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List of Publications by Year
in descending order

398 papers	28,580 citations	7069 78 h-index	7931 149 g-index
432 all docs	432 docs citations	432 times ranked	13568 citing authors

#	Article	IF	Citations
1	Refinement of the AMBER Force Field for Nucleic Acids: Improving the Description of Î±/Î³ Conformers. Biophysical Journal, 2007, 92, 3817-3829.	0.2	2,036
2	Benchmark database of accurate (MP2 and CCSD(T) complete basis set limit) interaction energies of small model complexes, DNA base pairs, and amino acid pairs. Physical Chemistry Chemical Physics, 2006, 8, 1985-1993.	1.3	1,635
3	Structure, Energetics, and Dynamics of the Nucleic Acid Base Pairs:â€‰ Nonempirical Ab Initio Calculations. Chemical Reviews, 1999, 99, 3247-3276.	23.0	984
4	Refinement of the Cornell et al. Nucleic Acids Force Field Based on Reference Quantum Chemical Calculations of Glycosidic Torsion Profiles. Journal of Chemical Theory and Computation, 2011, 7, 2886-2902.	2.3	873
5	Density functional theory and molecular clusters. Journal of Computational Chemistry, 1995, 16, 1315-1325.	1.5	503
6	Accurate Interaction Energies of Hydrogen-Bonded Nucleic Acid Base Pairs. Journal of the American Chemical Society, 2004, 126, 10142-10151.	6.6	444
7	Electronic properties, hydrogen bonding, stacking, and cation binding of DNA and RNA bases. Biopolymers, 2001, 61, 3-31.	1.2	408
8	RNA Structural Dynamics As Captured by Molecular Simulations: A Comprehensive Overview. Chemical Reviews, 2018, 118, 4177-4338.	23.0	408
9	Nature of Nucleic Acidâ^'Base Stacking: Nonempirical ab Initio and Empirical Potential Characterization of 10 Stacked Base Dimers. Comparison of Stacked and H-Bonded Base Pairs. The Journal of Physical Chemistry, 1996, 100, 5590-5596.	2.9	404
10	Structures and Energies of Hydrogen-Bonded DNA Base Pairs. A Nonempirical Study with Inclusion of Electron Correlation. The Journal of Physical Chemistry, 1996, 100, 1965-1974.	2.9	400
11	Refinement of the Sugarâ€“Phosphate Backbone Torsion Beta for AMBER Force Fields Improves the Description of Z- and B-DNA. Journal of Chemical Theory and Computation, 2015, 11, 5723-5736.	2.3	392
12	Toward True DNA Base-Stacking Energies:â€‰ MP2, CCSD(T), and Complete Basis Set Calculations. Journal of the American Chemical Society, 2002, 124, 11802-11808.	6.6	376
13	Assessing the Current State of Amber Force Field Modifications for DNA. Journal of Chemical Theory and Computation, 2016, 12, 4114-4127.	2.3	351
14	A systematic molecular dynamics study of nearest-neighbor effects on base pair and base pair step conformations and fluctuations in B-DNA. Nucleic Acids Research, 2010, 38, 299-313.	6.5	349
15	Performance of Molecular Mechanics Force Fields for RNA Simulations: Stability of UUCG and GNRA Hairpins. Journal of Chemical Theory and Computation, 2010, 6, 3836-3849.	2.3	339
16	Nature and magnitude of aromatic stacking of nucleic acid bases. Physical Chemistry Chemical Physics, 2008, 10, 2595.	1.3	317
17	Intercalators. 1. Nature of Stacking Interactions between Intercalators (Ethidium, Daunomycin,) Tj ETQq1 1 0.784314 rgBT /Overlock Functional Theory, and Empirical Potential Study. Journal of the American Chemical Society, 2002, 124, 3366-3376.	6.6	293
18	Toward Improved Description of DNA Backbone: Revisiting Epsilon and Zeta Torsion Force Field Parameters. Journal of Chemical Theory and Computation, 2013, 9, 2339-2354.	2.3	255

