

# Darrin M York

## List of Publications by Year in descending order

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189  
papers

40,640  
citations

41258

49  
h-index

3476

182  
g-index

195  
all docs

195  
docs citations

195  
times ranked

37187  
citing authors

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

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19	Solvent Structure and Hammerhead Ribozyme Catalysis. <i>Chemistry and Biology</i> , 2008, 15, 332-342.	6.2	104
20	Role of Mg <sup>2+</sup> in Hammerhead Ribozyme Catalysis from Molecular Simulation. <i>Journal of the American Chemical Society</i> , 2008, 130, 3053-3064.	6.6	102
21	Ion Counting from Explicit-Solvent Simulations and 3D-RISM. <i>Biophysical Journal</i> , 2014, 106, 883-894.	0.2	102
22	Force Field for Mg <sup>2+</sup> , Mn <sup>2+</sup> , Zn <sup>2+</sup> , and Cd <sup>2+</sup> Ions That Have Balanced Interactions with Nucleic Acids. <i>Journal of Physical Chemistry B</i> , 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. <i>Journal of the American Chemical Society</i> , 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. <i>Journal of Chemical Theory and Computation</i> , 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. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 2067-2084.	2.3	87
26	Quantum Mechanical/Molecular Mechanical Simulation Study of the Mechanism of Hairpin Ribozyme Catalysis. <i>Journal of the American Chemical Society</i> , 2008, 130, 4680-4691.	6.6	79
27	Comparison of structural, thermodynamic, kinetic and mass transport properties of Mg <sup>2+</sup> ion models commonly used in biomolecular simulations. <i>Journal of Computational Chemistry</i> , 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. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 3070.	1.3	76
29	A New Maximum Likelihood Approach for Free Energy Profile Construction from Molecular Simulations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 153-164.	2.3	76
30	Fast, Accurate, and Reliable Protocols for Routine Calculations of Protein-Ligand Binding Affinities in Drug Design Projects Using AMBER GPU-TI with ff14SB/GAFF. <i>ACS Omega</i> , 2020, 5, 4611-4619.	1.6	74
31	Hybrid QM/MM Study of Thio Effects in Transphosphorylation Reactions. <i>Journal of the American Chemical Society</i> , 2003, 125, 7178-7179.	6.6	73
32	Ellipticity: A Convenient Tool To Characterize Electrocyclic Reactions. <i>Chemistry - A European Journal</i> , 2005, 11, 1734-1738.	1.7	71
33	Nucleophilic Attack on Phosphate Diesters: A Density Functional Study of In-Line Reactivity in Dianionic, Monoanionic, and Neutral Systems. <i>Journal of Physical Chemistry B</i> , 2006, 110, 11525-11539.	1.2	71
34	Transesterification Thio Effects of Phosphate Diesters: Free Energy Barriers and Kinetic and Equilibrium Isotope Effects from Density-Functional Theory. <i>Biochemistry</i> , 2006, 45, 10043-10053.	1.2	67
35	Quantum Mechanical Treatment of Biological Macromolecules in Solution Using Linear-Scaling Electronic Structure Methods. <i>Physical Review Letters</i> , 1998, 80, 5011-5014.	2.9	65
