Kenneth M Merz Jr

List of Publications by Year
in descending order

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471	42,938	8732 75	2375 198
papers	citations	h-index	g-index

489	489	489	34192
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A Second Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules. Journal of the American Chemical Society, 1995, 117, 5179-5197.	6.6	12,116
2	The Amber biomolecular simulation programs. Journal of Computational Chemistry, 2005, 26, 1668-1688.	1.5	7,742
3	Atomic charges derived from semiempirical methods. Journal of Computational Chemistry, 1990, 11, 431-439.	1.5	3,004
4	Prediction of Drug Absorption Using Multivariate Statistics. Journal of Medicinal Chemistry, 2000, 43, 3867-3877.	2.9	1,254
5	Rational Design of Particle Mesh Ewald Compatible Lennard-Jones Parameters for +2 Metal Cations in Explicit Solvent. Journal of Chemical Theory and Computation, 2013, 9, 2733-2748.	2.3	559
6	MCPB.py: A Python Based Metal Center Parameter Builder. Journal of Chemical Information and Modeling, 2016, 56, 599-604.	2.5	416
7	Structural Survey of Zinc-Containing Proteins and Development of the Zinc AMBER Force Field (ZAFF). Journal of Chemical Theory and Computation, 2010, 6, 2935-2947.	2.3	378
8	Systematic Parameterization of Monovalent Ions Employing the Nonbonded Model. Journal of Chemical Theory and Computation, 2015, 11, 1645-1657.	2.3	334
9	Combined Quantum Mechanical/Molecular Mechanical Methodologies Applied to Biomolecular Systems. Accounts of Chemical Research, 1999, 32, 904-911.	7.6	325
10	Assessment of the â€œ6-31+G** + LANL2DZâ€•Mixed Basis Set Coupled with Density Functional Theory Methods and the Effective Core Potential: Prediction of Heats of Formation and Ionization Potentials for First-Row-Transition-Metal Complexes. Journal of Physical Chemistry A, 2009, 113, 9843-9851.	1.1	313
11	Taking into Account the Ion-Induced Dipole Interaction in the Nonbonded Model of Ions. Journal of Chemical Theory and Computation, 2014, 10, 289-297.	2.3	305
12	Critical Assessment of the Performance of Density Functional Methods for Several Atomic and Molecular Properties. Journal of Chemical Theory and Computation, 2007, 3, 407-433.	2.3	295
13	High throughput docking for library design and library prioritization. Proteins: Structure, Function and Bioinformatics, 2001, 43, 113-124.	1.5	283
14	d10-d10 Interactions: multinuclear copper(I) complexes. Inorganic Chemistry, 1988, 27, 2120-2127.	1.9	272
15	Metal Ion Modeling Using Classical Mechanics. Chemical Reviews, 2017, 117, 1564-1686.	23.0	266
16	Force field design for metalloproteins. Journal of the American Chemical Society, 1991, 113, 8262-8270.	6.6	265
17	Semiempirical molecular orbital calculations with linear system size scaling. Journal of Chemical Physics, 1996, 104, 6643-6649.	1.2	258
18	Parameterization of Highly Charged Metal Ions Using the 12-6-4 LJ-Type Nonbonded Model in Explicit Water. Journal of Physical Chemistry B, 2015, 119, 883-895.	1.2	237

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19	The role of quantum mechanics in structure-based drug design. Drug Discovery Today, 2007, 12, 725-731.	3.2	226
20	Prediction of Aqueous Solubility of a Diverse Set of Compounds Using Quantitative Structureâ^'Property Relationships. Journal of Medicinal Chemistry, 2003, 46, 3572-3580.	2.9	211
21	Fast, accurate semiempirical molecular orbital calculations for macromolecules. Journal of Chemical Physics, 1997, 107, 879-893.	1.2	208
22	Large-Scale Validation of a Quantum Mechanics Based Scoring Function:Â Predicting the Binding Affinity and the Binding Mode of a Diverse Set of Proteinâ^'Ligand Complexes. Journal of Medicinal Chemistry, 2005, 48, 4558-4575.	2.9	193
23	A comparison of DMPC- and DLPE-based lipid bilayers. Biophysical Journal, 1994, 66, 1076-1087.	0.2	163
