Darrin M York

List of Publications by Year in Descending Order

186 papers	31,975 citations	47 h-index	178 g-index
195 ext. papers	36,840 ext. citations	6 avg, IF	7.02 L-index

#	Paper	IF	Citations
186	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	6.4	14
185	Beneath the Surface: An Investigation of General Chemistry StudentsSStudy Skills to Predict Course Outcomes. *Journal of Chemical Education*, **2021**, 98, 281-292	2.4	3
184	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	2.8	4
183	Peripheral Methionine Residues Impact Flavin Photoreduction and Protonation in an Engineered LOV Domain Light Sensor. *Biochemistry*, **2021**, 60, 1148-1164	3.2	1
182	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	6.4	6
181	CHARMM-GUI Free Energy Calculator for Practical Ligand Binding Free Energy Simulations with AMBER. *Journal of Chemical Information and Modeling*, **2021**, 61, 4145-4151	6.1	4
180	Validation of Free Energy Methods in AMBER. *Journal of Chemical Information and Modeling*, **2020**, 60, 5296-5300	6.1	7
179	Fast, Accurate, and Reliable Protocols for Routine Calculations of Protein-Ligand Binding Affinities in Drug Design Projects Using AMBER GPU-TI with ff14SB/GAFF. *ACS Omega*, **2020**, 5, 4611-4619	3.9	31
178	Confluence of theory and experiment reveals the catalytic mechanism of the Varkud satellite ribozyme. *Nature Chemistry*, **2020**, 12, 193-201	17.6	14
177	The L-platform/L-scaffold framework: a blueprint for RNA-cleaving nucleic acid enzyme design. *Rna*, **2020**, 26, 111-125	5.8	10
176	Improved Alchemical Free Energy Calculations with Optimized Smoothstep Softcore Potentials. *Journal of Chemical Theory and Computation*, **2020**, 16, 5512-5525	6.4	17
175	Through the Looking CLASS: When Peer Leader Learning Attitudes Are Not What They Seem. *Journal of Chemical Education*, **2020**, 97, 2078-2090	2.4	3
174	Alchemical Binding Free Energy Calculations in AMBER20: Advances and Best Practices for Drug Discovery. *Journal of Chemical Information and Modeling*, **2020**, 60, 5595-5623	6.1	56
173	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	16.4	27
172	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	13.1	17
171	Development of a Robust Indirect Approach for MM -oQM Free Energy Calculations That Combines Force-Matched Reference Potential and BennettSs Acceptance Ratio Methods. *Journal of Chemical Theory and Computation*, **2019**, 15, 5543-5562	6.4	31
170	Dynamical ensemble of the active state and transition state mimic for the RNA-cleaving 8-17 DNAzyme in solution. *Nucleic Acids Research*, **2019**, 47, 10282-10295	20.1	15

169	Using AMBER18 for Relative Free Energy Calculations. *Journal of Chemical Information and Modeling*, **2019**, 59, 3128-3135	6.1	62
168	Cleaning Up Mechanistic Debris Generated by Twister Ribozymes Using Computational RNA Enzymology. *ACS Catalysis*, **2019**, 9, 5803-5815	13.1	15
167	An Ontology for Facilitating Discussion of Catalytic Strategies of RNA-Cleaving Enzymes. *ACS Chemical Biology*, **2019**, 14, 1068-1076	4.9	25
166	Framework for Conducting and Analyzing Crystal Simulations of Nucleic Acids to Aid in Modern Force Field Evaluation. *Journal of Physical Chemistry B*, **2019**, 123, 4611-4624	3.4	3
165	Quantum Suppression of Intramolecular Deuterium Kinetic Isotope Effects in a Pericyclic Hydrogen Transfer Reaction. *Journal of Physical Chemistry A*, **2019**, 123, 3647-3654	2.8	1
164	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	5.8	12
163	A GPU-Accelerated Parameter Interpolation Thermodynamic Integration Free Energy Method. *Journal of Chemical Theory and Computation*, **2018**, 14, 1564-1582	6.4	26
162	On the convergence of multi-scale free energy simulations. *Molecular Simulation*, **2018**, 44, 1062-1081	2	30
161	A Comparison of QM/MM Simulations with and without the Drude Oscillator Model Based on Hydration Free Energies of Simple Solutes. *Molecules*, **2018**, 23,	4.8	23
160	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	6.1	165
159	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	6.4	66
158	Divalent Metal Ion Activation of a Guanine General Base in the Hammerhead Ribozyme: Insights from Molecular Simulations. *Biochemistry*, **2017**, 56, 2985-2994	3.2	35
157	Quantum mechanical force fields for condensed phase molecular simulations. *Journal of Physics Condensed Matter*, **2017**, 29, 383002	1.8	18
156	A Multidimensional B-Spline Correction for Accurate Modeling Sugar Puckering in QM/MM Simulations. *Journal of Chemical Theory and Computation*, **2017**, 13, 3975-3984	6.4	9
155	Model for the Functional Active State of the TS Ribozyme from Molecular Simulation. *Angewandte Chemie - International Edition*, **2017**, 56, 13392-13395	16.4	16
154	Model for the Functional Active State of the TS Ribozyme from Molecular Simulation. *Angewandte Chemie*, **2017**, 129, 13577-13580	3.6	5
153	Kinetic Isotope Effect Analysis of RNA 2SO-Transphosphorylation. *Methods in Enzymology*, **2017**, 596, 433-457	1.7	1
152	Creation of Academic Social Networks (ASNs) for Effective Online eLearning Communities. *ACS Symposium Series*, **2016**, 109-126	0.4	1

