 2017, 5, 4571-4577.	2.7	23
30	Comparison of RP-3 Pyrolysis Reactions between Surrogates and 45-Component Model by ReaxFF Molecular Dynamics Simulations. <i>Energy & Fuels</i> , 2019, 33, 7176-7187.	2.5	23
31	Understanding the selectivity of inhibitors toward PI4KIII [±] and PI4KIII ² based molecular modeling. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 22103-22112.	1.3	22
32	Exploring the Chemical Space of Linear Alkane Pyrolysis via Deep Potential GENERator. <i>Energy & Fuels</i> , 2021, 35, 762-769.	2.5	22
33	Development of an Effective Polarizable Bond Method for Biomolecular Simulation. <i>Journal of Physical Chemistry B</i> , 2013, 117, 14885-14893.	1.2	19
34	A test of AMBER force fields in predicting the secondary structure of α -helical and β -hairpin peptides. <i>Chemical Physics Letters</i> , 2017, 679, 112-118.	1.2	19
35	An Electrochemical Biosensor with Dual Signal Outputs: Toward Simultaneous Quantification of pH and O_2 in the Brain upon Ischemia and in a Tumor during Cancer Starvation Therapy. <i>Angewandte Chemie</i> , 2017, 129, 10607-10611.	1.6	19
36	Optimization of convergence criteria for fragmentation methods. <i>Chemical Physics Letters</i> , 2017, 687, 163-170.	1.2	18

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37	Effect of Substituents in Different Positions of Aminothiazole Hinge-Binding Scaffolds on Inhibitorâ€™s CDK2 Association Probed by Interaction Entropy Method. ACS Omega, 2018, 3, 18052-18064.	1.6	18
38	A Fragment Quantum Mechanical Method for Metalloproteins. Journal of Chemical Theory and Computation, 2019, 15, 1430-1439.	2.3	17
39	Structural basis of the stereoselective formation of the spirooxindole ring in the biosynthesis of citrinadins. Nature Communications, 2021, 12, 4158.	5.8	17
40	Asp120Asn mutation impairs the catalytic activity of NDM-1 metallo-Î²-lactamase: experimental and computational study. Physical Chemistry Chemical Physics, 2014, 16, 6709.	1.3	16
41	Binding modes and conformational changes of FK506-binding protein 51 induced by inhibitor bindings: insight into molecular mechanisms based on multiple simulation technologies. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2141-2155.	2.0	16
42	Naphthalimide end-capping molecular rotors with different donor cores: Tuning emission in wide gamut and cell imaging. Dyes and Pigments, 2020, 179, 108431.	2.0	16
43	Correct folding of an Î±-helix and a Î²-hairpin using a polarized 2D torsional potential. Scientific Reports, 2015, 5, 10359.	1.6	15
44	A systematic study on RNA NMR chemical shift calculation based on the automated fragmentation QM/MM approach. RSC Advances, 2016, 6, 108590-108602.	1.7	14
45	Reduction-Triggered Release of CPT from Acid-Degradable Polymeric Prodrug Micelles Bearing Boronate Ester Bonds with Enhanced Cellular Uptake. ACS Biomaterials Science and Engineering, 2017, 3, 3364-3375.	2.6	14
46	Automated Fragmentation QM/MM Calculation of NMR Chemical Shifts for Protein-Ligand Complexes. Frontiers in Chemistry, 2018, 6, 150.	1.8	14
47	Antitumor activity of TY-011 against gastric cancer by inhibiting Aurora A, Aurora B and VEGFR2 kinases. Journal of Experimental and Clinical Cancer Research, 2016, 35, 183.	3.5	13
48	Direct folding simulation of helical proteins using an effective polarizable bond force field. Physical Chemistry Chemical Physics, 2017, 19, 15273-15284.	1.3	13
49	Ab initio neural network MD simulation of thermal decomposition of a high energy material CL-20/TNT. Physical Chemistry Chemical Physics, 2022, 24, 11801-11811.	1.3	13
50	PBSA_E: A PBSA-Based Free Energy Estimator for Proteinâ€™s Ligand Binding Affinity. Journal of Chemical Information and Modeling, 2016, 56, 854-861.	2.5	12
51	Discovery of core-structurally novel PTP1B inhibitors with specific selectivity containing oxindole-fused spirotetrahydrofurochroman by one-pot reaction. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 1105-1108.	1.0	12
52	A method for efficient calculation of thermal stability of proteins upon point mutations. Physical Chemistry Chemical Physics, 2020, 22, 8461-8466.	1.3	12