24	Carbon dioxide binding to human carbonic anhydrase II. Journal of the American Chemical Society, 1991, 113, 406-411.	6.6	160
25	Insights into the Strength and Origin of Halogen Bonding:Â The Halobenzeneâ^'Formaldehyde Dimer. Journal of Physical Chemistry A, 2007, 111, 1688-1694.	1.1	157
26	A Quantum Mechanics-Based Scoring Function:â€‰ Study of Zinc Ion-Mediated Ligand Binding. Journal of the American Chemical Society, 2004, 126, 1020-1021.	6.6	150
27	Application of the NosÃ©â^'Hoover Chain Algorithm to the Study of Protein Dynamics. The Journal of Physical Chemistry, 1996, 100, 1927-1937.	2.9	149
28	Computer modeling of the interactions of complex molecules. Accounts of Chemical Research, 1990, 23, 246-252.	7.6	146
29	Calculation of solvation free energies using a density functional/molecular dynamics coupled potential. The Journal of Physical Chemistry, 1993, 97, 11868-11870.	2.9	146
30	Free energy perturbation simulations of the inhibition of thermolysin: prediction of the free energy of binding of a new inhibitor. Journal of the American Chemical Society, 1989, 111, 5649-5658.	6.6	145
31	Using AMBER18 for Relative Free Energy Calculations. Journal of Chemical Information and Modeling, 2019, 59, 3128-3135.	2.5	138
32	Density functional transition states of organic and organometallic reactions. Journal of Chemical Physics, 1994, 100, 434-443.	1.2	135
33	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	18.7	128
34	Formal Estimation of Errors in Computed Absolute Interaction Energies of Proteinâ^'Ligand Complexes. Journal of Chemical Theory and Computation, 2011, 7, 790-797.	2.3	127
35	The mode of action of carbonic anhydrase. Journal of the American Chemical Society, 1989, 111, 5636-5649.	6.6	126
36	Divide and Conquer Hartreeâ^'Fock Calculations on Proteins. Journal of Chemical Theory and Computation, 2010, 6, 405-411.	2.3	124

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37	Free energy calculations on protein stability: Thr-157 .fwdarw. Val-157 mutation of T4 lysozyme. Journal of the American Chemical Society, 1989, 111, 8505-8508.	6.6	123
38	Rapid approximation to molecular surface area via the use of Boolean logic and look-up tables. Journal of Computational Chemistry, 1993, 14, 349-352.	1.5	123
39	A force field for monosaccharides and (1 ? 4) linked polysaccharides. Journal of Computational Chemistry, 1994, 15, 1019-1040.	1.5	121
40	Solvent Dynamics and Mechanism of Proton Transfer in Human Carbonic Anhydrase II. Journal of the American Chemical Society, 1999, 121, 2290-2302.	6.6	120
41	Analysis of a large data base of electrostatic potential derived atomic charges. Journal of Computational Chemistry, 1992, 13, 749-767.	1.5	114
42	Study of hydrogen bonding interactions relevant to biomolecular structure and function. Journal of Computational Chemistry, 1992, 13, 1151-1169.	1.5	114
43	3,4-Connected carbon nets: through-space and through-bond interactions in the solid state. Journal of the American Chemical Society, 1987, 109, 6742-6751.	6.6	113
44	The Ecstasy and Agony of Assay Interference Compounds. Journal of Medicinal Chemistry, 2017, 60, 2165-2168.	2.9	113
45	Explicitly Representing the Solvation Shell in Continuum Solvent Calculations. Journal of Physical Chemistry A, 2009, 113, 6404-6409.	1.1	112
46	Mechanism of the human carbonic anhydrase II-catalyzed hydration of carbon dioxide. Journal of the American Chemical Society, 1992, 114, 10498-10507.	6.6	108
47	Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, 10881-10905.	1.7	108
48	Structure and dynamics of the dilauroylphosphatidylethanolamine lipid bilayer. Biochemistry, 1992, 31, 7656-7664.	1.2	103
49	Insights into the function of the zinc hydroxide-Thr199-Glu106 hydrogen bonding network in carbonic anhydrases. Journal of Molecular Biology, 1990, 214, 799-802.	2.0	102
50	Head group-water interactions in lipid bilayers: a comparison between DMPC- and DLPE-based lipid bilayers. Langmuir, 1993, 9, 1179-1183.	1.6	101