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19	Performance of empirical potentials (AMBER, CFF95, CVFF, CHARMM, OPLS, POLTEV), semiempirical quantum chemical methods (AM1, MNDO/M, PM3), andab initio Hartree-Fock method for interaction of DNA bases: Comparison with nonempirical beyond Hartree-Fock results. , 1997, 18, 1136-1150.		251
20	Nonplanar geometries of DNA bases. Ab initio second-order Moeller-Plesset study. The Journal of Physical Chemistry, 1994, 98, 3161-3164.	2.9	242
21	DNA Basepair Step Deformability Inferred from Molecular Dynamics Simulations. Biophysical Journal, 2003, 85, 2872-2883.	0.2	237
22	Reference Simulations of Noncanonical Nucleic Acids with Different Ï‡ Variants of the AMBER Force Field: Quadruplex DNA, Quadruplex RNA, and Z-DNA. Journal of Chemical Theory and Computation, 2012, 8, 2506-2520.	2.3	231
23	Hydrogen Bonding and Stacking of DNA Bases: A Review of Quantum-chemicalab initioStudies. Journal of Biomolecular Structure and Dynamics, 1996, 14, 117-135.	2.0	222
24	Interaction of DNA Base Pairs with Various Metal Cations (Mg2+, Ca2+, Sr2+, Ba2+, Cu+, Ag+, Au+, Zn2+,) Tj ETQq0 0 0 rgBT /Overlock Interaction. Journal of Physical Chemistry B, 1997, 101, 9670-9677.	1.2	222
25	Ab Initio Study of the Interaction of Guanine and Adenine with Various Mono- and Bivalent Metal Cations (Li+, Na+, K+, Rb+, Cs+; Cu+, Ag+, Au+; Mg2+, Ca2+, Sr2+, Ba2+; Zn2+, Cd2+, and Hg2+). The Journal of Physical Chemistry, 1996, 100, 7250-7255.	2.9	214
26	Nature of Base Stacking: Reference Quantum-Chemical Stacking Energies in Ten Unique B-DNA Base-Pair Steps. Chemistry - A European Journal, 2006, 12, 2854-2865.	1.7	211
27	DNA base amino groups and their role in molecular interactions: Ab initio and preliminary density functional theory calculations. , 1996, 57, 959-970.		197
28	H-Bonded and Stacked DNA Base Pairs: Cytosine Dimer. An Ab Initio Second-Order Moeller-Plesset Study. Journal of the American Chemical Society, 1995, 117, 792-798.	6.6	187
29	Correlated ab initio study of nucleic acid bases and their tautomers in the gas phase, in a microhydrated environment and in aqueous solution : Part 1. Cytosine. Physical Chemistry Chemical Physics, 2002, 4, 4192-4203.	1.3	187
30	Î¼ABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. Nucleic Acids Research, 2014, 42, 12272-12283.	6.5	186
31	Interaction between the Guanineâ^'Cytosine Watsonâ^'Crick DNA Base Pair and Hydrated Group IIa (Mg2+,) Tj ETQq1 1 0.784314 rgBT / 102, 5951-5957.	1.1	171
32	Nanosecond Molecular Dynamics Simulations of Parallel and Antiparallel Guanine Quadruplex DNA Molecules. Journal of the American Chemical Society, 1999, 121, 5519-5534.	6.6	162
33	High-energy chemistry of formamide: A unified mechanism of nucleobase formation. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 657-662.	3.3	159
34	Classification and energetics of the base-phosphate interactions in RNA. Nucleic Acids Research, 2009, 37, 4898-4918.	6.5	156
35	Molecular Dynamics and Quantum Mechanics of RNA: Conformational and Chemical Change We Can Believe In. Accounts of Chemical Research, 2010, 43, 40-47.	7.6	155
36	Thermodynamic Parameters for Stacking and Hydrogen Bonding of Nucleic Acid Bases in Aqueous Solution:Â Ab Initio/Langevin Dipoles Study. Journal of Physical Chemistry B, 1999, 103, 884-892.	1.2	150