151	RepEx: A Flexible Framework for Scalable Replica Exchange Molecular Dynamics Simulations **2016**,		6
150	VR-SCOSMO: A smooth conductor-like screening model with charge-dependent radii for modeling chemical reactions. *Journal of Chemical Physics*, **2016**, 144, 164115	3.9	2
149	A Two-Metal-Ion-Mediated Conformational Switching Pathway for HDV Ribozyme Activation. *ACS Catalysis*, **2016**, 6, 1853-1869	13.1	22
148	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, 3058-65	16.4	46
147	Isotope effect analyses provide evidence for an altered transition state for RNA 2SO-transphosphorylation catalyzed by Zn(2+). *Chemical Communications*, **2016**, 52, 4462-5	5.8	8
146	An active site rearrangement within the Tetrahymena group I ribozyme releases nonproductive interactions and allows formation of catalytic interactions. *Rna*, **2016**, 22, 32-48	5.8	5
145	Improved ligand geometries in crystallographic refinement using AFITT in PHENIX. *Acta Crystallographica Section D: Structural Biology*, **2016**, 72, 1062-72	5.5	22
144	A Modified Divide-and-Conquer Linear-Scaling Quantum Force Field with Multipolar Charge Densities **2016**, 3-31		3
143	Ambient-Potential Composite Ewald Method for ab Initio Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation. *Journal of Chemical Theory and Computation*, **2016**, 12, 2611-32	6.4	26
142	The importance of protonation and tautomerization in relative binding affinity prediction: a comparison of AMBER TI and Schrödinger FEP. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 533-9	4.2	15
141	Comparison of structural, thermodynamic, kinetic and mass transport properties of Mg(2+) ion models commonly used in biomolecular simulations. *Journal of Computational Chemistry*, **2015**, 36, 970-82	3.5	52
140	Effect of Zn2+ binding and enzyme active site on the transition state for RNA 2SO-transphosphorylation interpreted through kinetic isotope effects. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2015**, 1854, 1795-800	4	15
139	Heavy atom labeled nucleotides for measurement of kinetic isotope effects. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2015**, 1854, 1737-45	4	8
138	Determination of hepatitis delta virus ribozyme N(-1) nucleobase and functional group specificity using internal competition kinetics. *Analytical Biochemistry*, **2015**, 483, 12-20	3.1	6
137	Multiscale methods for computational RNA enzymology. *Methods in Enzymology*, **2015**, 553, 335-74	1.7	15
136	Nucleic acid reactivity: challenges for next-generation semiempirical quantum models. *Journal of Computational Chemistry*, **2015**, 36, 1370-89	3.5	13
135	Integration of kinetic isotope effect analyses to elucidate ribonuclease mechanism. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2015**, 1854, 1801-8	4	18
134	Force Field for Mg(2+), Mn(2+), Zn(2+), and Cd(2+) Ions That Have Balanced Interactions with Nucleic Acids. *Journal of Physical Chemistry B*, **2015**, 119, 15460-70	3.4	66