36	Cation-Anion Interactions within the Nucleic Acid Ion Atmosphere Revealed by Ion Counting. <i>Journal of the American Chemical Society</i> , 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. <i>Journal of Chemical Physics</i> , 2004, 120, 9903-9906.	1.2	63
38	Experimental and computational analysis of the transition state for ribonuclease A-catalyzed RNA 2'-O-phosphorylation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 13002-13007.	3.3	62
39	Quantum Mechanical Study of Aqueous Polarization Effects on Biological Macromolecules. <i>Journal of the American Chemical Society</i> , 1996, 118, 10940-10941.	6.6	61
40	Roadmaps through Free Energy Landscapes Calculated Using the Multidimensional vFEP Approach. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 24-34.	2.3	58
41	Density-functional calculations of the structure and stability of C <sub>240</sub> . <i>Physical Review B</i> , 1994, 49, 8526-8528.	1.1	56
42	Hybrid QM/MM Study of Thio Effects in Transphosphorylation Reactions: The Role of Solvation. <i>Journal of the American Chemical Society</i> , 2004, 126, 7504-7513.	6.6	56
43	Charge-dependent model for many-body polarization, exchange, and dispersion interactions in hybrid quantum mechanical-molecular mechanical calculations. <i>Journal of Chemical Physics</i> , 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. <i>Chemical Physics Letters</i> , 1996, 263, 297-304.	1.2	55
45	A Variational Linear-Scaling Framework to Build Practical, Efficient Next-Generation Orbital-Based Quantum Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1417-1427.	2.3	55
46	Pseudorotation Barriers of Biological Oxyphosphoranes: A Challenge for Simulations of Ribozyme Catalysis. <i>Chemistry - A European Journal</i> , 2005, 11, 2081-2093.	1.7	54
47	Development of a Robust Indirect Approach for MM $\hat{\rho}$ QM Free Energy Calculations That Combines Force-Matched Reference Potential and Bennett's Acceptance Ratio Methods. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5543-5562.	2.3	54
48	Improvement of semiempirical response properties with charge-dependent response density. <i>Journal of Chemical Physics</i> , 2005, 123, 164108.	1.2	53
49	Enzyme Dynamics and Tunneling Enhanced by Compression in the Hydrogen Abstraction Catalyzed by Soybean Lipoxygenase-1. <i>Journal of Physical Chemistry B</i> , 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. <i>Journal of the American Chemical Society</i> , 2016, 138, 3058-3065.	6.6	51
51	Quantum descriptors for biological macromolecules from linear-scaling electronic structure methods. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 56, 724-737.	1.5	50
52	Solvent Polarization and Kinetic Isotope Effects in Nitroethane Deprotonation and Implications to the Nitroalkane Oxidase Reaction. <i>Journal of the American Chemical Society</i> , 2005, 127, 16374-16375.	6.6	50
53	Active Participation of the Mg <sup>2+</sup> Ion in the Reaction Coordinate of RNA Self-Cleavage Catalyzed by the Hammerhead Ribozyme. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1-3.	2.3	50
54	Improvement of DNA and RNA Sugar Pucker Profiles from Semiempirical Quantum Methods. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1538-1545.	2.3	50

