Darrin M York

List of Publications by Year
in descending order

189 papers	40,640 citations	41323 49 h-index	3482 182 g-index
195 all docs	195 docs citations	195 times ranked	37187 citing authors

#	Article	IF	Citations
1	Particle mesh Ewald: AnNâ‹…log(N) method for Ewald sums in large systems. Journal of Chemical Physics, 1993, 98, 10089-10092.	1.2	24,656
2	CHARMM: The biomolecular simulation program. Journal of Computational Chemistry, 2009, 30, 1545-1614.	1.5	7,077
3	The effect of longâ€range electrostatic interactions in simulations of macromolecular crystals: A comparison of the Ewald and truncated list methods. Journal of Chemical Physics, 1993, 99, 8345-8348.	1.2	611
4	A Smooth Solvation Potential Based on the Conductor-Like Screening Model. Journal of Physical Chemistry A, 1999, 103, 11060-11079.	1.1	381
5	GPU-Accelerated Molecular Dynamics and Free Energy Methods in Amber18: Performance Enhancements and New Features. Journal of Chemical Information and Modeling, 2018, 58, 2043-2050.	2.5	293
6	Extension of the Self-Consistent-Charge Density-Functional Tight-Binding Method:â€‰ Third-Order Expansion of the Density Functional Theory Total Energy and Introduction of a Modified Effective Coulomb Interaction. Journal of Physical Chemistry A, 2007, 111, 10861-10873.	1.1	265
7	An Efficient Linear-Scaling Ewald Method for Long-Range Electrostatic Interactions in Combined QM/MM Calculations. Journal of Chemical Theory and Computation, 2005, 1, 2-13.	2.3	258
8	A chemical potential equalization method for molecular simulations. Journal of Chemical Physics, 1996, 104, 159-172.	1.2	219
9	Constant pH Replica Exchange Molecular Dynamics in Explicit Solvent Using Discrete Protonation States: Implementation, Testing, and Validation. Journal of Chemical Theory and Computation, 2014, 10, 1341-1352.	2.3	210
10	Atomic-level accuracy in simulations of large protein crystals.. Proceedings of the National Academy of Sciences of the United States of America, 1994, 91, 8715-8718.	3.3	183
11	Linearâ€scaling semiempirical quantum calculations for macromolecules. Journal of Chemical Physics, 1996, 105, 2744-2750.	1.2	178
12	Alchemical Binding Free Energy Calculations in AMBER20: Advances and Best Practices for Drug Discovery. Journal of Chemical Information and Modeling, 2020, 60, 5595-5623.	2.5	177
13	Toward the Accurate Modeling of DNA: The Importance of Long-Range Electrostatics. Journal of the American Chemical Society, 1995, 117, 5001-5002.	6.6	172
14	Specific Reaction Parametrization of the AM1/d Hamiltonian for Phosphoryl Transfer Reactions:â€‰ H, O, and P Atoms. Journal of Chemical Theory and Computation, 2007, 3, 486-504.	2.3	138
15	Using AMBER18 for Relative Free Energy Calculations. Journal of Chemical Information and Modeling, 2019, 59, 3128-3135.	2.5	138
16	Accurate Proton Affinity and Gas-Phase Basicity Values for Molecules Important in Biocatalysis. Journal of Physical Chemistry B, 2010, 114, 13911-13921.	1.2	127
17	The fast Fourier Poisson method for calculating Ewald sums. Journal of Chemical Physics, 1994, 101, 3298-3300.	1.2	112
18	Theoretical methods that help understanding the structure and reactivity of gas phase ions. International Journal of Mass Spectrometry, 2005, 240, 37-99.	0.7	104

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19	Solvent Structure and Hammerhead RibozymeÂCatalysis. Chemistry and Biology, 2008, 15, 332-342.	6.2	104
20	Role of Mg²⁺ in Hammerhead Ribozyme Catalysis from Molecular Simulation. Journal of the American Chemical Society, 2008, 130, 3053-3064.	6.6	102