133	Cation-Anion Interactions within the Nucleic Acid Ion Atmosphere Revealed by Ion Counting. *Journal of the American Chemical Society*, **2015**, 137, 14705-15	16.4	48
132	Charge-dependent many-body exchange and dispersion interactions in combined QM/MM simulations. *Journal of Chemical Physics*, **2015**, 143, 234111	3.9	15
131	Structural fidelity and NMR relaxation analysis in a prototype RNA hairpin. *Rna*, **2015**, 21, 963-74	5.8	24
130	Assessment of metal-assisted nucleophile activation in the hepatitis delta virus ribozyme from molecular simulation and 3D-RISM. *Rna*, **2015**, 21, 1566-77	5.8	16
129	Competitive interaction of monovalent cations with DNA from 3D-RISM. *Nucleic Acids Research*, **2015**, 43, 8405-15	20.1	32
128	Multipolar Ewald methods, 2: applications using a quantum mechanical force field. *Journal of Chemical Theory and Computation*, **2015**, 11, 451-61	6.4	17
127	Interpretation of pH-activity profiles for acid-base catalysis from molecular simulations. *Biochemistry*, **2015**, 54, 1307-13	3.2	27
126	Multipolar Ewald methods, 1: theory, accuracy, and performance. *Journal of Chemical Theory and Computation*, **2015**, 11, 436-50	6.4	30
125	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, 373-7	6.4	9
124	Quantum mechanical study of solvent effects in a prototype SN2 reaction in solution: Cl- attack on CH3Cl. *Journal of Chemical Physics*, **2014**, 140, 054109	3.9	15
123	Ab initio path-integral calculations of kinetic and equilibrium isotope effects on base-catalyzed RNA transphosphorylation models. *Journal of Computational Chemistry*, **2014**, 35, 1302-16	3.5	11
122	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, 7789-92	16.4	29
121	Linear free energy relationships in RNA transesterification: theoretical models to aid experimental interpretations. *Physical Chemistry Chemical Physics*, **2014**, 16, 15846-55	3.6	14
120	Parametrization of an Orbital-Based Linear-Scaling Quantum Force Field for Noncovalent Interactions. *Journal of Chemical Theory and Computation*, **2014**, 10, 1086-1098	6.4	27
119	Improvement of DNA and RNA Sugar Pucker Profiles from Semiempirical Quantum Methods. *Journal of Chemical Theory and Computation*, **2014**, 10, 1538-1545	6.4	38
118	Roadmaps through free energy landscapes calculated using the multi-dimensional vFEP approach. *Journal of Chemical Theory and Computation*, **2014**, 10, 24-34	6.4	45
117	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	6.4	149
116	Altered (transition) states: mechanisms of solution and enzyme catalyzed RNA 2SO-transphosphorylation. *Current Opinion in Chemical Biology*, **2014**, 21, 96-102	9.7	28

115	Ion counting from explicit-solvent simulations and 3D-RISM. *Biophysical Journal*, **2014**, 106, 883-94	2.9	77
114	Recent advances toward a general purpose linear-scaling quantum force field. *Accounts of Chemical Research*, **2014**, 47, 2812-20	24.3	34
113	Molecular Dynamics Simulation of Nitrobenzene Dioxygenase Using AMBER Force Field. *Journal of Chemical Theory and Computation*, **2014**, 10, 2246-2254	6.4	20
112	Mechanistic insights into RNA transphosphorylation from kinetic isotope effects and linear free energy relationships of model reactions. *Chemistry - A European Journal*, **2014**, 20, 14336-43	4.8	26
111	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	6.4	48
110	A New Maximum Likelihood Approach for Free Energy Profile Construction from Molecular Simulations. *Journal of Chemical Theory and Computation*, **2013**, 9, 153-164	6.4	59
109	Molecular simulations of RNA 2SO-transesterification reaction models in solution. *Journal of Physical Chemistry B*, **2013**, 117, 94-103	3.4	21
108	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	4	8
107	Experimental and computational analysis of the transition state for ribonuclease A-catalyzed RNA 2SO-transphosphorylation. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 13002-7	11.5	52
106	A framework for flexible and scalable replica-exchange on production distributed CI **2013**,		2
105	Experimental and computational evidence that ribonuclease A alters the transition state for RNA 2?-O-transphosphorylation. *FASEB Journal*, **2013**, 27, 998.6	0.9	
104	Characterization of the reaction path and transition states for RNA transphosphorylation models from theory and experiment. *Angewandte Chemie - International Edition*, **2012**, 51, 647-51	16.4	43
103	Inside Back Cover: Characterization of the Reaction Path and Transition States for RNA Transphosphorylation Models from Theory and Experiment (Angew. Chem. Int. Ed. 3/2012). *Angewandte Chemie - International Edition*, **2012**, 51, 823-823	16.4	
102	Exact Relation between Potential of Mean Force and Free-Energy Profile. *Journal of Chemical Theory and Computation*, **2012**, 8, 3998-4003	6.4	21
101	Innenr□ktitelbild: Characterization of the Reaction Path and Transition States for RNA Transphosphorylation Models from Theory and Experiment (Angew. Chem. 3/2012). *Angewandte Chemie*, **2012**, 124, 847-847	3.6	
100	Extended polarization in third-order SCC-DFTB from chemical-potential equalization. *Journal of Physical Chemistry A*, **2012**, 116, 9131-41	2.8	38
99	Mapping L1 ligase ribozyme conformational switch. *Journal of Molecular Biology*, **2012**, 423, 106-22	6.5	6
98	Characterization of the Reaction Path and Transition States for RNA Transphosphorylation Models from Theory and Experiment. *Angewandte Chemie*, **2012**, 124, 671-675	3.6	3

