Tong Zhu

List of Publications by Year
in descending order

97 papers	3,170 citations	218381 26 h-index	168136 53 g-index
112 all docs	112 docs citations	112 times ranked	3936 citing authors

#	Article	IF	Citations
1	Novel 2-phenyl-3-(Pyridin-2-yl) thiazolidin-4-one derivatives as potent inhibitors for proliferation of osteosarcoma cells inÂvitro and inÂvivo. European Journal of Medicinal Chemistry, 2022, 228, 114010.	2.6	2
2	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
3	Exploring the Chemical Space of Linear Alkane Pyrolysis via Deep Potential GENerator. Energy & Fuels, 2021, 35, 762-769.	2.5	22
4	Molecular mechanism related to the binding of fluorophores to Mango-II revealed by multiple-replica molecular dynamics simulations. Physical Chemistry Chemical Physics, 2021, 23, 10636-10649.	1.3	6
5	Cyclopentadienyl radical formation from the reaction of excited nitrogen atoms with benzene: a theoretical study. Physical Chemistry Chemical Physics, 2021, 23, 12408-12420.	1.3	9
6	Engineering the biomimetic cofactors of NMNH for cytochrome P450 BM3 based on binding conformation refinement. RSC Advances, 2021, 11, 12036-12042.	1.7	4
7	Influences of Vibrio cholerae Lipid A Types on LPS Bilayer Properties. Journal of Physical Chemistry B, 2021, 125, 2105-2112.	1.2	10
8	Fragment-Based Ab Initio Molecular Dynamics Simulation for Combustion. Molecules, 2021, 26, 3120.	1.7	1
9	Automatically Constructed Neural Network Potentials for Molecular Dynamics Simulation of Zinc Proteins. Frontiers in Chemistry, 2021, 9, 692200.	1.8	10
10	Structural basis of the stereoselective formation of the spirooxindole ring in the biosynthesis of citrinadins. Nature Communications, 2021, 12, 4158.	5.8	17
11	Benchmark Force Fields for the Molecular Dynamic Simulation of G-Quadruplexes. Molecules, 2021, 26, 5379.	1.7	12
12	CHARMM-GUI Supports Hydrogen Mass Repartitioning and Different Protonation States of Phosphates in Lipopolysaccharides. Journal of Chemical Information and Modeling, 2021, 61, 831-839.	2.5	59
13	Automated Construction of Neural Network Potential Energy Surface: The Enhanced Self-Organizing Incremental Neural Network Deep Potential Method. Journal of Chemical Information and Modeling, 2021, 61, 5425-5437.	2.5	6
14	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
15	Decoding molecular mechanism of inhibitor bindings to CDK2 using molecular dynamics simulations and binding free energy calculations. Journal of Biomolecular Structure and Dynamics, 2020, 38, 985-996.	2.0	29
16	Preferred conformations of lipooligosaccharides and oligosaccharides of Moraxella catarrhalis. Glycobiology, 2020, 30, 86-94.	1.3	6
17	ReacNetGenerator: an automatic reaction network generator for reactive molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 683-691.	1.3	54
18	Design, synthesis, and structure activity relationship (SAR) studies of novel imidazo[1,2-a] pyridine derivatives as Nek2 inhibitors. Bioorganic and Medicinal Chemistry, 2020, 28, 115775.	1.4	4

