Yingkai Zhang

List of Publications by Year
in descending order

115 papers	9,625 citations	57758 44 h-index	37204 96 g-index
117 all docs	117 docs citations	117 times ranked	9340 citing authors

#	Article	IF	Citations
1	De novo Design of SARS-CoV-2 Main Protease Inhibitors. Synlett, 2022, 33, 458-463.	1.8	6
2	Peptide Tethering: Pocket-Directed Fragment Screening for Peptidomimetic Inhibitor Discovery. Journal of the American Chemical Society, 2022, 144, 1198-1204.	13.7	12
3	Unified Deep Learning Model for Multitask Reaction Predictions with Explanation. Journal of Chemical Information and Modeling, 2022, 62, 1376-1387.	5.4	19
4	Accurate Prediction of Aqueous Free Solvation Energies Using 3D Atomic Feature-Based Graph Neural Network with Transfer Learning. Journal of Chemical Information and Modeling, 2022, 62, 1840-1848.	5.4	24
5	Delta Machine Learning to Improve Scoring-Ranking-Screening Performances of Protein–Ligand Scoring Functions. Journal of Chemical Information and Modeling, 2022, 62, 2696-2712.	5.4	26
6	Protein–Ligand Docking in the Machine-Learning Era. Molecules, 2022, 27, 4568.	3.8	37
7	EGCG binds intrinsically disordered N-terminal domain of p53 and disrupts p53-MDM2 interaction. Nature Communications, 2021, 12, 986.	12.8	77
8	Dataset Construction to Explore Chemical Space with 3D Geometry and Deep Learning. Journal of Chemical Information and Modeling, 2021, 61, 1095-1104.	5.4	11
9	Dominant role of CDKN2B/p15INK4B of 9p21.3 tumor suppressor hub in inhibition of cell-cycle and glycolysis. Nature Communications, 2021, 12, 2047.	12.8	30
10	Selective and noncovalent targeting of RAS mutants for inhibition and degradation. Nature Communications, 2021, 12, 2656.	12.8	51
11	Identification of Secondary Binding Sites on Protein Surfaces for Rational Elaboration of Synthetic Protein Mimics. ACS Chemical Biology, 2021, 16, 1179-1183.	3.4	6
12	Lin_F9: A Linear Empirical Scoring Function for Protein–Ligand Docking. Journal of Chemical Information and Modeling, 2021, 61, 4630-4644.	5.4	13
13	Targeting Amyloidogenic Processing of APP in Alzheimer's Disease. Frontiers in Molecular Neuroscience, 2020, 13, 137.	2.9	73
14	Substrate–Enzyme Interactions in Intramembrane Proteolysis: γ-Secretase as the Prototype. Frontiers in Molecular Neuroscience, 2020, 13, 65.	2.9	3
15	An in silico mechanistic insight into HDAC8 activation facilitates the discovery of new small-molecule activators. Bioorganic and Medicinal Chemistry, 2020, 28, 115607.	3.0	5
16	Inhibition of striatal-enriched protein tyrosine phosphatase by targeting computationally revealed cryptic pockets. European Journal of Medicinal Chemistry, 2020, 190, 112131.	5.5	3
17	Molecular basis for receptor tyrosine kinase A-loop tyrosine transphosphorylation. Nature Chemical Biology, 2020, 16, 267-277.	8.0	31
18	AlphaSpace 2.0: Representing Concave Biomolecular Surfaces Using β-Clusters. Journal of Chemical Information and Modeling, 2020, 60, 1494-1508.	5.4	7