97	Density-functional expansion methods: Grand challenges. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	27
96	Active participation of Mg ion in the reaction coordinate of RNA self-cleavage catalyzed by the hammerhead ribozyme. *Journal of Chemical Theory and Computation*, **2011**, 7, 1-3	6.4	47
95	Characterization of the Structure and Dynamics of the HDV Ribozyme at Different Stages Along the Reaction Path. *Journal of Physical Chemistry Letters*, **2011**, 2, 2538-2543	6.4	30
94	Density-functional expansion methods: generalization of the auxiliary basis. *Journal of Chemical Physics*, **2011**, 134, 194103	3.9	10
93	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	7.1	37
92	Insights into the Role of Conformational Transitions and Metal Ion Binding in RNA Catalysis from Molecular Simulations. *Annual Reports in Computational Chemistry*, **2010**, 6, 168-200	1.8	1
91	Density-functional expansion methods: evaluation of LDA, GGA, and meta-GGA functionals and different integral approximations. *Journal of Chemical Physics*, **2010**, 133, 244107	3.9	27
90	Identification of dynamical hinge points of the L1 ligase molecular switch. *Rna*, **2010**, 16, 769-80	5.8	6
89	Exocyclic deoxyadenosine adducts of 1,2,3,4-diepoxybutane: synthesis, structural elucidation, and mechanistic studies. *Chemical Research in Toxicology*, **2010**, 23, 118-33	4	34
88	Computational mutagenesis studies of hammerhead ribozyme catalysis. *Journal of the American Chemical Society*, **2010**, 132, 13505-18	16.4	17
87	Molecular dynamics simulation of bovine pancreatic ribonuclease A-CpA and transition state-like complexes. *Journal of Physical Chemistry B*, **2010**, 114, 7371-82	3.4	20
86	Accurate proton affinity and gas-phase basicity values for molecules important in biocatalysis. *Journal of Physical Chemistry B*, **2010**, 114, 13911-21	3.4	105
85	CHARMM: the biomolecular simulation program. *Journal of Computational Chemistry*, **2009**, 30, 1545-614	3.5	5515
84	Density Functional Study of the Influence of C5 Cytosine Substitution in Base Pairs with Guanine. *Theoretical Chemistry Accounts*, **2009**, 122, 179-188	1.9	17
83	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	6.5	38
82	Unraveling the Mechanisms of Ribozyme Catalysis with Multiscale Simulations. *Challenges and Advances in Computational Chemistry and Physics*, **2009**, 377-408	0.7	1
81	Spherical tensor gradient operator method for integral rotation: a simple, efficient, and extendable alternative to Slater-Koster tables. *Journal of Chemical Physics*, **2008**, 129, 016102	3.9	5
80	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	6.4	76