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19	Reaction mechanism and product branching ratios of OH+C2H3F reaction: A theoretical study. Chinese Journal of Chemical Physics, 2020, 33, 203-209.	0.6	1
20	Complex reaction processes in combustion unraveled by neural network-based molecular dynamics simulation. Nature Communications, 2020, 11, 5713.	5.8	111
21	Pharmacological activation of the p53 pathway by a new compound CYZ2017 exerts anti-tumor effects. Biochemical and Biophysical Research Communications, 2020, 533, 1069-1075.	1.0	0
22	An Approach to Computing Solvent Reorganization Energy. Journal of Chemical Theory and Computation, 2020, 16, 6513-6519.	2.3	3
23	Modeling and Simulation of Bacterial Outer Membranes with Lipopolysaccharides and Enterobacterial Common Antigen. Journal of Physical Chemistry B, 2020, 124, 5948-5956.	1.2	26
24	An ab initio/RRKM study of the reaction mechanism and product branching ratios of CH3OH+ and CH3OH++ dissociation. Journal of Molecular Structure, 2020, 1217, 128410.	1.8	4
25	Design, Synthesis, and Biological Evaluation of Imidazo[1,2-a]pyridine Derivatives as Novel PI3K/mTOR Dual Inhibitors. Journal of Medicinal Chemistry, 2020, 63, 3028-3046.	2.9	50
26	Effect of mutations on drug resistance of smoothened receptor toward inhibitors probed by molecular modeling. Chemical Physics Letters, 2020, 741, 137126.	1.2	0
27	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
28	A method for efficient calculation of thermal stability of proteins upon point mutations. Physical Chemistry Chemical Physics, 2020, 22, 8461-8466.	1.3	12
29	Broadband mid-infrared 2.0 Î¼m emission in Yb3+/Ho3+ co-doped silicate-germanate glasses for mid-infrared fiber amplifiers. Optical Engineering, 2020, 59, 1.	0.5	3
30	Comparison of RP-3 Pyrolysis Reactions between Surrogates and 45-Component Model by ReaxFF Molecular Dynamics Simulations. Energy & Fuels, 2019, 33, 7176-7187.	2.5	23
31	Molecular Dynamics Simulation of Zinc Ion in Water with an ab Initio Based Neural Network Potential. Journal of Physical Chemistry A, 2019, 123, 6587-6595.	1.1	24
32	A Fragment Quantum Mechanical Method for Metalloproteins. Journal of Chemical Theory and Computation, 2019, 15, 1430-1439.	2.3	17
33	Effect of mutations on binding of ligands to guanine riboswitch probed by free energy perturbation and molecular dynamics simulations. Nucleic Acids Research, 2019, 47, 6618-6631.	6.5	130
34	Self-Assembly of Metallo-Nucleoside Hydrogels for Injectable Materials That Promote Wound Closure. ACS Applied Materials & Interfaces, 2019, 11, 19743-19750.	4.0	55
35	Insights into the binding mechanisms of inhibitors of MDM2 based on molecular dynamics simulations and binding free energy calculations. Chemical Physics Letters, 2019, 728, 94-101.	1.2	4
36	Understanding Aldose Reductase-Inhibitors interactions with free energy simulation. Journal of Molecular Graphics and Modelling, 2019, 91, 10-21.	1.3	10

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37	L-4, a Well-Tolerated and Orally Active Inhibitor of Hedgehog Pathway, Exhibited Potent Anti-tumor Effects Against Medulloblastoma in vitro and in vivo. Frontiers in Pharmacology, 2019, 10, 89.	1.6	7
38	Understanding the selectivity of inhibitors toward PI4KIIIÎ± and PI4KIIIÎ² based molecular modeling. Physical Chemistry Chemical Physics, 2019, 21, 22103-22112.	1.3	22
39	Formation mechanism and spectroscopy of C₆H radicals in extreme environments: a theoretical study. Physical Chemistry Chemical Physics, 2019, 21, 23044-23055.	1.3	5
40	A quantum mechanical computational method for modeling electrostatic and solvation effects of protein. Scientific Reports, 2018, 8, 5475.	1.6	10
41	Donor Engineering for NIR-II Molecular Fluorophores with Enhanced Fluorescent Performance. Journal of the American Chemical Society, 2018, 140, 1715-1724.	6.6	379
42	Camptothecin prodrug nanomicelle based on a boronate ester-linked diblock copolymer as the carrier of doxorubicin with enhanced cellular uptake. Journal of Biomaterials Science, Polymer Edition, 2018, 29, 160-180.	1.9	11
43	800 nm Bandwidth Amplified Spontaneous Emission of Divalent Cobalt Ion-doped Fiber Pumped at 550 nm. Transactions of the Indian Ceramic Society, 2018, 77, 188-191.	0.4	0
44	Effect of Substituents in Different Positions of Aminothiazole Hinge-Binding Scaffolds on Inhibitorâ€“CDK2 Association Probed by Interaction Entropy Method. ACS Omega, 2018, 3, 18052-18064.	1.6	18
45	Developing a Bright NIRâ€II Fluorophore with Fast Renal Excretion and Its Application in Molecular Imaging of Immune Checkpoint PDâ€L1. Advanced Functional Materials, 2018, 28, 1804956.	7.8	85
46	Exploring drug-resistant mechanisms of I84V mutation in HIV-1 protease toward different inhibitors by thermodynamics integration and solvated interaction energy method. Chemical Physics Letters, 2018, 706, 400-408.	1.2	30
47	Comparison of the unfolding and oligomerization of human prion protein under acidic and neutral environments by molecular dynamics simulations. Chemical Physics Letters, 2018, 706, 594-600.	1.2	5
48	Automated Fragmentation QM/MM Calculation of NMR Chemical Shifts for Protein-Ligand Complexes. Frontiers in Chemistry, 2018, 6, 150.	1.8	14
49	A Force Balanced Fragmentation Method for ab Initio Molecular Dynamic Simulation of Protein. Frontiers in Chemistry, 2018, 6, 189.	1.8	5
50	Evaluation of the Coupled Two-Dimensional Main Chain Torsional Potential in Modeling Intrinsically Disordered Proteins. Journal of Chemical Information and Modeling, 2017, 57, 267-274.	2.5	6
51	A test of AMBER force fields in predicting the secondary structure of Î±-helical and Î²-hairpin peptides. Chemical Physics Letters, 2017, 679, 112-118.	1.2	19
52	Direct folding simulation of helical proteins using an effective polarizable bond force field. Physical Chemistry Chemical Physics, 2017, 19, 15273-15284.	1.3	13
53	An Electrochemical Biosensor with Dual Signal Outputs: Toward Simultaneous Quantification of pH and O₂ in the Brain upon Ischemia and in a Tumor during Cancer Starvation Therapy. Angewandte Chemie - International Edition, 2017, 56, 10471-10475.	7.2	84
54	Single Biosensor for Simultaneous Quantification of Glucose and pH in a Rat Brain of Diabetic Model Using Both Current and Potential Outputs. Analytical Chemistry, 2017, 89, 6656-6662.	3.2	45