21	Ion Counting from Explicit-Solvent Simulations and 3D-RISM. Biophysical Journal, 2014, 106, 883-894.	0.2	102
22	Force Field for Mg²⁺, Mn²⁺, Zn²⁺, and Cd²⁺ Ions That Have Balanced Interactions with Nucleic Acids. Journal of Physical Chemistry B, 2015, 119, 15460-15470.	1.2	95
23	The Structure and Stability of Biological Metaphosphate, Phosphate, and Phosphorane Compounds in the Gas Phase and in Solution. Journal of the American Chemical Society, 2004, 126, 1654-1665.	6.6	94
24	Toward Fast and Accurate Binding Affinity Prediction with pmemdGTI: An Efficient Implementation of GPU-Accelerated Thermodynamic Integration. Journal of Chemical Theory and Computation, 2017, 13, 3077-3084.	2.3	93
25	Description of Phosphate Hydrolysis Reactions with the Self-Consistent-Charge Density-Functional-Tight-Binding (SCC-DFTB) Theory. 1. Parameterization. Journal of Chemical Theory and Computation, 2008, 4, 2067-2084.	2.3	87
26	Quantum Mechanical/Molecular Mechanical Simulation Study of the Mechanism of Hairpin Ribozyme Catalysis. Journal of the American Chemical Society, 2008, 130, 4680-4691.	6.6	79
27	Comparison of structural, thermodynamic, kinetic and mass transport properties of Mg²⁺ ion models commonly used in biomolecular simulations. Journal of Computational Chemistry, 2015, 36, 970-982.	1.5	79
28	Benchmark calculations of proton affinities and gas-phase basicities of molecules important in the study of biological phosphoryl transfer. Physical Chemistry Chemical Physics, 2005, 7, 3070.	1.3	76
29	A New Maximum Likelihood Approach for Free Energy Profile Construction from Molecular Simulations. Journal of Chemical Theory and Computation, 2013, 9, 153-164.	2.3	76
30	Fast, Accurate, and Reliable Protocols for Routine Calculations of Proteinâ€“Ligand Binding Affinities in Drug Design Projects Using AMBER GPU-TI with ff14SB/GAFF. ACS Omega, 2020, 5, 4611-4619.	1.6	74
31	Hybrid QM/MM Study of Thio Effects in Transphosphorylation Reactions. Journal of the American Chemical Society, 2003, 125, 7178-7179.	6.6	73
32	Ellipticity: A Convenient Tool To Characterize Electrocyclic Reactions. Chemistry - A European Journal, 2005, 11, 1734-1738.	1.7	71
33	Nucleophilic Attack on Phosphate Diesters:Â A Density Functional Study of Inâ^'Line Reactivity in Dianionic, Monoanionic, and Neutral Systems. Journal of Physical Chemistry B, 2006, 110, 11525-11539.	1.2	71
34	Transesterification Thio Effects of Phosphate Diesters:Â Free Energy Barriers and Kinetic and Equilibrium Isotope Effects from Density-Functional Theoryâ€. Biochemistry, 2006, 45, 10043-10053.	1.2	67
35	Quantum Mechanical Treatment of Biological Macromolecules in Solution Using Linear-Scaling Electronic Structure Methods. Physical Review Letters, 1998, 80, 5011-5014.	2.9	65
36	Cationâ€“Anion Interactions within the Nucleic Acid Ion Atmosphere Revealed by Ion Counting. Journal of the American Chemical Society, 2015, 137, 14705-14715.	6.6	65

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37	Many-body force field models based solely on pairwise Coulomb screening do not simultaneously reproduce correct gas-phase and condensed-phase polarizability limits. Journal of Chemical Physics, 2004, 120, 9903-9906.	1.2	63
38	Experimental and computational analysis of the transition state for ribonuclease A-catalyzed RNA 2â€²-O -transphosphorylation. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 13002-13007.	3.3	62
39	Quantum Mechanical Study of Aqueous Polarization Effects on Biological Macromolecules. Journal of the American Chemical Society, 1996, 118, 10940-10941.	6.6	61
40	Roadmaps through Free Energy Landscapes Calculated Using the Multidimensional vFEP Approach. Journal of Chemical Theory and Computation, 2014, 10, 24-34.	2.3	58