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19	Substrate interaction inhibits γ-secretase production of amyloid-β peptides. Chemical Communications, 2020, 56, 2578-2581.	4.1	3
20	Modulation of virus-induced NF-κB signaling by NEMO coiled coil mimics. Nature Communications, 2020, 11, 1786.	12.8	30
21	A Conserved Allosteric Pathway in Tyrosine Kinase Regulation. Structure, 2019, 27, 1308-1315.e3.	3.3	16
22	Incorporating Explicit Water Molecules and Ligand Conformation Stability in Machine-Learning Scoring Functions. Journal of Chemical Information and Modeling, 2019, 59, 4540-4549.	5.4	66
23	Predicting Molecular Energy Using Force-Field Optimized Geometries and Atomic Vector Representations Learned from an Improved Deep Tensor Neural Network. Journal of Chemical Theory and Computation, 2019, 15, 4113-4121.	5.3	25
24	Identification and structure–function analyses of an allosteric inhibitor of the tyrosine phosphatase PTPN22. Journal of Biological Chemistry, 2019, 294, 8653-8663.	3.4	8
25	Intrinsic cleavage of RNA polymerase II adopts a nucleobase-independent mechanism assisted by transcript phosphate. Nature Catalysis, 2019, 2, 228-235.	34.4	13
26	Exploring fragment-based target-specific ranking protocol with machine learning on cathepsin S. Journal of Computer-Aided Molecular Design, 2019, 33, 1095-1105.	2.9	10
27	Two symmetric arginine residues play distinct roles in *Thermus thermophilus* Argonaute DNA guide strand-mediated DNA target cleavage. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 845-853.	7.1	15
28	Synergistic effects of H3 and H4 nucleosome tails on structure and dynamics of a lesion-containing DNA: Binding of a displaced lesion partner base to the H3 tail for GG-NER recognition. DNA Repair, 2018, 65, 73-78.	2.8	10
29	Computational Strategy for Bound State Structure Prediction in Structure-Based Virtual Screening: A Case Study of Protein Tyrosine Phosphatase Receptor Type O Inhibitors. Journal of Chemical Information and Modeling, 2018, 58, 2331-2342.	5.4	8
30	Lesion Sensing during Initial Binding by Yeast XPC/Rad4: Toward Predicting Resistance to Nucleotide Excision Repair. Chemical Research in Toxicology, 2018, 31, 1260-1268.	3.3	20
31	Functional loop dynamics of the S-component of ECF transporter FolT. Molecular Physics, 2018, 116, 2613-2621.	1.7	0
32	Nucleotide Excision Repair Lesion-Recognition Protein Rad4 Captures a Pre-Flipped Partner Base in a Benzo[*a*]pyrene-Derived DNA Lesion: How Structure Impacts the Binding Pathway. Chemical Research in Toxicology, 2017, 30, 1344-1354.	3.3	32
33	Design, synthesis and biological evaluation of quinoline derivatives as HDAC class I inhibitors. European Journal of Medicinal Chemistry, 2017, 133, 11-23.	5.5	35
34	Nucleosome Histone Tail Conformation and Dynamics: Impacts of Lysine Acetylation and a Nearby Minor Groove Benzo[*a*]pyrene-Derived Lesion. Biochemistry, 2017, 56, 1963-1973.	2.5	20
35	Targeting Unoccupied Surfaces on Protein–Protein Interfaces. Journal of the American Chemical Society, 2017, 139, 15560-15563.	13.7	41
36	Improving scoring-docking-screening powers of protein-ligand scoring functions using random forest. Journal of Computational Chemistry, 2017, 38, 169-177.	3.3	201

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37	Resveratrol serves as a protein-substrate interaction stabilizer in human SIRT1 activation. Scientific Reports, 2016, 6, 38186.	3.3	71
38	Born–Oppenheimer Ab Initio QM/MM Molecular Dynamics Simulations of Enzyme Reactions. Methods in Enzymology, 2016, 577, 105-118.	1.0	23
39	Bimetallic C–C Bond-Forming Reductive Elimination from Nickel. Journal of the American Chemical Society, 2016, 138, 4779-4786.	13.7	70
40	Amide Rotation Hindrance Predicts Proteolytic Resistance of Cystine-Knot Peptides. Journal of Physical Chemistry Letters, 2016, 7, 1138-1142.	4.6	6
41	Entrapment of a Histone Tail by a DNA Lesion in a Nucleosome Suggests the Lesion Impacts Epigenetic Marking: A Molecular Dynamics Study. Biochemistry, 2016, 55, 239-242.	2.5	10
42	Thiol versus hydroxamate as zinc binding group in <scp>HDAC</scp> inhibition: An <i>Ab initio</i><scp>QM</scp>/<scp>MM</scp> molecular dynamics study. Journal of Computational Chemistry, 2015, 36, 2228-2235.	3.3	22
43	Computational Design of a Time-Dependent Histone Deacetylase 2 Selective Inhibitor. ACS Chemical Biology, 2015, 10, 687-692.	3.4	41
44	AlphaSpace: Fragment-Centric Topographical Mapping To Target Protein–Protein Interaction Interfaces. Journal of Chemical Information and Modeling, 2015, 55, 1585-1599.	5.4	47
45	Recognition of Damaged DNA for Nucleotide Excision Repair: A Correlated Motion Mechanism with a Mismatched <i>cis-syn</i> Thymine Dimer Lesion. Biochemistry, 2015, 54, 5263-5267.	2.5	26
46	Mechanistic Insights into a Classic Wonder Drug—Aspirin. Journal of the American Chemical Society, 2015, 137, 70-73.	13.7	66
47	Improved parameterization of interatomic potentials for rare gas dimers with density-based energy decomposition analysis. Journal of Chemical Physics, 2014, 140, 214117.	3.0	8
48	Structural and Dynamic Characterization of Polymerase κ's Minor Groove Lesion Processing Reveals How Adduct Topology Impacts Fidelity. Biochemistry, 2014, 53, 5683-5691.	2.5	16
49	How Is Acetylcholinesterase Phosphonylated by Soman? An <i>Ab Initio</i> QM/MM Molecular Dynamics Study. Journal of Physical Chemistry A, 2014, 118, 9132-9139.	2.5	24
50	Peptide Conformation Analysis Using an Integrated Bayesian Approach. Journal of Chemical Theory and Computation, 2014, 10, 4152-4159.	5.3	19
51	DNA Cytosine Methylation: Structural and Thermodynamic Characterization of the Epigenetic Marking Mechanism. Biochemistry, 2013, 52, 2828-2838.	2.5	33
52	Free Energy Profiles of Base Flipping in Intercalative Polycyclic Aromatic Hydrocarbon-Damaged DNA Duplexes: Energetic and Structural Relationships to Nucleotide Excision Repair Susceptibility. Chemical Research in Toxicology, 2013, 26, 1115-1125.	3.3	18
53	Sirtuin Deacetylation Mechanism and Catalytic Role of the Dynamic Cofactor Binding Loop. Journal of Physical Chemistry Letters, 2013, 4, 491-495.	4.6	29
54	Preferred WMSA catalytic mechanism of the nucleotidyl transfer reaction in human DNA polymerase κ elucidates error-free bypass of a bulky DNA lesion. Nucleic Acids Research, 2012, 40, 9193-9205.	14.5	34