51	Free Energy Perturbation Study of Octanol/Water Partition Coefficients:â€‰Comparison with Continuum GB/SA Calculations. Journal of Physical Chemistry B, 1999, 103, 714-726.	1.2	100
52	Hybrid QM/MM and DFT Investigations of the Catalytic Mechanism and Inhibition of the Dinuclear Zinc Metallo-Î²-Lactamase CcrA fromBacteroidesfragilis. Journal of the American Chemical Society, 2005, 127, 4232-4241.	6.6	100
53	X-ray diffraction "fingerprinting" of DNA structure in solution for quantitative evaluation of molecular dynamics simulation. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 3534-3539.	3.3	100
54	Ice-binding mechanism of winter flounder antifreeze proteins. Biophysical Journal, 1997, 73, 2851-2873.	0.2	98

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55	An examination of a density functional/molecular mechanical coupled potential. Journal of Computational Chemistry, 1995, 16, 113-128.	1.5	96
56	The Role of Polarization and Charge Transfer in the Solvation of Biomolecules. Journal of the American Chemical Society, 1999, 121, 9182-9190.	6.6	96
57	Protein dynamics and solvation in aqueous and nonaqueous environments. Journal of the American Chemical Society, 1993, 115, 6529-6537.	6.6	95
58	Assessment of Density Functional Theory Methods for the Computation of Heats of Formation and Ionization Potentials of Systems Containing Third Row Transition Metals. Journal of Physical Chemistry A, 2007, 111, 6044-6053.	1.1	94
59	Fully Quantum Mechanical Description of Proteins in Solution. Combining Linear Scaling Quantum Mechanical Methodologies with the Poissonâ^'Boltzmann Equation. Journal of Physical Chemistry A, 1999, 103, 5171-5188.	1.1	91
60	One-Dimensional Molecular Representations and Similarity Calculations:Â Methodology and Validation. Journal of Medicinal Chemistry, 2001, 44, 3795-3809.	2.9	90
61	Protein NMR Chemical Shift Calculations Based on the Automated Fragmentation QM/MM Approach. Journal of Physical Chemistry B, 2009, 113, 10380-10388.	1.2	90
62	Assigning the Protonation States of the Key Aspartates in Î²-Secretase Using QM/MM X-ray Structure Refinement. Journal of Chemical Theory and Computation, 2006, 2, 1057-1069.	2.3	89
63	New developments in applying quantum mechanics to proteins. Current Opinion in Structural Biology, 2001, 11, 217-223.	2.6	88
64	Using Quantum Mechanical Approaches to Study Biological Systems. Accounts of Chemical Research, 2014, 47, 2804-2811.	7.6	86
65	Charge-Transfer Interactions in Macromolecular Systems:â€‰ A New View of the Protein/Water Interface. Journal of the American Chemical Society, 1998, 120, 5593-5594.	6.6	84
66	Zinc Metallo-Î²-Lactamase from Bacteroides fragilis:â€‰ A Quantum Chemical Study on Model Systems of the Active Site. Journal of the American Chemical Society, 2000, 122, 4197-4208.	6.6	84
67	Divide and Conquer Interaction Energy Decomposition. Journal of Physical Chemistry A, 1999, 103, 3321-3329.	1.1	83
68	Limits of Free Energy Computation for Proteinâ^'Ligand Interactions. Journal of Chemical Theory and Computation, 2010, 6, 1769-1776.	2.3	83
69	Ureases:â€‰ Quantum Chemical Calculations on Cluster Models. Journal of the American Chemical Society, 2003, 125, 15324-15337.	6.6	82
70	Further analysis and comparative study of intermolecular interactions using dimers from the S22 database. Journal of Chemical Physics, 2009, 131, 065102.	1.2	82
71	The BioFragment Database (BFDb): An open-data platform for computational chemistry analysis of noncovalent interactions. Journal of Chemical Physics, 2017, 147, 161727.	1.2	82
72	Parameterization of Monovalent Ions for the OPC3, OPC, TIP3P-FB, and TIP4P-FB Water Models. Journal of Chemical Information and Modeling, 2021, 61, 869-880.	2.5	81

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73	Linear scaling molecular orbital calculations of biological systems using the semiempirical divide and conquer method. Journal of Computational Chemistry, 2000, 21, 1494-1504.	1.5	80