53	Benchmark Force Fields for the Molecular Dynamic Simulation of G-Quadruplexes. Molecules, 2021, 26, 5379.	1.7	12
54	Direct folding simulation of a long helix in explicit water. Applied Physics Letters, 2013, 102, .	1.5	11

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55	A theoretical study of the substituent effect on reactions of amines, carbon dioxide and ethylene oxide catalyzed by binary ionic liquids. <i>RSC Advances</i> , 2017, 7, 51521-51527.	1.7	11
56	Camptothecin prodrug nanomicelle based on a boronate ester-linked diblock copolymer as the carrier of doxorubicin with enhanced cellular uptake. <i>Journal of Biomaterials Science, Polymer Edition</i> , 2018, 29, 160-180.	1.9	11
57	Preclinical activity of MBM-5 in gastrointestinal cancer by inhibiting NEK2 kinase activity. <i>Oncotarget</i> , 2016, 7, 79327-79341.	0.8	11
58	A quantum mechanical computational method for modeling electrostatic and solvation effects of protein. <i>Scientific Reports</i> , 2018, 8, 5475.	1.6	10
59	Understanding Aldose Reductase-Inhibitors interactions with free energy simulation. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 91, 10-21.	1.3	10
60	Influences of <i>Vibrio cholerae</i> Lipid A Types on LPS Bilayer Properties. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2105-2112.	1.2	10
61	Automatically Constructed Neural Network Potentials for Molecular Dynamics Simulation of Zinc Proteins. <i>Frontiers in Chemistry</i> , 2021, 9, 692200.	1.8	10
62	Electronic polarization stabilizes tertiary structure prediction of HP-36. <i>Journal of Molecular Modeling</i> , 2014, 20, 2195.	0.8	9
63	Cyclopentadienyl radical formation from the reaction of excited nitrogen atoms with benzene: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 12408-12420.	1.3	9
64	The intrinsic helical propensities of the helical fragments in prion protein under neutral and low pH conditions: a replica exchange molecular dynamics study. <i>Journal of Molecular Modeling</i> , 2013, 19, 4897-4908.	0.8	8
65	Correction of erroneously packed protein's side chains in the NMR structure based on ab initio chemical shift calculations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 18163.	1.3	8
66	New peptide deformylase inhibitors design, synthesis and pharmacokinetic assessment. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2016, 26, 3714-3718.	1.0	8
67	Origins of Protons in C-H Bond Insertion Products of Phenols: Proton-Self-Sufficient Function via Water Molecules. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6523-6529.	1.1	8
68	Energetics of protein backbone hydrogen bonds and their local electrostatic environment. <i>Science China Chemistry</i> , 2014, 57, 1708-1715.	4.2	7
69	Coupled Two-Dimensional Main-Chain Torsional Potential for Protein Dynamics II: Performance and Validation. <i>Journal of Physical Chemistry B</i> , 2015, 119, 4188-4193.	1.2	7
70	L-4, a Well-Tolerated and Orally Active Inhibitor of Hedgehog Pathway, Exhibited Potent Anti-tumor Effects Against Medulloblastoma in vitro and in vivo. <i>Frontiers in Pharmacology</i> , 2019, 10, 89.	1.6	7
71	Evaluation of the Coupled Two-Dimensional Main Chain Torsional Potential in Modeling Intrinsically Disordered Proteins. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 267-274.	2.5	6
72	Preferred conformations of lipooligosaccharides and oligosaccharides of <i>Moraxella catarrhalis</i> . <i>Glycobiology</i> , 2020, 30, 86-94.	1.3	6

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73	Molecular mechanism related to the binding of fluorophores to Mango-II revealed by multiple-replica molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 10636-10649.	1.3	6
74	Automated Construction of Neural Network Potential Energy Surface: The Enhanced Self-Organizing Incremental Neural Network Deep Potential Method. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5425-5437.	2.5	6
75	Protein-water hydrogen bonds are stabilized by electrostatic polarization. <i>Molecular Physics</i> , 2012, 110, 595-604.	0.8	5