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55	QM/MM Molecular Dynamics Study of Purine-Specific Nucleoside Hydrolase. Journal of Physical Chemistry B, 2012, 116, 1984-1991.	2.6	23
56	Aging Mechanism of Soman Inhibited Acetylcholinesterase. Journal of Physical Chemistry B, 2012, 116, 12199-12207.	2.6	51
57	Revelation of a Catalytic Calcium-Binding Site Elucidates Unusual Metal Dependence of a Human Apyrase. Journal of the American Chemical Society, 2012, 134, 15595-15603.	13.7	23
58	An Internal Water-Retention Site in the Rhomboid Intramembrane Protease GlpG Ensures Catalytic Efficiency. Structure, 2012, 20, 1255-1263.	3.3	36
59	Serine protease acylation proceeds with a subtle re-orientation of the histidine ring at the tetrahedral intermediate. Chemical Communications, 2011, 47, 1577-1579.	4.1	47
60	Ab Initio QM/MM Free-Energy Studies of Arginine Deiminase Catalysis: The Protonation State of the Cys Nucleophile. Journal of Physical Chemistry B, 2011, 115, 3725-3733.	2.6	22
61	Molecular Mechanism for Eliminylation, a Newly Discovered Post-Translational Modification. Journal of the American Chemical Society, 2011, 133, 11103-11105.	13.7	28
62	Directional Dependence of Hydrogen Bonds: A Density-Based Energy Decomposition Analysis and Its Implications on Force Field Development. Journal of Chemical Theory and Computation, 2011, 7, 4038-4049.	5.3	35
63	A Transferable Nonbonded Pairwise Force Field to Model Zinc Interactions in Metalloproteins. Journal of Chemical Theory and Computation, 2011, 7, 433-443.	5.3	47
64	Zinc Chelation with Hydroxamate in Histone Deacetylases Modulated by Water Access to the Linker Binding Channel. Journal of the American Chemical Society, 2011, 133, 6110-6113.	13.7	91
65	Flexibility of Catalytic Zinc Coordination in Thermolysin and HDAC8: A Born–Oppenheimer ab Initio QM/MM Molecular Dynamics Study. Journal of Chemical Theory and Computation, 2010, 6, 337-343.	5.3	76
66	Base Flipping Free Energy Profiles for Damaged and Undamaged DNA. Chemical Research in Toxicology, 2010, 23, 1868-1870.	3.3	26
67	A Proton-Shuttle Reaction Mechanism for Histone Deacetylase 8 and the Catalytic Role of Metal Ions. Journal of the American Chemical Society, 2010, 132, 9471-9479.	13.7	121
68	Catalytic Reaction Mechanism of Acetylcholinesterase Determined by Born–Oppenheimer Ab Initio QM/MM Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 8817-8825.	2.6	109
69	Reaction Mechanism of Monoethanolamine with CO_2 in Aqueous Solution from Molecular Modeling. Journal of Physical Chemistry A, 2010, 114, 11844-11852.	2.5	161
70	Introducing sampling entropy in repository based adaptive umbrella sampling. Journal of Chemical Physics, 2009, 131, 214105.	3.0	2
71	Increasing the time step with mass scaling in Born–Oppenheimer *ab initio* QM/MM molecular dynamics simulations. Journal of Computational Chemistry, 2009, 30, 2706-2711.	3.3	31
72	Side chain specificity of ADP-ribosylation by a sirtuin. FEBS Journal, 2009, 276, 7159-7176.	4.7	26