74	The Hydrolysis of Urea and the Proficiency of Urease. Journal of the American Chemical Society, 2004, 126, 6932-6944.	6.6	78
75	Mixed Quantum Mechanics/Molecular Mechanics Scoring Function To Predict Proteinâ^'Ligand Binding Affinity. Journal of Chemical Theory and Computation, 2010, 6, 3079-3091.	2.3	78
76	The Ecstasy and Agony of Assay Interference Compounds. ACS Central Science, 2017, 3, 143-147.	5.3	78
77	Binding of Bicarbonate to Human Carbonic Anhydrase II:Â A Continuum of Binding States. Journal of the American Chemical Society, 1997, 119, 863-871.	6.6	77
78	Quantum mechanical/quantum mechanical methods. I. A divide and conquer strategy for solving the SchrÃ¶dinger equation for large molecular systems using a composite density functionalâ€“semiempirical Hamiltonian. Journal of Chemical Physics, 2000, 113, 5604-5613.	1.2	77
79	Molecular Dynamics Study of Ethanolamine as a Pure Liquid and in Aqueous Solution. Journal of Physical Chemistry B, 2007, 111, 3695-3703.	1.2	77
80	Molecular Dynamics Simulations of the Mononuclear Zinc-Î²-lactamase fromBacillus Cereus. Journal of the American Chemical Society, 2001, 123, 3759-3770.	6.6	75
81	Molecular Dynamics Study of the IIA Binding Site in Human Serum Albumin:Â Influence of the Protonation State of Lys195 and Lys199. Journal of Medicinal Chemistry, 2001, 44, 250-260.	2.9	74
82	Insights into the Structure and Dynamics of the Dinuclear Zinc Î²-Lactamase Site fromBacteroides fragilisâ€. Biochemistry, 2002, 41, 6615-6630.	1.2	74
83	AM1 parameters for zinc. Organometallics, 1988, 7, 522-524.	1.1	70
84	Novel Acyclic Diaminocarbene Ligands with Increased Steric Demand and Their Application in Gold Catalysis. Organic Letters, 2010, 12, 4860-4863.	2.4	70
85	Importance of Dispersion and Electron Correlation in ab Initio Protein Folding. Journal of Physical Chemistry B, 2009, 113, 5290-5300.	1.2	67
86	Molecular Dynamics Simulations of the Mononuclear Zinc-Î²-lactamase fromBacilluscereusComplexed with Benzylpenicillin and a Quantum Chemical Study of the Reaction Mechanism. Journal of the American Chemical Society, 2001, 123, 9867-9879.	6.6	66
87	Evolution of Alchemical Free Energy Methods in Drug Discovery. Journal of Chemical Information and Modeling, 2020, 60, 5308-5318.	2.5	66
88	Gas-phase and solution-phase potential energy surfaces for carbon dioxide + n-water (n = 1,2). Journal of the American Chemical Society, 1990, 112, 7973-7980.	6.6	64
89	Determination of pKas of ionizable groups in proteins: the pKa of Glu 7 and 35 in hen eggs white lysozyme and Glu 106 in human carbonic anhydrase II. Journal of the American Chemical Society, 1991, 113, 3572-3575.	6.6	64
90	Disruption of the Active Site Solvent Network in Carbonic Anhydrase II Decreases the Efficiency of Proton Transferâ€. Biochemistry, 1996, 35, 16421-16428.	1.2	64

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91	Stability and Activity of Mesophilic Subtilisin E and Its Thermophilic Homolog:â€‰ Insights from Molecular Dynamics Simulations. Journal of the American Chemical Society, 1999, 121, 6895-6903.	6.6	64
92	Are Many-Body Effects Important in Protein Folding?. Journal of Physical Chemistry B, 2000, 104, 9554-9563.	1.2	64
93	Dynamic Force Field Models: Molecular Dynamics Simulations of Human Carbonic Anhydrase II Using a Quantum Mechanical/Molecular Mechanical Coupled Potential. The Journal of Physical Chemistry, 1995, 99, 11266-11275.	2.9	63
94	Mass spectral and computational free energy studies of alkali metal ion-containing water clusters. The Journal of Physical Chemistry, 1995, 99, 7829-7836.	2.9	62
95	Charge transfer in small hydrogen bonded clusters. Journal of Chemical Physics, 2002, 116, 7380-7388.	1.2	62