41	Density-functional calculations of the structure and stability ofC240. Physical Review B, 1994, 49, 8526-8528.	1.1	56
42	Hybrid QM/MM Study of Thio Effects in Transphosphorylation Reactions:Â The Role of Solvation. Journal of the American Chemical Society, 2004, 126, 7504-7513.	6.6	56
43	Charge-dependent model for many-body polarization, exchange, and dispersion interactions in hybrid quantum mechanicalâ^•molecular mechanical calculations. Journal of Chemical Physics, 2007, 127, 194101.	1.2	56
44	Parameterization and efficient implementation of a solvent model for linear-scaling semiempirical quantum mechanical calculations of biological macromolecules. Chemical Physics Letters, 1996, 263, 297-304.	1.2	55
45	A Variational Linear-Scaling Framework to Build Practical, Efficient Next-Generation Orbital-Based Quantum Force Fields. Journal of Chemical Theory and Computation, 2013, 9, 1417-1427.	2.3	55
46	Pseudorotation Barriers of Biological Oxyphosphoranes: A Challenge for Simulations of Ribozyme Catalysis. Chemistry - A European Journal, 2005, 11, 2081-2093.	1.7	54
47	Development of a Robust Indirect Approach for MM â†' QM Free Energy Calculations That Combines Force-Matched Reference Potential and Bennettâ€™s Acceptance Ratio Methods. Journal of Chemical Theory and Computation, 2019, 15, 5543-5562.	2.3	54
48	Improvement of semiempirical response properties with charge-dependent response density. Journal of Chemical Physics, 2005, 123, 164108.	1.2	53
49	Enzyme Dynamics and Tunneling Enhanced by Compression in the Hydrogen Abstraction Catalyzed by Soybean Lipoxygenase-1. Journal of Physical Chemistry B, 2006, 110, 24708-24719.	1.2	51
50	Ribozyme Catalysis with a Twist: Active State of the Twister Ribozyme in Solution Predicted from Molecular Simulation. Journal of the American Chemical Society, 2016, 138, 3058-3065.	6.6	51
51	Quantum descriptors for biological macromolecules from linear-scaling electronic structure methods. Proteins: Structure, Function and Bioinformatics, 2004, 56, 724-737.	1.5	50
52	Solvent Polarization and Kinetic Isotope Effects in Nitroethane Deprotonation and Implications to the Nitroalkane Oxidase Reaction. Journal of the American Chemical Society, 2005, 127, 16374-16375.	6.6	50
53	Active Participation of the Mg²⁺ Ion in the Reaction Coordinate of RNA Self-Cleavage Catalyzed by the Hammerhead Ribozyme. Journal of Chemical Theory and Computation, 2011, 7, 1-3.	2.3	50
54	Improvement of DNA and RNA Sugar Pucker Profiles from Semiempirical Quantum Methods. Journal of Chemical Theory and Computation, 2014, 10, 1538-1545.	2.3	50

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55	Spectroscopic Properties of Tyrosyl Radicals in Dipeptides. Journal of the American Chemical Society, 2002, 124, 5496-5505.	6.6	49
56	CHARMM force field parameters for simulation of reactive intermediates in native and thio-substituted ribozymes. Journal of Computational Chemistry, 2007, 28, 495-507.	1.5	49
57	Characterization of the Reaction Path and Transition States for RNA Transphosphorylation Models from Theory and Experiment. Angewandte Chemie - International Edition, 2012, 51, 647-651.	7.2	49
58	A GPU-Accelerated Parameter Interpolation Thermodynamic Integration Free Energy Method. Journal of Chemical Theory and Computation, 2018, 14, 1564-1582.	2.3	48
59	Electrostatic interactions in the hairpin ribozyme account for the majority of the rate acceleration without chemical participation by nucleobases. Rna, 2008, 14, 1501-1507.	1.6	47