79	Role of Mg2+ in hammerhead ribozyme catalysis from molecular simulation. *Journal of the American Chemical Society*, **2008**, 130, 3053-64	16.4	93
78	Quantum mechanical/molecular mechanical simulation study of the mechanism of hairpin ribozyme catalysis. *Journal of the American Chemical Society*, **2008**, 130, 4680-91	16.4	74
77	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, 7168-9	16.4	17
76	Contracted auxiliary Gaussian basis integral and derivative evaluation. *Journal of Chemical Physics*, **2008**, 128, 064104	3.9	19
75	Electrostatic interactions in the hairpin ribozyme account for the majority of the rate acceleration without chemical participation by nucleobases. *Rna*, **2008**, 14, 1501-7	5.8	44
74	Extension of adaptive tree code and fast multipole methods to high angular momentum particle charge densities. *Journal of Computational Chemistry*, **2008**, 29, 1895-904	3.5	15
73	Solvent structure and hammerhead ribozyme catalysis. *Chemistry and Biology*, **2008**, 15, 332-42		92
72	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. *Journal of Physical Chemistry A*, **2007**, 111, 10861-73	2.8	221
71	Specific Reaction Parametrization of the AM1/d Hamiltonian for Phosphoryl Transfer Reactions: H, O, and P Atoms. *Journal of Chemical Theory and Computation*, **2007**, 3, 486-504	6.4	131
70	Insight into the role of Mg in hammerhead ribozyme catalysis from X-ray crystallography and molecular dynamics simulation. *Journal of Chemical Theory and Computation*, **2007**, 3, 325-327	6.4	37
69	CHARMM force field parameters for simulation of reactive intermediates in native and thio-substituted ribozymes. *Journal of Computational Chemistry*, **2007**, 28, 495-507	3.5	38
68	Charge-dependent model for many-body polarization, exchange, and dispersion interactions in hybrid quantum mechanical/molecular mechanical calculations. *Journal of Chemical Physics*, **2007**, 127, 194101	3.9	53
67	A charge-scaling implementation of the variational electrostatic projection method. *Journal of Computational Chemistry*, **2006**, 27, 103-15	3.5	9
66	Enzyme dynamics and tunneling enhanced by compression in the hydrogen abstraction catalyzed by soybean lipoxygenase-1. *Journal of Physical Chemistry B*, **2006**, 110, 24708-19	3.4	49
65	Nucleophilic attack on phosphate diesters: a density functional study of in-line reactivity in dianionic, monoanionic, and neutral systems. *Journal of Physical Chemistry B*, **2006**, 110, 11525-39	3.4	66
64	Normal modes of redox-active tyrosine: conformation dependence and comparison to experiment. *Journal of Physical Chemistry B*, **2006**, 110, 10970-81	3.4	31
63	Multilevel and density functional electronic structure calculations of proton affinities and gas-phase basicities involved in biological phosphoryl transfer. *Journal of Physical Chemistry A*, **2006** , 110, 791-7	2.8	17
62	QCRNA 1.0: a database of quantum calculations for RNA catalysis. *Journal of Molecular Graphics and Modelling*, **2006**, 25, 423-33	2.8	25

61	Transesterification thio effects of phosphate diesters: free energy barriers and kinetic and equilibrium isotope effects from density-functional theory. *Biochemistry*, **2006**, 45, 10043-53	3.2	64
60	The contribution of phosphate-phosphate repulsions to the free energy of DNA bending. *Nucleic Acids Research*, **2005**, 33, 1257-68	20.1	30
59	Kinetic isotope effects on thio-substituted biological phosphoryl transfer reactions from density-functional theory. *Chemical Communications*, **2005**, 3909-11	5.8	17
58	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	6.4	217
57	Smooth solvation method for d-orbital semiempirical calculations of biological reactions. 1. Implementation. *Journal of Physical Chemistry B*, **2005**, 109, 9799-809	3.4	30
56	Density functional study of the in-line mechanism of methanolysis of cyclic phosphate and thiophosphate esters in solution: insight into thio effects in RNA transesterification. *Journal of Physical Chemistry B*, **2005**, 109, 19987-20003	3.4	33
55	A Semiempirical Quantum Model for Hydrogen-Bonded Nucleic Acid Base Pairs. *Journal of Chemical Theory and Computation*, **2005**, 1, 1275-85	6.4	42
54	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, 536-56	3.4	25
53	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, 3070-9	3.6	72
52	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, 9810-7	3.4	18
51	Theoretical studies of dissociative phosphoryl transfer in interconversion of phosphoenolpyruvate to phosphonopyruvate: solvent effects, thio effects, and implications for enzymatic reactions. *Journal of Physical Chemistry B*, **2005**, 109, 13827-34	3.4	18
50	Solvent polarization and kinetic isotope effects in nitroethane deprotonation and implications to the nitroalkane oxidase reaction. *Journal of the American Chemical Society*, **2005**, 127, 16374-5	16.4	50
49	Theoretical methods that help understanding the structure and reactivity of gas phase ions. *International Journal of Mass Spectrometry*, **2005**, 240, 37-99	1.9	95
48	Pseudorotation barriers of biological oxyphosphoranes: a challenge for simulations of ribozyme catalysis. *Chemistry - A European Journal*, **2005**, 11, 2081-93	4.8	51
47	Ellipticity: a convenient tool to characterize electrocyclic reactions. *Chemistry - A European Journal*, **2005**, 11, 1734-8	4.8	64
46	High-order discretization schemes for biochemical applications of boundary element solvation and variational electrostatic projection methods. *Journal of Chemical Physics*, **2005**, 122, 194110	3.9	14
45	Improvement of semiempirical response properties with charge-dependent response density. *Journal of Chemical Physics*, **2005**, 123, 164108	3.9	49
44	Design and application of a multicoefficient correlation method for dispersion interactions. *Journal of Chemical Physics*, **2004**, 120, 590-602	3.9	7