96	A Fast QM/MM (Quantum Mechanical/Molecular Mechanical) Approach to Calculate Nuclear Magnetic Resonance Chemical Shifts for Macromolecules. Journal of Chemical Theory and Computation, 2006, 2, 209-215.	2.3	62
97	Insights into the Acylation Mechanism of Class A Î²-Lactamases from Molecular Dynamics Simulations of the TEM-1 Enzyme Complexed with Benzylpenicillin. Journal of the American Chemical Society, 2003, 125, 672-684.	6.6	61
98	Simulation of Liquid Water Using Semiempirical Hamiltonians and the Divide and Conquer Approach. Journal of Physical Chemistry A, 2005, 109, 3425-3432.	1.1	60
99	Tunneling dynamics of cyclobutadiene. Journal of the American Chemical Society, 1984, 106, 4040-4041.	6.6	59
100	GB/SA water model for the Merck molecular force field (MMFF). Journal of Molecular Graphics and Modelling, 2000, 18, 273-282.	1.3	59
101	Protein flexibility in aqueous and nonaqueous solutions. Journal of the American Chemical Society, 1992, 114, 10113-10116.	6.6	58
102	Systematic Parametrization of Divalent Metal Ions for the OPC3, OPC, TIP3P-FB, and TIP4P-FB Water Models. Journal of Chemical Theory and Computation, 2020, 16, 4429-4442.	2.3	58
103	Acceleration of Electron Repulsion Integral Evaluation on Graphics Processing Units via Use of Recurrence Relations. Journal of Chemical Theory and Computation, 2013, 9, 965-976.	2.3	57
104	Computation of the physio-chemical properties and data mining of large molecular collections. Journal of Computational Chemistry, 2002, 23, 172-183.	1.5	56
105	Inhibition of carbonic anhydrase. Journal of the American Chemical Society, 1991, 113, 4484-4490.	6.6	55
106	The application of the genetic algorithm to the minimization of potential energy functions. Journal of Global Optimization, 1993, 3, 49-66.	1.1	55
107	Quantum mechanical and molecular dynamics simulations of ureases and Zn Î²-lactamases. Journal of Computational Chemistry, 2006, 27, 1240-1262.	1.5	55
108	Molecular Recognition of K+ and Na+ by Valinomycin in Methanol. Journal of the American Chemical Society, 1995, 117, 779-791.	6.6	54

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109	Molecular dynamics simulations of lipid bilayers. Current Opinion in Structural Biology, 1997, 7, 511-517.	2.6	54
110	Ionic Conduction in Polyphosphazene Solids and Gels:Â13C,31P, and15N NMR Spectroscopy and Molecular Dynamics Simulations. Macromolecules, 1999, 32, 732-741.	2.2	54
111	Competitive Hydrolytic and Elimination Mechanisms in the Urease Catalyzed Decomposition of Urea. Journal of Physical Chemistry B, 2007, 111, 10263-10274.	1.2	53
112	Insight into the Cationâ^'Ï€ Interaction at the Metal Binding Site of the Copper Metallochaperone CusF. Journal of the American Chemical Society, 2011, 133, 19330-19333.	6.6	53
113	Molecular dynamics simulations of the dinuclear zinc-Î²-lactamase from Bacteroides fragilis complexed with imipenem. Journal of Computational Chemistry, 2002, 23, 1587-1600.	1.5	52
114	Insights into Cu(I) Exchange in HAH1 Using Quantum Mechanical and Molecular Simulations. Biochemistry, 2007, 46, 8816-8826.	1.2	52
115	QM/MM X-ray refinement of zinc metalloenzymes. Journal of Inorganic Biochemistry, 2010, 104, 512-522.	1.5	52
116	Potential of Mean Force Calculations on the SN1 Fragmentation of tert-Butyl Chloride. The Journal of Physical Chemistry, 1995, 99, 384-390.	2.9	51
117	Refinement of protein crystal structures using energy restraints derived from linear-scaling quantum mechanics. Acta Crystallographica Section D: Biological Crystallography, 2005, 61, 322-332.	2.5	51
118	MNDO calculations for compounds containing mercury. Organometallics, 1985, 4, 1964-1966.	1.1	50
119	Ground states of molecules. Part 84. MNDO calculations for compounds containing zinc. Organometallics, 1986, 5, 1494-1496.	1.1	50
120	Theoretical investigation of the CO2 + OH- .fwdarw. HCO3- reaction in the gas and aqueous phases. Journal of the American Chemical Society, 1993, 115, 9640-9647.	6.6	50