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73	Reaction Pathway and Free-Energy Barrier for Reactivation of Dimethylphosphoryl-Inhibited Human Acetylcholinesterase. Journal of Physical Chemistry B, 2009, 113, 16226-16236.	2.6	53
74	Importance of Charge Independent Effects in Readout of the Trimethyllysine Mark by HP1 Chromodomain. Journal of the American Chemical Society, 2009, 131, 14928-14931.	13.7	22
75	Polymerase-Tailored Variations in the Water-Mediated and Substrate-Assisted Mechanism for Nucleotidyl Transfer: Insights from a Study of T7 DNA Polymerase. Journal of Molecular Biology, 2009, 389, 787-796.	4.2	28
76	Active Site Cysteine Is Protonated in the PAD4 Michaelis Complex: Evidence from Bornâˆ'Oppenheimer Ab Initio QM/MM Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 12750-12758.	2.6	36
77	Density-based energy decomposition analysis for intermolecular interactions with variationally determined intermediate state energies. Journal of Chemical Physics, 2009, 131, 164112.	3.0	125
78	Bornâˆ'Oppenheimer ab Initio QM/MM Molecular Dynamics Simulations of the Hydrolysis Reaction Catalyzed by Protein Arginine Deiminase 4. Journal of Physical Chemistry B, 2009, 113, 16705-16710.	2.6	37
79	Ab Initio Quantum Mechanical/Molecular Mechanical Studies of Histone Modifying Enzymes. Challenges and Advances in Computational Chemistry and Physics, 2009, , 341-350.	0.6	1
80	Highly Dissociative and Concerted Mechanism for the Nicotinamide Cleavage Reaction in Sir2Tm Enzyme Suggested by Ab Initio QM/MM Molecular Dynamics Simulations. Journal of the American Chemical Society, 2008, 130, 16721-16728.	13.7	77
81	How Do SET-Domain Protein Lysine Methyltransferases Achieve the Methylation State Specificity? Revisited by Ab Initio QM/MM Molecular Dynamics Simulations. Journal of the American Chemical Society, 2008, 130, 3806-3813.	13.7	84
82	Interfacing ab Initio Quantum Mechanical Method with Classical Drude Osillator Polarizable Model for Molecular Dynamics Simulation of Chemical Reactions. Journal of Chemical Theory and Computation, 2008, 4, 1237-1248.	5.3	67
83	Determination of free energy profiles by repository based adaptive umbrella sampling: Bridging nonequilibrium and quasiequilibrium simulations. Journal of Chemical Physics, 2008, 128, 204106.	3.0	10
84	Design-atom approach for the quantum mechanical/molecular mechanical covalent boundary: A design-carbon atom with five valence electrons. Journal of Chemical Physics, 2007, 127, 124102.	3.0	20
85	Catalytic Mechanism and Metal Specificity of Bacterial Peptide Deformylase:Â A Density Functional Theory QM/MM Study. Journal of Physical Chemistry B, 2007, 111, 6229-6235.	2.6	26
86	A Water-Mediated and Substrate-Assisted Catalytic Mechanism forSulfolobus solfataricusDNA Polymerase IV. Journal of the American Chemical Society, 2007, 129, 4731-4737.	13.7	118
87	Ab Initio Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation of Enzyme Catalysis:â€‰ The Case of Histone Lysine Methyltransferase SET7/9. Journal of Physical Chemistry B, 2007, 111, 3758-3764.	2.6	78
88	Tuning the Membrane Selectivity of Antimicrobial Peptides by Using Multivalent Design. ChemBioChem, 2007, 8, 2063-2065.	2.6	55
89	Catalytic Mechanism and Product Specificity of the Histone Lysine Methyltransferase SET7/9:Â An ab Initio QM/MM-FE Study with Multiple Initial Structures. Journal of the American Chemical Society, 2006, 128, 1272-1278.	13.7	141
90	Unexpected Deacetylation Mechanism Suggested by a Density Functional Theory QM/MM Study of Histone-Deacetylase-Like Protein. Journal of the American Chemical Society, 2006, 128, 4530-4531.	13.7	98