43	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, 9903-6	3.9	59
42	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, 7939-48	3.9	27
41	Structure and binding of Mg(II) ions and di-metal bridge complexes with biological phosphates and phosphoranes. *Journal of Biological Inorganic Chemistry*, **2004**, 9, 807-17	3.7	27
40	Quantum descriptors for biological macromolecules from linear-scaling electronic structure methods. *Proteins: Structure, Function and Bioinformatics*, **2004**, 56, 724-37	4.2	46
39	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	2.1	33
38	Pseudorotation of natural and chemically modified biological phosphoranes: implications for RNA catalysis. *ChemPhysChem*, **2004**, 5, 1045-9	3.2	29
37	Pseudorotation of Natural and Chemically Modified Biological Phosphoranes: Implications for RNA Catalysis. *ChemPhysChem*, **2004**, 5, 1266-1266	3.2	1
36	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, 1654-65	16.4	92
35	Hybrid QM/MM study of thio effects in transphosphorylation reactions: the role of solvation. *Journal of the American Chemical Society*, **2004**, 126, 7504-13	16.4	54
34	Theoretical study of the vinyl allene oxide to cyclopent-2-en-1-one rearrangement: mechanism, torquoselectivity and solvent effects. *Journal of Organic Chemistry*, **2004**, 69, 3635-44	4.2	35
33	Parameterization of semiempirical methods to treat nucleophilic attacks to biological phosphates: AM1/d parameters for phosphorus. *Theoretical Chemistry Accounts*, **2003**, 109, 149-159	1.9	37
32	Fast approximate methods for calculating nucleic acid base pair interaction energies. *Journal of Computational Chemistry*, **2003**, 24, 57-67	3.5	30
31	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	6.5	36
30	Examination of the correlation energy and second virial coefficients from accurate ab initio calculations of rare-gas dimers. *Journal of Chemical Physics*, **2003**, 119, 2618-2622	3.9	27
29	Hybrid QM/MM study of thio effects in transphosphorylation reactions. *Journal of the American Chemical Society*, **2003**, 125, 7178-9	16.4	69
28	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		5
27	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	2.1	40
26	Quantum Mechanical Characterization of Nucleic Acids in Solution:A Linear-Scaling Study of Charge Fluctuations in DNA and RNA. *Journal of Physical Chemistry B*, **2002**, 106, 7693-7703	3.4	19

25	Spectroscopic properties of tyrosyl radicals in dipeptides. *Journal of the American Chemical Society*, **2002**, 124, 5496-505	16.4	46
24	Electronic structure properties of solvated biomolecules: A quantum approach for macromolecular characterization. *Journal of Computational Chemistry*, **2000**, 21, 1562-1571	3.5	18
23	A Smooth Solvation Potential Based on the Conductor-Like Screening Model. *Journal of Physical Chemistry A*, **1999**, 103, 11060-11079	2.8	306
22	Quantum Mechanical Treatment of Biological Macromolecules in Solution Using Linear-Scaling Electronic Structure Methods. *Physical Review Letters*, **1998**, 80, 5011-5014	7.4	63
21	Application of Linear-Scaling Electronic Structure Methods to the Study of Polarization of Proteins and DNA in Solution. *ACS Symposium Series*, **1998**, 275-287	0.4	2
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