60	Competitive interaction of monovalent cations with DNA from 3D-RISM. Nucleic Acids Research, 2015, 43, 8405-8415.	6.5	47
61	Development of Range-Corrected Deep Learning Potentials for Fast, Accurate Quantum Mechanical/Molecular Mechanical Simulations of Chemical Reactions in Solution. Journal of Chemical Theory and Computation, 2021, 17, 6993-7009.	2.3	47
62	Divalent Metal Ion Activation of a Guanine General Base in the Hammerhead Ribozyme: Insights from Molecular Simulations. Biochemistry, 2017, 56, 2985-2994.	1.2	46
63	Predicting Site-Binding Modes of Ions and Water to Nucleic Acids Using Molecular Solvation Theory. Journal of the American Chemical Society, 2019, 141, 2435-2445.	6.6	46
64	A Semiempirical Quantum Model for Hydrogen-Bonded Nucleic Acid Base Pairs. Journal of Chemical Theory and Computation, 2005, 1, 1275-1285.	2.3	45
65	An Ontology for Facilitating Discussion of Catalytic Strategies of RNA-Cleaving Enzymes. ACS Chemical Biology, 2019, 14, 1068-1076.	1.6	45
66	Threshold Occupancy and Specific Cation Binding Modes in the Hammerhead Ribozyme Active Site are Required for Active Conformation. Journal of Molecular Biology, 2009, 388, 195-206.	2.0	43
67	Extended Polarization in Third-Order SCC-DFTB from Chemical-Potential Equalization. Journal of Physical Chemistry A, 2012, 116, 9131-9141.	1.1	42
68	On the convergence of multi-scale free energy simulations. Molecular Simulation, 2018, 44, 1062-1081.	0.9	42
69	Theoretical studies on the hydrolysis of phosphate diesters in the gas phase, solution, and RNase A. International Journal of Quantum Chemistry, 2002, 86, 10-26.	1.0	41
70	Parameterization of semiempirical methods to treat nucleophilic attacks to biological phosphates: AM1/d parameters for phosphorus. Theoretical Chemistry Accounts, 2003, 109, 149-159.	0.5	40
71	Influence of C-5 substituted cytosine and related nucleoside analogs on the formation of benzo[a]pyrene diol epoxide-dG adducts at CG base pairs of DNA. Nucleic Acids Research, 2011, 39, 3988-4006.	6.5	40
72	Ambient-Potential Composite Ewald Method for ab Initio Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2016, 12, 2611-2632.	2.3	40

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73	Insights into the Regioselectivity and RNA-binding Affinity of HIV-1 Nucleocapsid Protein from Linear-scaling Quantum Methods. Journal of Molecular Biology, 2003, 330, 993-1004.	2.0	38
74	Insight into the Role of Mg2+ in Hammerhead Ribozyme Catalysis from X-ray Crystallography and Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2007, 3, 325-327.	2.3	38
75	Recent Advances toward a General Purpose Linear-Scaling Quantum Force Field. Accounts of Chemical Research, 2014, 47, 2812-2820.	7.6	38
76	Density-functional expansion methods: Evaluation of LDA, GGA, and meta-GGA functionals and different integral approximations. Journal of Chemical Physics, 2010, 133, 244107.	1.2	37
77	High-level ab initio methods for calculation of potential energy surfaces of van der Waals complexes. International Journal of Quantum Chemistry, 2004, 98, 388-408.	1.0	35
78	Theoretical Study of the Vinyl Allene Oxide to Cyclopent-2-en-1-one Rearrangement:â€‰ Mechanism, Torquoselectivity and Solvent Effects. Journal of Organic Chemistry, 2004, 69, 3635-3644.	1.7	35
79	The contribution of phosphate-phosphate repulsions to the free energy of DNA bending. Nucleic Acids Research, 2005, 33, 1257-1268.	6.5	35
80	Multipolar Ewald Methods, 1: Theory, Accuracy, and Performance. Journal of Chemical Theory and Computation, 2015, 11, 436-450.	2.3	35
81	Improved Alchemical Free Energy Calculations with Optimized Smoothstep Softcore Potentials. Journal of Chemical Theory and Computation, 2020, 16, 5512-5525.	2.3	35