121	An Examination of a Hartree-Fock/Molecular Mechanical Coupled Potential. The Journal of Physical Chemistry, 1995, 99, 17344-17348.	2.9	50
122	Enzymatic Catalysis of Urea Decomposition:Â Elimination or Hydrolysis?. Journal of the American Chemical Society, 2004, 126, 11832-11842.	6.6	50
123	Rationalization of the Enantioselectivity of Subtilisin in DMF. Journal of the American Chemical Society, 1999, 121, 3486-3493.	6.6	49
124	Molecular recognition of potassium ion by the naturally occurring antibiotic ionophore nonactin. Journal of the American Chemical Society, 1992, 114, 7542-7549.	6.6	48
125	Effects of Fluorine Substitution on the Edge-to-Face Interaction of the Benzene Dimer. Journal of Physical Chemistry B, 2005, 109, 17752-17756.	1.2	48
126	Development of the Knowledge-Based and Empirical Combined Scoring Algorithm (KECSA) To Score Proteinâ€“Ligand Interactions. Journal of Chemical Information and Modeling, 2013, 53, 1073-1083.	2.5	48

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127	The Energy Computation Paradox and ab initio Protein Folding. PLoS ONE, 2011, 6, e18868.	1.1	48
128	Accurate assessment of the strain energy in a proteinâ€bound drug using QM/MM Xâ€ray refinement and converged quantum chemistry. Journal of Computational Chemistry, 2011, 32, 2587-2597.	1.5	47
129	Quantum Chemistry Calculations for Metabolomics. Chemical Reviews, 2021, 121, 5633-5670.	23.0	47
130	Accurate macromolecular crystallographic refinement: incorporation of the linear scaling, semiempirical quantum-mechanics programDivConinto thePHENIXrefinement package. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 1233-1247.	2.5	46
131	Hydration of zinc ions: theoretical study of [Zn(H2O)4](H2O)82+ and [Zn(H2O)6](H2O)62+. Chemical Physics Letters, 2000, 326, 288-292.	1.2	45
132	Critical assessment of the performance of the semiempirical divide and conquer method for single point calculations and geometry optimizations of large chemical systems. Journal of Chemical Physics, 2000, 113, 10512-10523.	1.2	45
133	Computational Studies of the Farnesyltransferase Ternary Complex Part I:Â Substrate Bindingâ€. Biochemistry, 2005, 44, 16513-16523.	1.2	45
134	The Reformatskii reaction. Journal of the American Chemical Society, 1987, 109, 6553-6554.	6.6	44
135	Free energy calculations on the relative solvation free energies of benzene, anisole, and 1,2,3-trimethoxybenzene: theoretical and experimental analysis of aromatic methoxy solvation. The Journal of Physical Chemistry, 1991, 95, 6661-6666.	2.9	44
136	Wide-Open Flaps Are Key to Urease Activity. Journal of the American Chemical Society, 2012, 134, 9934-9937.	6.6	44
137	Utility of the Hard/Soft Acidâ€"Base Principle via the Fukui Function in Biological Systems. Journal of Chemical Theory and Computation, 2010, 6, 548-559.	2.3	43
138	Binding Preferences of Hydroxamate Inhibitors of the Matrix Metalloproteinase Human Fibroblast Collagenase. Journal of Medicinal Chemistry, 1999, 42, 1225-1234.	2.9	42
139	Acylation of Class A Î²-lactamases by Penicillins:â€‰ A Theoretical Examination of the Role of Serine 130 and the Î²-lactam Carboxylate Group. Journal of Physical Chemistry B, 2001, 105, 11302-11313.	1.2	42
140	Solution Structure of Mycobacterium tuberculosis NmtR in the Apo State: Insights into Ni(II)-Mediated Allostery. Biochemistry, 2012, 51, 2619-2629.	1.2	42
141	Simulations of Allosteric Motions in the Zinc Sensor CzrA. Journal of the American Chemical Society, 2012, 134, 3367-3376.	6.6	42
142	Critical assessment of quantum mechanics based energy restraints in protein crystal structure refinement. Protein Science, 2006, 15, 2773-2784.	3.1	41
143	Potential energy surfaces and tunneling dynamics of some Jahn-Teller active molecules. The Journal of Physical Chemistry, 1985, 89, 4739-4744.	2.9	40
144	Interaction of small peptides with lipid bilayers. Biophysical Journal, 1995, 69, 1299-1308.	0.2	40