76	An implementation of hydrophobic force in implicit solvent molecular dynamics simulation for packed proteins. <i>Journal of Molecular Modeling</i> , 2013, 19, 2605-2612.	0.8	5
77	Comparison of the unfolding and oligomerization of human prion protein under acidic and neutral environments by molecular dynamics simulations. <i>Chemical Physics Letters</i> , 2018, 706, 594-600.	1.2	5
78	A Force Balanced Fragmentation Method for ab Initio Molecular Dynamic Simulation of Protein. <i>Frontiers in Chemistry</i> , 2018, 6, 189.	1.8	5
79	Formation mechanism and spectroscopy of $C_{6}H$ radicals in extreme environments: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 23044-23055.	1.3	5
80	Insights into the binding mechanisms of inhibitors of MDM2 based on molecular dynamics simulations and binding free energy calculations. <i>Chemical Physics Letters</i> , 2019, 728, 94-101.	1.2	4
81	Design, synthesis, and structure activity relationship (SAR) studies of novel imidazo[1,2-a] pyridine derivatives as Nek2 inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , 2020, 28, 115775.	1.4	4
82	An ab initio/RRKM study of the reaction mechanism and product branching ratios of CH_3OH^+ and CH_3OH^{++} dissociation. <i>Journal of Molecular Structure</i> , 2020, 1217, 128410.	1.8	4
83	Engineering the biomimetic cofactors of NMNH for cytochrome P450 BM3 based on binding conformation refinement. <i>RSC Advances</i> , 2021, 11, 12036-12042.	1.7	4
84	Quasi-classical trajectory study of the reaction $O(3P) + HCl \hat{\rightarrow} OH + Cl$ and $O(3P) + DCl \hat{\rightarrow} OD + Cl$: Vector and scalar properties. <i>Computational and Theoretical Chemistry</i> , 2010, 948, 36-42.	1.5	3
85	An Approach to Computing Solvent Reorganization Energy. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6513-6519.	2.3	3
86	Quantum Calculation of Protein NMR Chemical Shifts Based on the Automated Fragmentation Method. <i>Advances in Experimental Medicine and Biology</i> , 2015, 827, 49-70.	0.8	3
87	Broadband mid-infrared $2.0\text{ }\mu\text{m}$ emission in Yb^{3+}/Ho^{3+} co-doped silicate-germanate glasses for mid-infrared fiber amplifiers. <i>Optical Engineering</i> , 2020, 59, 1.	0.5	3
88	Quasi-classical Trajectory Study of Reaction $O(3P) + HCl(\nu = 2; j = 1, 6, 9) \hat{\rightarrow} OH + Cl$. <i>Chinese Physics Letters</i> , 2010, 27, 033102.	1.3	2
89	THE EFFECT OF VIBRATIONAL EXCITATION OF THE REACTION $O(3P) + HCl \hat{\rightarrow} OH + Cl$ FOR THE $A^3\Sigma^+$ ELECTRONIC STATES. <i>Journal of Theoretical and Computational Chemistry</i> , 2010, 09, 1033-1042.	1.8	2
90	Predicted PAR1 inhibitors from multiple computational methods. <i>Chemical Physics Letters</i> , 2016, 659, 295-303.	1.2	2

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91	Discovery of Bisindole as a Novel Scaffold for Protein Tyrosine Phosphatase 1B Inhibitors. <i>Archiv Der Pharmazie</i> , 2017, 350, e1600173.	2.1	2
92	Novel 2-phenyl-3-(Pyridin-2-yl) thiazolidin-4-one derivatives as potent inhibitors for proliferation of osteosarcoma cells in <i>in vitro</i> and <i>in vivo</i> . <i>European Journal of Medicinal Chemistry</i> , 2022, 228, 114010.	2.6	2
93	Reaction mechanism and product branching ratios of OH+C ₂ H ₃ F reaction: A theoretical study. <i>Chinese Journal of Chemical Physics</i> , 2020, 33, 203-209.	0.6	1
94	Fragment-Based Ab Initio Molecular Dynamics Simulation for Combustion. <i>Molecules</i> , 2021, 26, 3120.	1.7	1
95	800 nm Bandwidth Amplified Spontaneous Emission of Divalent Cobalt Ion-doped Fiber Pumped at 550 nm. <i>Transactions of the Indian Ceramic Society</i> , 2018, 77, 188-191.	0.4	0
96	Pharmacological activation of the p53 pathway by a new compound CYZ2017 exerts anti-tumor effects. <i>Biochemical and Biophysical Research Communications</i> , 2020, 533, 1069-1075.	1.0	0
97	Effect of mutations on drug resistance of smoothened receptor toward inhibitors probed by molecular modeling. <i>Chemical Physics Letters</i> , 2020, 741, 137126.	1.2	0