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55	Spectroscopic Properties of Tyrosyl Radicals in Dipeptides. <i>Journal of the American Chemical Society</i> , 2002, 124, 5496-5505.	6.6	49
56	CHARMM force field parameters for simulation of reactive intermediates in native and thio-substituted ribozymes. <i>Journal of Computational Chemistry</i> , 2007, 28, 495-507.	1.5	49
57	Characterization of the Reaction Path and Transition States for RNA Transphosphorylation Models from Theory and Experiment. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 647-651.	7.2	49
58	A GPU-Accelerated Parameter Interpolation Thermodynamic Integration Free Energy Method. <i>Journal of Chemical Theory and Computation</i> , 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. <i>Rna</i> , 2008, 14, 1501-1507.	1.6	47
60	Competitive interaction of monovalent cations with DNA from 3D-RISM. <i>Nucleic Acids Research</i> , 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. <i>Journal of Chemical Theory and Computation</i> , 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. <i>Biochemistry</i> , 2017, 56, 2985-2994.	1.2	46
63	Predicting Site-Binding Modes of Ions and Water to Nucleic Acids Using Molecular Solvation Theory. <i>Journal of the American Chemical Society</i> , 2019, 141, 2435-2445.	6.6	46
64	A Semiempirical Quantum Model for Hydrogen-Bonded Nucleic Acid Base Pairs. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 1275-1285.	2.3	45
65	An Ontology for Facilitating Discussion of Catalytic Strategies of RNA-Cleaving Enzymes. <i>ACS Chemical Biology</i> , 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. <i>Journal of Molecular Biology</i> , 2009, 388, 195-206.	2.0	43
67	Extended Polarization in Third-Order SCC-DFTB from Chemical-Potential Equalization. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9131-9141.	1.1	42
68	On the convergence of multi-scale free energy simulations. <i>Molecular Simulation</i> , 2018, 44, 1062-1081.	0.9	42
69	Theoretical studies on the hydrolysis of phosphate diesters in the gas phase, solution, and RNase A. <i>International Journal of Quantum Chemistry</i> , 2002, 86, 10-26.	1.0	41
70	Parameterization of semiempirical methods to treat nucleophilic attacks to biological phosphates: AM1/d parameters for phosphorus. <i>Theoretical Chemistry Accounts</i> , 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. <i>Nucleic Acids Research</i> , 2011, 39, 3988-4006.	6.5	40
72	Ambient-Potential Composite Ewald Method for <i>ab Initio</i> Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation. <i>Journal of Chemical Theory and Computation</i> , 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. <i>Journal of Molecular Biology</i> , 2003, 330, 993-1004.	2.0	38
74	Insight into the Role of Mg <sup>2+</sup> in Hammerhead Ribozyme Catalysis from X-ray Crystallography and Molecular Dynamics Simulation. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 325-327.	2.3	38
75	Recent Advances toward a General Purpose Linear-Scaling Quantum Force Field. <i>Accounts of Chemical Research</i> , 2014, 47, 2812-2820.	7.6	38
76	Density-functional expansion methods: Evaluation of LDA, GGA, and meta-GGA functionals and different integral approximations. <i>Journal of Chemical Physics</i> , 2010, 133, 244107.	1.2	37
77	High-level ab initio methods for calculation of potential energy surfaces of van der Waals complexes. <i>International Journal of Quantum Chemistry</i> , 2004, 98, 388-408.	1.0	35
78	Theoretical Study of the Vinyl Allene Oxide to Cyclopent-2-en-1-one Rearrangement: Mechanism, Torquoselectivity and Solvent Effects. <i>Journal of Organic Chemistry</i> , 2004, 69, 3635-3644.	1.7	35
79	The contribution of phosphate-phosphate repulsions to the free energy of DNA bending. <i>Nucleic Acids Research</i> , 2005, 33, 1257-1268.	6.5	35
80	Multipolar Ewald Methods, 1: Theory, Accuracy, and Performance. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 436-450.	2.3	35
81	Improved Alchemical Free Energy Calculations with Optimized Smoothstep Softcore Potentials. <i>Journal of Chemical Theory and Computation</i> , 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. <i>Journal of Chemical Physics</i> , 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: An Insight into Thio Effects in RNA Transesterification. <i>Journal of Physical Chemistry B</i> , 2005, 109, 19987-20003.	1.2	34
84	Exocyclic Deoxyadenosine Adducts of 1,2,3,4-Diepoxybutane: Synthesis, Structural Elucidation, and Mechanistic Studies. <i>Chemical Research in Toxicology</i> , 2010, 23, 118-133.	1.7	34
85	Altered (transition) states: mechanisms of solution and enzyme catalyzed RNA 2'-O-transphosphorylation. <i>Current Opinion in Chemical Biology</i> , 2014, 21, 96-102.	2.8	34
86	Interpretation of pH-Activity Profiles for Acid-Base Catalysis from Molecular Simulations. <i>Biochemistry</i> , 2015, 54, 1307-1313.	1.2	33
87	Confluence of theory and experiment reveals the catalytic mechanism of the Varkud satellite ribozyme. <i>Nature Chemistry</i> , 2020, 12, 193-201.	6.6	33
88	Pseudorotation of Natural and Chemically Modified Biological Phosphoranes: Implications for RNA Catalysis. <i>ChemPhysChem</i> , 2004, 5, 1045-1049.	1.0	32
89	Normal Modes of Redox-Active Tyrosine: A Conformation Dependence and Comparison to Experiment. <i>Journal of Physical Chemistry B</i> , 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. <i>Journal of the American Chemical Society</i> , 2014, 136, 7789-7792.	6.6	31