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91	Geometric Preferences in Iron(II) and Zinc(II) Model Complexes of Peptide Deformylase. Inorganic Chemistry, 2006, 45, 1409-1411.	4.0	15
92	How does activation loop phosphorylation modulate catalytic activity in the cAMP-dependent protein kinase: A theoretical study. Protein Science, 2006, 15, 672-683.	7.6	55
93	Pseudobond ab initio QM/MM approach and its applications to enzyme reactions. Theoretical Chemistry Accounts, 2006, 116, 43-50.	1.4	148
94	Molecular docking of balanol to dynamics snapshots of protein kinase A. Proteins: Structure, Function and Bioinformatics, 2005, 61, 850-858.	2.6	60
95	An efficient approach for ab initio energy calculation of biopolymers. Journal of Chemical Physics, 2005, 122, 184105.	3.0	96
96	Improved pseudobonds for combined ab initio quantum mechanical/molecular mechanical methods. Journal of Chemical Physics, 2005, 122, 024114.	3.0	147
97	How Does the cAMP-Dependent Protein Kinase Catalyze the Phosphorylation Reaction:Â An ab Initio QM/MM Study. Journal of the American Chemical Society, 2005, 127, 1553-1562.	13.7	140
98	An efficient linear scaling method for ab initio calculation of electron density of proteins. Chemical Physics Letters, 2004, 394, 293-297.	2.6	100
99	Studying the roles of W86, E202, and Y337 in binding of acetylcholine to acetylcholinesterase using a combined molecular dynamics and multiple docking approach. Protein Science, 2003, 12, 2675-2684.	7.6	41
100	Influence of Structural Fluctuation on Enzyme Reaction Energy Barriers in Combined Quantum Mechanical/Molecular Mechanical Studies. Journal of Physical Chemistry B, 2003, 107, 4459-4463.	2.6	108
101	Ab Initio QM/MM Study Shows There Is No General Acid in the Reaction Catalyzed by 4-Oxalocrotonate Tautomerase. Journal of the American Chemical Society, 2003, 125, 10384-10393.	13.7	89
102	Studying the affinity and kinetics of molecular association with molecular-dynamics simulation. Journal of Chemical Physics, 2003, 118, 1821-1827.	3.0	26
103	Role of the Catalytic Triad and Oxyanion Hole in Acetylcholinesterase Catalysis:â€‰ An ab initio QM/MM Study. Journal of the American Chemical Society, 2002, 124, 10572-10577.	13.7	243
104	Studying Enzyme Binding Specificity in Acetylcholinesterase Using a Combined Molecular Dynamics and Multiple Docking Approach. Journal of the American Chemical Society, 2002, 124, 8260-8267.	13.7	101
105	Ab Initio QM/MM and Free Energy Calculations of Enzyme Reactions. Lecture Notes in Computational Science and Engineering, 2002, , 333-355.	0.3	6
106	Density functional study of a weakly hydrogen-bonded benzene-ammonia complex: The importance of the exchange functional. International Journal of Quantum Chemistry, 2000, 79, 325-329.	2.0	15
107	Perspective on "Density-functional theory for fractional particle number: derivative discontinuities of the energy". Theoretical Chemistry Accounts, 2000, 103, 346-348.	1.4	124
108	Degenerate Ground States and a Fractional Number of Electrons in Density and Reduced Density Matrix Functional Theory. Physical Review Letters, 2000, 84, 5172-5175.	7.8	390

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109	Free energy calculation on enzyme reactions with an efficient iterative procedure to determine minimum energy paths on a combined ab initio QM/MM potential energy surface. Journal of Chemical Physics, 2000, 112, 3483-3492.	3.0	434
110	Perspective on â€œDensity-functional theory for fractional particle number: derivative discontinuities of the energyâ€. , 2000, , 346-348.		14
111	How Is the Active Site of Enolase Organized To Catalyze Two Different Reaction Steps?. Journal of the American Chemical Society, 2000, 122, 6560-6570.	13.7	103
112	A pseudobond approach to combining quantum mechanical and molecular mechanical methods. Journal of Chemical Physics, 1999, 110, 46-54.	3.0	460
113	Comment on â€œGeneralized Gradient Approximation Made Simpleâ€. Physical Review Letters, 1998, 80, 890-890.	7.8	2,323
114	A challenge for density functionals: Self-interaction error increases for systems with a noninteger number of electrons. Journal of Chemical Physics, 1998, 109, 2604-2608.	3.0	524
115	Describing van der Waals Interaction in diatomic molecules with generalized gradient approximations: The role of the exchange functional. Journal of Chemical Physics, 1997, 107, 7921-7925.	3.0	282