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55	Invisible photochromism and optical anti-counterfeiting based on Dâ€“A type inverse diarylethene. Journal of Materials Chemistry C, 2017, 5, 4571-4577.	2.7	23
56	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
57	Discovery of Bisindole as a Novel Scaffold for Protein Tyrosine Phosphatase 1B Inhibitors. Archiv Der Pharmazie, 2017, 350, e1600173.	2.1	2
58	Structure-based design and synthesis of imidazo[1,2-a]pyridine derivatives as novel and potent Nek2 inhibitors with inÂvitro and inÂvivo antitumor activities. European Journal of Medicinal Chemistry, 2017, 126, 1083-1106.	2.6	41
59	Optimization of convergence criteria for fragmentation methods. Chemical Physics Letters, 2017, 687, 163-170.	1.2	18
60	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
61	Origins of Protons in Câ€“H Bond Insertion Products of Phenols: Proton-Self-Sufficient Function via Water Molecules. Journal of Physical Chemistry A, 2017, 121, 6523-6529.	1.1	8
62	A theoretical study of the substituent effect on reactions of amines, carbon dioxide and ethylene oxide catalyzed by binary ionic liquids. RSC Advances, 2017, 7, 51521-51527.	1.7	11
63	An Electrochemical Biosensor with Dual Signal Outputs: Toward Simultaneous Quantification of pH and O₂ in the Brain upon Ischemia and in a Tumor during Cancer Starvation Therapy. Angewandte Chemie, 2017, 129, 10607-10611.	1.6	19
64	Ferroceneâ€Grafted Photochromic Triads Based on a Sterically Hindered Ethene Bridge: Redoxâ€Switchable Fluorescence and Gated Photochromism. Advanced Optical Materials, 2016, 4, 1410-1416.	3.6	32
65	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
66	PBSA_E: A PBSA-Based Free Energy Estimator for Proteinâ€“Ligand Binding Affinity. Journal of Chemical Information and Modeling, 2016, 56, 854-861.	2.5	12
67	Predicted PAR1 inhibitors from multiple computational methods. Chemical Physics Letters, 2016, 659, 295-303.	1.2	2
68	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
69	New peptide deformylase inhibitors design, synthesis and pharmacokinetic assessment. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 3714-3718.	1.0	8
70	Enabling Light Work in Helical Self-Assembly for Dynamic Amplification of Chirality with Photoreversibility. Journal of the American Chemical Society, 2016, 138, 2219-2224.	6.6	142
71	Preclinical activity of MBM-5 in gastrointestinal cancer by inhibiting NEK2 kinase activity. Oncotarget, 2016, 7, 79327-79341.	0.8	11
72	Correct folding of an Î±-helix and a Î²-hairpin using a polarized 2D torsional potential. Scientific Reports, 2015, 5, 10359.	1.6	15