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91	Fast approximate methods for calculating nucleic acid base pair interaction energies. <i>Journal of Computational Chemistry</i> , 2003, 24, 57-67.	1.5	30
92	Smooth Solvation Method for d-Orbital Semiempirical Calculations of Biological Reactions. 1. Implementation. <i>Journal of Physical Chemistry B</i> , 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. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2538-2543.	2.1	30
94	Density-functional expansion methods: grand challenges. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	30
95	Mechanistic Insights into RNA Transphosphorylation from Kinetic Isotope Effects and Linear Free Energy Relationships of Model Reactions. <i>Chemistry - A European Journal</i> , 2014, 20, 14336-14343.	1.7	29
96	Parametrization of an Orbital-Based Linear-Scaling Quantum Force Field for Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 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. <i>Molecules</i> , 2018, 23, 2695.	1.7	29
98	Improved ligand geometries in crystallographic refinement using <i>AFIT</i> in <i>PHENIX</i> . <i>Acta Crystallographica Section D: Structural Biology</i> , 2016, 72, 1062-1072.	1.1	29
99	Examination of the correlation energy and second virial coefficients from accurate ab initio calculations of rare-gas dimers. <i>Journal of Chemical Physics</i> , 2003, 119, 2618-2622.	1.2	28
100	Structure and binding of Mg(II) ions and di-metal bridge complexes with biological phosphates and phosphoranates. <i>Journal of Biological Inorganic Chemistry</i> , 2004, 9, 807-817.	1.1	27
101	Molecular Dynamics Simulation of Nitrobenzene Dioxygenase Using AMBER Force Field. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2246-2254.	2.3	27
102	Structural fidelity and NMR relaxation analysis in a prototype RNA hairpin. <i>Rna</i> , 2015, 21, 963-974.	1.6	27
103	Dynamical ensemble of the active state and transition state mimic for the RNA-cleaving 8 <sup>17</sup> DNAzyme in solution. <i>Nucleic Acids Research</i> , 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. <i>Journal of Physical Chemistry B</i> , 2005, 109, 536-556.	1.2	26
105	QCRNA 1.0: A database of quantum calculations for RNA catalysis. <i>Journal of Molecular Graphics and Modelling</i> , 2006, 25, 423-433.	1.3	26
106	Molecular Dynamics Simulation of Bovine Pancreatic Ribonuclease A <sup>~</sup> CpA and Transition State-like Complexes. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7371-7382.	1.2	25
107	Exact Relation between Potential of Mean Force and Free-Energy Profile. <i>Journal of Chemical Theory and Computation</i> , 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 Schrödinger FEP. <i>Journal of Computer-Aided Molecular Design</i> , 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. <i>Rna</i> , 2020, 26, 111-125.	1.6	25
110	A Two-Metal-Ion-Mediated Conformational Switching Pathway for HDV Ribozyme Activation. <i>ACS Catalysis</i> , 2016, 6, 1853-1869.	5.5	24
111	Cleaning Up Mechanistic Debris Generated by Twister Ribozymes Using Computational RNA Enzymology. <i>ACS Catalysis</i> , 2019, 9, 5803-5815.	5.5	24
112	CHARMM-GUI Free Energy Calculator for Practical Ligand Binding Free Energy Simulations with AMBER. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4145-4151.	2.5	24
113	Free Energy Methods in Drug Discovery—Introduction. <i>ACS Symposium Series</i> , 0, , 1-38.	0.5	24
114	Contracted auxiliary Gaussian basis integral and derivative evaluation. <i>Journal of Chemical Physics</i> , 2008, 128, 064104.	1.2	23
115	Quantum mechanical force fields for condensed phase molecular simulations. <i>Journal of Physics Condensed Matter</i> , 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. <i>ACS Catalysis</i> , 2019, 9, 10612-10617.	5.5	22
117	Molecular Simulations of RNA 2'-O <sup>2</sup> -Transesterification Reaction Models in Solution. <i>Journal of Physical Chemistry B</i> , 2013, 117, 94-103.	1.2	21
118	Theoretical Studies of Dissociative Phosphoryl Transfer in Interconversion of Phosphoenolpyruvate to Phosphonopyruvate: Solvent Effects, Thio Effects, and Implications for Enzymatic Reactions. <i>Journal of Physical Chemistry B</i> , 2005, 109, 13827-13834.	1.2	20
119	Charge-dependent many-body exchange and dispersion interactions in combined QM/MM simulations. <i>Journal of Chemical Physics</i> , 2015, 143, 234111.	1.2	20
120	Integration of kinetic isotope effect analyses to elucidate ribonuclease mechanism. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 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. <i>Rna</i> , 2019, 25, 1439-1456.	1.6	20
122	Quantum Mechanical Characterization of Nucleic Acids in Solution: A Linear-Scaling Study of Charge Fluctuations in DNA and RNA. <i>Journal of Physical Chemistry B</i> , 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. <i>Journal of the American Chemical Society</i> , 2008, 130, 7168-7169.	6.6	19
124	Computational Mutagenesis Studies of Hammerhead Ribozyme Catalysis. <i>Journal of the American Chemical Society</i> , 2010, 132, 13505-13518.	6.6	19
125	Multipolar Ewald Methods, 2: Applications Using a Quantum Mechanical Force Field. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 451-461.	2.3	19
126	Validation of Free Energy Methods in AMBER. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5296-5300.	2.5	19