82	Complete basis set extrapolated potential energy, dipole, and polarizability surfaces of alkali halide ion-neutral weakly avoided crossings with and without applied electric fields. Journal of Chemical Physics, 2004, 120, 7939-7948.	1.2	34
83	Density Functional Study of the In-Line Mechanism of Methanolysis of Cyclic Phosphate and Thiophosphate Esters in Solution:Â Insight into Thio Effects in RNA Transesterification. Journal of Physical Chemistry B, 2005, 109, 19987-20003.	1.2	34
84	Exocyclic Deoxyadenosine Adducts of 1,2,3,4-Diepoxybutane: Synthesis, Structural Elucidation, and Mechanistic Studies. Chemical Research in Toxicology, 2010, 23, 118-133.	1.7	34
85	Altered (transition) states: mechanisms of solution and enzyme catalyzed RNA 2â€²-O-transphosphorylation. Current Opinion in Chemical Biology, 2014, 21, 96-102.	2.8	34
86	Interpretation of pHâ€“Activity Profiles for Acidâ€“Base Catalysis from Molecular Simulations. Biochemistry, 2015, 54, 1307-1313.	1.2	33
87	Confluence of theory and experiment reveals the catalytic mechanism of the Varkud satellite ribozyme. Nature Chemistry, 2020, 12, 193-201.	6.6	33
88	Pseudorotation of Natural and Chemically Modified Biological Phosphoranes: Implications for RNA Catalysis. ChemPhysChem, 2004, 5, 1045-1049.	1.0	32
89	Normal Modes of Redox-Active Tyrosine:Â Conformation Dependence and Comparison to Experiment. Journal of Physical Chemistry B, 2006, 110, 10970-10981.	1.2	31
90	Evidence for the Role of Active Site Residues in the Hairpin Ribozyme from Molecular Simulations along the Reaction Path. Journal of the American Chemical Society, 2014, 136, 7789-7792.	6.6	31

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91	Fast approximate methods for calculating nucleic acid base pair interaction energies. Journal of Computational Chemistry, 2003, 24, 57-67.	1.5	30
92	Smooth Solvation Method for d-Orbital Semiempirical Calculations of Biological Reactions. 1. Implementation. Journal of Physical Chemistry B, 2005, 109, 9799-9809.	1.2	30
93	Characterization of the Structure and Dynamics of the HDV Ribozyme in Different Stages Along the Reaction Path. Journal of Physical Chemistry Letters, 2011, 2, 2538-2543.	2.1	30
94	Density-functional expansion methods: grand challenges. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	30
95	Mechanistic Insights into RNA Transphosphorylation from Kinetic Isotope Effects and Linear Free Energy Relationships of Model Reactions. Chemistry - A European Journal, 2014, 20, 14336-14343.	1.7	29
96	Parametrization of an Orbital-Based Linear-Scaling Quantum Force Field for Noncovalent Interactions. Journal of Chemical Theory and Computation, 2014, 10, 1086-1098.	2.3	29
97	A Comparison of QM/MM Simulations with and without the Drude Oscillator Model Based on Hydration Free Energies of Simple Solutes. Molecules, 2018, 23, 2695.	1.7	29
98	Improved ligand geometries in crystallographic refinement usingAFITTinPHENIX. Acta Crystallographica Section D: Structural Biology, 2016, 72, 1062-1072.	1.1	29
99	Examination of the correlation energy and second virial coefficients from accurateab initiocalculations of rare-gas dimers. Journal of Chemical Physics, 2003, 119, 2618-2622.	1.2	28
100	Structure and binding of Mg(II) ions and di-metal bridge complexes with biological phosphates and phosphoranes. Journal of Biological Inorganic Chemistry, 2004, 9, 807-817.	1.1	27
101	Molecular Dynamics Simulation of Nitrobenzene Dioxygenase Using AMBER Force Field. Journal of Chemical Theory and Computation, 2014, 10, 2246-2254.	2.3	27