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145	Pairwise Decomposition of Residue Interaction Energies Using Semiempirical Quantum Mechanical Methods in Studies of Proteinâ^'Ligand Interaction. Journal of the American Chemical Society, 2005, 127, 6583-6594.	6.6	40
146	Molecular Recognition and Drug-Lead Identification: What Can Molecular Simulations Tell Us?. Current Medicinal Chemistry, 2010, 17, 25-41.	1.2	39
147	Density functional study of symmetric proton transfers. Journal of Chemical Physics, 1994, 101, 6658-6665.	1.2	38
148	Relative Configuration of Natural Products Using NMR Chemical Shifts. Journal of Natural Products, 2009, 72, 709-713.	1.5	38
149	Can we separate active from inactive conformations?. Journal of Computer-Aided Molecular Design, 2002, 16, 105-112.	1.3	37
150	Haptic applications for molecular structure manipulation. Journal of Molecular Graphics and Modelling, 2007, 25, 801-805.	1.3	37
151	Extended Zinc AMBER Force Field (EZAFF). Journal of Chemical Theory and Computation, 2018, 14, 242-254.	2.3	37
152	Conformational preferences for hydroxyl groups in substituted tetrahydropyrans. Journal of Computational Chemistry, 1992, 13, 772-791.	1.5	36
153	Thiosemicarbazones as Aedes aegypti larvicidal. European Journal of Medicinal Chemistry, 2015, 100, 162-175.	2.6	36
154	Determination of Atomic Charges Including solvation and Conformational Effects. The Journal of Physical Chemistry, 1994, 98, 1341-1343.	2.9	35
155	Solvation and Dynamics of Chymotrypsin in Hexane. Journal of the American Chemical Society, 1996, 118, 6490-6498.	6.6	35
156	A Critical Assessment of the Performance of Proteinâ^'Ligand Scoring Functions Based on NMR Chemical Shift Perturbations. Journal of Medicinal Chemistry, 2007, 50, 5128-5134.	2.9	35
157	The Ecstasy and Agony of Assay Interference Compounds. ACS Medicinal Chemistry Letters, 2017, 8, 379-382.	1.3	35
158	The Important Role of Active Site Water in the Catalytic Mechanism of Human Carbonic Anhydrase II ? A Semiempirical MO Approach to the Hydration of CO 2 ?. Journal of Molecular Modeling, 1998, 4, 355-365.	0.8	34
159	Pose Scoring by NMR. Journal of the American Chemical Society, 2004, 126, 11430-11431.	6.6	34
160	Aspects of organotin chemistry. Journal of the American Chemical Society, 1984, 106, 6773-6777.	6.6	33
161	Interaction of the Fusion Inhibiting Peptide Carbobenzoxy-D-Phe-L-Phe-Gly with N-Methyldioleoylphosphatidylethanolamine Lipid Bilayers. Journal of the American Chemical Society, 1995, 117, 6561-6571.	6.6	33
162	The Concept of Solvent Compatibility and Its Impact on Protein Stability and Activity Enhancement in Nonaqueous Solvents. Journal of the American Chemical Society, 1997, 119, 9939-9948.	6.6	33

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163	Implementation and Testing of a Frozen Density Matrixâ"Divide and Conquer Algorithm. Journal of Physical Chemistry A, 1999, 103, 1868-1875.	1.1	33
164	Chapter 9 Calculating Binding Free Energy in Proteinâ€"Ligand Interaction. Annual Reports in Computational Chemistry, 2005, 1, 113-130.	0.9	33
165	Catalyzed Decomposition of Urea. Molecular Dynamics Simulations of the Binding of Urea to Urease. Biochemistry, 2006, 45, 4429-4443.	1.2	33
166	Catalytic Mechanism of Aromatic Prenylation by NphB. Biochemistry, 2012, 51, 2606-2618.	1.2	33
167	PM3-compatible zinc parameters optimized for metalloenzyme active sites. Journal of Computational Chemistry, 2004, 25, 1677-1692.	1.5	32
168	Transferability of ion models. The Journal of Physical Chemistry, 1993, 97, 6524-6529.	2.9	31
169	Theoretical examination of the mechanism of aldoseâ€"ketose isomerization. Protein Engineering, Design and Selection, 1993, 6, 479-484.	1.0	31
170	Sodium Parameters for AM1 and PM3 Optimized Using a Modified Genetic Algorithm. Journal of Physical Chemistry B, 2002, 106, 2779-2785.	1.2	31
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