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127	Electronic structure properties of solvated biomolecules: A quantum approach for macromolecular characterization. <i>Journal of Computational Chemistry</i> , 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. <i>Journal of Physical Chemistry B</i> , 2005, 109, 9810-9817.	1.2	18
129	Density functional study of the influence of C5 cytosine substitution in base pairs with guanine. <i>Theoretical Chemistry Accounts</i> , 2009, 122, 179-188.	0.5	18
130	Linear free energy relationships in RNA transesterification: theoretical models to aid experimental interpretations. <i>Physical Chemistry Chemical Physics</i> , 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. <i>Rna</i> , 2015, 21, 1566-1577.	1.6	18
132	Density-Functional Study of the Geometries, Stabilities, and Bond Energies of Group III <sup>V</sup> (13 <sup>15</sup> ) Four-Membered-Ring Compounds. <i>Journal of the American Chemical Society</i> , 1996, 118, 5732-5736.	6.6	17
133	Kinetic isotope effects on thio-substituted biological phosphoryl transfer reactions from density-functional theory. <i>Chemical Communications</i> , 2005, , 3909.	2.2	17
134	Multilevel and Density Functional Electronic Structure Calculations of Proton Affinities and Gas-Phase Basicities Involved in Biological Phosphoryl Transfer. <i>Journal of Physical Chemistry A</i> , 2006, 110, 791-797.	1.1	17
135	Extension of adaptive tree code and fast multipole methods to high angular momentum particle charge densities. <i>Journal of Computational Chemistry</i> , 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. <i>Journal of Chemical Theory and Computation</i> , 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. <i>International Journal of Quantum Chemistry</i> , 1992, 44, 145-166.	1.0	16
138	Quantum mechanical study of solvent effects in a prototype S <sub>N</sub> 2 reaction in solution: Cl <sup>-</sup> attack on CH <sub>3</sub> Cl. <i>Journal of Chemical Physics</i> , 2014, 140, 054109.	1.2	16
139	Effect of Zn <sup>2+</sup> binding and enzyme active site on the transition state for RNA 2 <sup>€</sup> -O-transphosphorylation interpreted through kinetic isotope effects. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2015, 1854, 1795-1800.	1.1	16
140	Multiscale Methods for Computational RNA Enzymology. <i>Methods in Enzymology</i> , 2015, 553, 335-374.	0.4	16
141	Model for the Functional Active State of the TS Ribozyme from Molecular Simulation. <i>Angewandte Chemie - International Edition</i> , 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. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1326-1336.	2.3	16
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