102	Structural fidelity and NMR relaxation analysis in a prototype RNA hairpin. Rna, 2015, 21, 963-974.	1.6	27
103	Dynamical ensemble of the active state and transition state mimic for the RNA-cleaving 8â€“17 DNAzyme in solution. Nucleic Acids Research, 2019, 47, 10282-10295.	6.5	27
104	Variational Electrostatic Projection (VEP) Methods for Efficient Modeling of the Macromolecular Electrostatic and Solvation Environment in Activated Dynamics Simulations. Journal of Physical Chemistry B, 2005, 109, 536-556.	1.2	26
105	QCRNA 1.0: A database of quantum calculations for RNA catalysis. Journal of Molecular Graphics and Modelling, 2006, 25, 423-433.	1.3	26
106	Molecular Dynamics Simulation of Bovine Pancreatic Ribonuclease Aâ”CpA and Transition State-like Complexes. Journal of Physical Chemistry B, 2010, 114, 7371-7382.	1.2	25
107	Exact Relation between Potential of Mean Force and Free-Energy Profile. Journal of Chemical Theory and Computation, 2012, 8, 3998-4003.	2.3	25
108	The importance of protonation and tautomerization in relative binding affinity prediction: a comparison of AMBER TI and SchrÃ¶dinger FEP. Journal of Computer-Aided Molecular Design, 2016, 30, 533-539.	1.3	25

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109	The L-platform/L-scaffold framework: a blueprint for RNA-cleaving nucleic acid enzyme design. Rna, 2020, 26, 111-125.	1.6	25
110	A Two-Metal-Ion-Mediated Conformational Switching Pathway for HDV Ribozyme Activation. ACS Catalysis, 2016, 6, 1853-1869.	5.5	24
111	Cleaning Up Mechanistic Debris Generated by Twister Ribozymes Using Computational RNA Enzymology. ACS Catalysis, 2019, 9, 5803-5815.	5.5	24
112	CHARMM-GUI Free Energy Calculator for Practical Ligand Binding Free Energy Simulations with AMBER. Journal of Chemical Information and Modeling, 2021, 61, 4145-4151.	2.5	24
113	Free Energy Methods in Drug Discoveryâ€"Introduction. ACS Symposium Series, 0, , 1-38.	0.5	24
114	Contracted auxiliary Gaussian basis integral and derivative evaluation. Journal of Chemical Physics, 2008, 128, 064104.	1.2	23
115	Quantum mechanical force fields for condensed phase molecular simulations. Journal of Physics Condensed Matter, 2017, 29, 383002.	0.7	22
116	Evidence for a Catalytic Strategy to Promote Nucleophile Activation in Metal-Dependent RNA-Cleaving Ribozymes and 8-17 DNAzyme. ACS Catalysis, 2019, 9, 10612-10617.	5.5	22
117	Molecular Simulations of RNA 2â€²-O-Transesterification Reaction Models in Solution. Journal of Physical Chemistry B, 2013, 117, 94-103.	1.2	21
118	Theoretical Studies of Dissociative Phosphoryl Transfer in Interconversion of Phosphoenolpyruvate to Phosphonopyruvate:Â Solvent Effects, Thio Effects, and Implications for Enzymatic Reactions. Journal of Physical Chemistry B, 2005, 109, 13827-13834.	1.2	20
119	Charge-dependent many-body exchange and dispersion interactions in combined QM/MM simulations. Journal of Chemical Physics, 2015, 143, 234111.	1.2	20
120	Integration of kinetic isotope effect analyses to elucidate ribonuclease mechanism. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 1801-1808.	1.1	20
121	Molecular simulations of the pistol ribozyme: unifying the interpretation of experimental data and establishing functional links with the hammerhead ribozyme. Rna, 2019, 25, 1439-1456.	1.6	20
122	Quantum Mechanical Characterization of Nucleic Acids in Solution:Â A Linear-Scaling Study of Charge Fluctuations in DNA and RNA. Journal of Physical Chemistry B, 2002, 106, 7693-7703.	1.2	19
123	Origin of Mutational Effects at the C3 and G8 Positions on Hammerhead Ribozyme Catalysis from Molecular Dynamics Simulations. Journal of the American Chemical Society, 2008, 130, 7168-7169.	6.6	19