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73	Coupled Two-Dimensional Main-Chain Torsional Potential for Protein Dynamics II: Performance and Validation. Journal of Physical Chemistry B, 2015, 119, 4188-4193.	1.2	7
74	Quantum Fragment Based ab Initio Molecular Dynamics for Proteins. Journal of Chemical Theory and Computation, 2015, 11, 5897-5905.	2.3	59
75	AFNMR: automated fragmentation quantum mechanical calculation of NMR chemical shifts for biomolecules. Journal of Biomolecular NMR, 2015, 63, 125-139.	1.6	56
76	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. Journal of Chemical Information and Modeling, 2015, 55, 1903-1913.	2.5	118
77	Quantum Calculation of Protein NMR Chemical Shifts Based on the Automated Fragmentation Method. Advances in Experimental Medicine and Biology, 2015, 827, 49-70.	0.8	3
78	Energetics of protein backbone hydrogen bonds and their local electrostatic environment. Science China Chemistry, 2014, 57, 1708-1715.	4.2	7
79	Fragment Quantum Mechanical Calculation of Proteins and Its Applications. Accounts of Chemical Research, 2014, 47, 2748-2757.	7.6	173
80	Correction of erroneously packed protein's side chains in the NMR structure based on ab initio chemical shift calculations. Physical Chemistry Chemical Physics, 2014, 16, 18163.	1.3	8
81	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
82	Electronic polarization stabilizes tertiary structure prediction of HP-36. Journal of Molecular Modeling, 2014, 20, 2195.	0.8	9
83	An implementation of hydrophobic force in implicit solvent molecular dynamics simulation for packed proteins. Journal of Molecular Modeling, 2013, 19, 2605-2612.	0.8	5
84	The intrinsic helical propensities of the helical fragments in prion protein under neutral and low pH conditions: a replica exchange molecular dynamics study. Journal of Molecular Modeling, 2013, 19, 4897-4908.	0.8	8
85	A New Quantum Calibrated Force Field for Zincâ€“Protein Complex. Journal of Chemical Theory and Computation, 2013, 9, 1788-1798.	2.3	44
86	Automated Fragmentation QM/MM Calculation of Amide Proton Chemical Shifts in Proteins with Explicit Solvent Model. Journal of Chemical Theory and Computation, 2013, 9, 2104-2114.	2.3	73
87	Development of an Effective Polarizable Bond Method for Biomolecular Simulation. Journal of Physical Chemistry B, 2013, 117, 14885-14893.	1.2	19
88	Direct folding simulation of a long helix in explicit water. Applied Physics Letters, 2013, 102, .	1.5	11
89	Fragment density functional theory calculation of NMR chemical shifts for proteins with implicit solvation. Physical Chemistry Chemical Physics, 2012, 14, 7837-7845.	1.3	74
90	Polarization of Intraprotein Hydrogen Bond Is Critical to Thermal Stability of Short Helix. Journal of Physical Chemistry B, 2012, 116, 549-554.	1.2	39

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91	Proteinâ€“water hydrogen bonds are stabilized by electrostatic polarization. Molecular Physics, 2012, 110, 595-604.	0.8	5
92	Folding of a Helix Is Critically Stabilized by Polarization of Backbone Hydrogen Bonds: Study in Explicit Water. Journal of Physical Chemistry B, 2012, 116, 3430-3435.	1.2	27
93	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. European Journal of Medicinal Chemistry, 2010, 45, 227-235.	2.6	30
94	Quasi-classical trajectory study of the reaction O(3P) + HCl â†' OH + Cl and O(3P) + DCl â†' OD + Cl: Vector and scalar properties. Computational and Theoretical Chemistry, 2010, 948, 36-42.	1.5	3
95	Quasi-classical Trajectory Study of Reaction O (3 P) + HCl (v = 2; j = 1,6,9) â†' OH + Cl. Chinese Physics Letters, 2010, 27, 033102.	1.3	2
96	THE EFFECT OF VIBRATIONAL EXCITATION OF THE REACTION O(³P) + HCl â†' OH + Cl FOR THE ³Aâ€³ ELECTRONIC STATES. Journal of Theoretical and Computational Chemistry, 2010, 09, 1033-1042.	1.8	2
97	Discovery of a Potent and Selective Inhibitor of Cyclin-Dependent Kinase 4/6. Journal of Medicinal Chemistry, 2005, 48, 2388-2406.	2.9	438