124	Computational Mutagenesis Studies of Hammerhead Ribozyme Catalysis. Journal of the American Chemical Society, 2010, 132, 13505-13518.	6.6	19
125	Multipolar Ewald Methods, 2: Applications Using a Quantum Mechanical Force Field. Journal of Chemical Theory and Computation, 2015, 11, 451-461.	2.3	19
126	Validation of Free Energy Methods in AMBER. Journal of Chemical Information and Modeling, 2020, 60, 5296-5300.	2.5	19

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127	Electronic structure properties of solvated biomolecules: A quantum approach for macromolecular characterization. Journal of Computational Chemistry, 2000, 21, 1562-1571.	1.5	18
128	Smooth Solvation Method for d-Orbital Semiempirical Calculations of Biological Reactions. 2. Application to Transphosphorylation Thio Effects in Solution. Journal of Physical Chemistry B, 2005, 109, 9810-9817.	1.2	18
129	Density functional study of the influence of C5 cytosine substitution in base pairs with guanine. Theoretical Chemistry Accounts, 2009, 122, 179-188.	0.5	18
130	Linear free energy relationships in RNA transesterification: theoretical models to aid experimental interpretations. Physical Chemistry Chemical Physics, 2014, 16, 15846-15855.	1.3	18
131	Assessment of metal-assisted nucleophile activation in the hepatitis delta virus ribozyme from molecular simulation and 3D-RISM. Rna, 2015, 21, 1566-1577.	1.6	18
132	Density-Functional Study of the Geometries, Stabilities, and Bond Energies of Group IIIâ^'V (13â^'15) Four-Membered-Ring Compounds. Journal of the American Chemical Society, 1996, 118, 5732-5736.	6.6	17
133	Kinetic isotope effects on thio-substituted biological phosphoryl transfer reactions from density-functional theory. Chemical Communications, 2005, , 3909.	2.2	17
134	Multilevel and Density Functional Electronic Structure Calculations of Proton Affinities and Gas-Phase Basicities Involved in Biological Phosphoryl Transferâ€. Journal of Physical Chemistry A, 2006, 110, 791-797.	1.1	17
135	Extension of adaptive tree code and fast multipole methods to high angular momentum particle charge densities. Journal of Computational Chemistry, 2008, 29, 1895-1904.	1.5	17
136	Combined QM/MM, Machine Learning Path Integral Approach to Compute Free Energy Profiles and Kinetic Isotope Effects in RNA Cleavage Reactions. Journal of Chemical Theory and Computation, 2022, 18, 4304-4317.	2.3	17
137	The interaction of Na(I), Ca(II), and Mg(II) metal ions with duplex DNA: A theoretical modeling study. International Journal of Quantum Chemistry, 1992, 44, 145-166.	1.0	16
138	Quantum mechanical study of solvent effects in a prototype SN2 reaction in solution: Clâ^' attack on CH3Cl. Journal of Chemical Physics, 2014, 140, 054109.	1.2	16
139	Effect of Zn2+ binding and enzyme active site on the transition state for RNA 2â€²-O-transphosphorylation interpreted through kinetic isotope effects. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 1795-1800.	1.1	16
140	Multiscale Methods for Computational RNA Enzymology. Methods in Enzymology, 2015, 553, 335-374.	0.4	16
141	Model for the Functional Active State of the TS Ribozyme from Molecular Simulation. Angewandte Chemie - International Edition, 2017, 56, 13392-13395.	7.2	16
142	Variational Method for Networkwide Analysis of Relative Ligand Binding Free Energies with Loop Closure and Experimental Constraints. Journal of Chemical Theory and Computation, 2021, 17, 1326-1336.	2.3	16
143	Extension of the Variational Free Energy Profile and Multistate Bennett Acceptance Ratio Methods for High-Dimensional Potential of Mean Force Profile Analysis. Journal of Physical Chemistry A, 2021, 125, 4216-4232.	1.1	15
144	High-order discretization schemes for biochemical applications of boundary element solvation and variational electrostatic projection methods. Journal of Chemical Physics, 2005, 122, 194110.	1.2	14

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145	Ab initio pathâ€integral calculations of kinetic and equilibrium isotope effects on baseâ€catalyzed RNA transphosphorylation models. Journal of Computational Chemistry, 2014, 35, 1302-1316.	1.5	14
146	Nucleic acid reactivity: Challenges for next-generation semiempirical quantum models. Journal of Computational Chemistry, 2015, 36, 1370-1389.	1.5	14
147	A generalized formulation of electronegativity equalization from density-functional theory. International Journal of Quantum Chemistry, 1995, 56, 385-394.	1.0	13
148	A new definition of atomic charges based on a variational principle for the electrostatic potential energy. Journal of Chemical Physics, 1995, 102, 7549-7556.	1.2	13
149	A Multidimensional B-Spline Correction for Accurate Modeling Sugar Puckering in QM/MM Simulations. Journal of Chemical Theory and Computation, 2017, 13, 3975-3984.	2.3	12
150	Density-functional expansion methods: Generalization of the auxiliary basis. Journal of Chemical Physics, 2011, 134, 194103.	1.2	11
151	A charge-scaling implementation of the variational electrostatic projection method. Journal of Computational Chemistry, 2006, 27, 103-115.	1.5	10
152	Characterization of the Three-Dimensional Free Energy Manifold for the Uracil Ribonucleoside from Asynchronous Replica Exchange Simulations. Journal of Chemical Theory and Computation, 2015, 11, 373-377.	2.3	10
153	Heavy atom labeled nucleotides for measurement of kinetic isotope effects. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 1737-1745.	1.1	10
154	Beneath the Surface: An Investigation of General Chemistry Studentsâ€™ Study Skills to Predict Course Outcomes. Journal of Chemical Education, 2021, 98, 281-292.	1.1	10
155	Robust, Efficient and Automated Methods for Accurate Prediction of Protein-Ligand Binding Affinities in AMBER Drug Discovery Boost. ACS Symposium Series, 0, , 161-204.	0.5	9
156	Time-dependent density functional theory calculations of molecular static and dynamic polarizabilities, cauchy coefficients and their anisotropies with atomic numerical basis functions. Computational and Theoretical Chemistry, 2002, 591, 255-266.	1.5	8
157	Design and application of a multicoefficient correlation method for dispersion interactions. Journal of Chemical Physics, 2004, 120, 590-602.	1.2	8
158	Bridging the Gap Between Theory and Experiment to Derive a Detailed Understanding of Hammerhead Ribozyme Catalysis. Progress in Molecular Biology and Translational Science, 2013, 120, 25-91.	0.9	8
159	Isotope effect analyses provide evidence for an altered transition state for RNA 2â€²-O-transphosphorylation catalyzed by Zn2+. Chemical Communications, 2016, 52, 4462-4465.	2.2	8
160	Identification of dynamical hinge points of the L1 ligase molecular switch. Rna, 2010, 16, 769-780.	1.6	7
161	An active site rearrangement within the Tetrahymena group I ribozyme releases nonproductive interactions and allows formation of catalytic interactions. Rna, 2016, 22, 32-48.	1.6	7
162	Spherical tensor gradient operator method for integral rotation: A simple, efficient, and extendable alternative to Slaterâ€“Koster tables. Journal of Chemical Physics, 2008, 129, 016102.	1.2	6

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