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37	Molecular Dynamics Simulations and Thermodynamics Analysis of DNAâˆ'Drug Complexes. Minor Groove Binding between 4â€˛,6-Diamidino-2-phenylindole and DNA Duplexes in Solution. Journal of the American Chemical Society, 2003, 125, 1759-1769.	6.6	150
38	Sequence-dependent elastic properties of DNA 1 1Edited by I. Tinoco. Journal of Molecular Biology, 2000, 299, 695-709.	2.0	149
39	The Effect of Metal Binding to the N7 Site of Purine Nucleotides on Their Structure, Energy, and Involvement in Base Pairing. Journal of Physical Chemistry B, 2000, 104, 7535-7544.	1.2	147
40	Metal-Stabilized Rare Tautomers and Mispairs of DNA Bases:â€‰ N6-Metalated Adenine and N4-Metalated Cytosine, Theoretical and Experimental Views. Journal of Physical Chemistry A, 1999, 103, 11406-11413.	1.1	145
41	Molecular Dynamics Simulations of Nucleic Acids. From Tetranucleotides to the Ribosome. Journal of Physical Chemistry Letters, 2014, 5, 1771-1782.	2.1	139
42	Bifurcated hydrogen bonds in DNA crystal structures. An ab initio quantum chemical study. Journal of the American Chemical Society, 1994, 116, 709-714.	6.6	137
43	Molecular dynamics simulations of RNA: Anin silico single molecule approach. Biopolymers, 2007, 85, 169-184.	1.2	137
44	Base Pair Fraying in Molecular Dynamics Simulations of DNA and RNA. Journal of Chemical Theory and Computation, 2014, 10, 3177-3189.	2.3	135
45	Formation Pathways of a Guanine-Quadruplex DNA Revealed by Molecular Dynamics and Thermodynamic Analysis of the Substates. Biophysical Journal, 2003, 85, 1787-1804.	0.2	128
46	Câ€'HÂ·Â·Â·O Contacts in the AdenineÂ·Â·Â·Uracil Watsonâ€'Crick and UracilÂ·Â·Â·Uracil Nucleic Acid Base Pairs:â€‰ Nonempirical ab Initio Study with Inclusion of Electron Correlation Effects. Journal of Physical Chemistry B, 2000, 104, 6286-6292.	1.2	125
47	Computer Folding of RNA Tetraloops: Identification of Key Force Field Deficiencies. Journal of Chemical Theory and Computation, 2016, 12, 4534-4548.	2.3	125
48	Cations and Hydration in Catalytic RNA: Molecular Dynamics of the Hepatitis Delta Virus Ribozyme. Biophysical Journal, 2006, 91, 626-638.	0.2	122
49	Single Stranded Loops of Quadruplex DNA As Key Benchmark for Testing Nucleic Acids Force Fields. Journal of Chemical Theory and Computation, 2009, 5, 2514-2530.	2.3	121
50	Explaining the varied glycosidic conformational, G-tract length and sequence preferences for anti-parallel G-quadruplexes. Nucleic Acids Research, 2011, 39, 4499-4512.	6.5	119
51	Molecular Dynamics Simulations of Guanine Quadruplex Loops: Advances and Force Field Limitations. Biophysical Journal, 2004, 87, 227-242.	0.2	116
52	Amino groups in nucleic acid bases, aniline, aminopyridines, and aminotriazine are nonplanar: Results of correlatedabinitioquantum chemical calculations and anharmonic analysis of the aniline inversion motion. Journal of Chemical Physics, 1996, 105, 11042-11050.	1.2	115
53	Base Stacking and Hydrogen Bonding in Protonated Cytosine Dimer: The Role of Molecular ion-dipole and Induction Interactions. Journal of Biomolecular Structure and Dynamics, 1996, 13, 695-706.	2.0	114
54	Molecular dynamics simulations of G-DNA and perspectives on the simulation of nucleic acid structures. Methods, 2012, 57, 25-39.	1.9	111

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55	Structural dynamics of possible late-stage intermediates in folding of quadruplex DNA studied by molecular simulations. Nucleic Acids Research, 2013, 41, 7128-7143.	6.5	111
56	On the potential role of the amino nitrogen atom as a hydrogen bond acceptor in macromolecules. Journal of Molecular Biology, 1998, 279, 1123-1136.	2.0	110
57	A prebiotically plausible synthesis of pyrimidine Î²-ribonucleosides and their phosphate derivatives involving photoanomerization. Nature Chemistry, 2017, 9, 303-309.	6.6	109
58	Uracil Dimer:â€‰ Potential Energy and Free Energy Surfaces. Ab Initio beyond Hartreeâ^'Fock and Empirical Potential Studies. Journal of Physical Chemistry A, 1998, 102, 6921-6926.	1.1	108
59	Non-Watson-Crick Basepairing and Hydration in RNA Motifs: Molecular Dynamics of 5S rRNA Loop E. Biophysical Journal, 2003, 84, 3564-3582.	0.2	108
60	Relative Stability of Different DNA Guanine Quadruplex Stem Topologies Derived Using Large-Scale Quantum-Chemical Computations. Journal of the American Chemical Society, 2013, 135, 9785-9796.	6.6	108
61	Nature and magnitude of aromatic base stacking in DNA and RNA: Quantum chemistry, molecular mechanics, and experiment. Biopolymers, 2013, 99, 978-988.	1.2	106
62	Interaction Energies of Hydrogen-Bonded Formamide Dimer, Formamidine Dimer, and Selected DNA Base Pairs Obtained with Large Basis Sets of Atomic Orbitals. Journal of Physical Chemistry A, 2000, 104, 4592-4597.	1.1	103
63	Interaction of the Adenineâ^'Thymine Watsonâ^'Crick and Adenineâ^'Adenine Reverse-Hoogsteen DNA Base Pairs with Hydrated Group IIa (Mg2+, Ca2+, Sr2+, Ba2+) and IIb (Zn2+, Cd2+, Hg2+) Metal Cations:Â Absence of the Base Pair Stabilization by Metal-Induced Polarization Effects. Journal of Physical Chemistry B, 1999, 103, 2528-2534.	1.2	102
64	Nonplanar DNA Base Pairs. Journal of Biomolecular Structure and Dynamics, 1996, 13, 827-833.	2.0	101
65	Molecular dynamics simulations and their application to four-stranded DNA. Methods, 2007, 43, 278-290.	1.9	97
66	Comparison of Intrinsic Stacking Energies of Ten Unique Dinucleotide Steps in A-RNA and B-DNA Duplexes. Can We Determine Correct Order of Stability by Quantum-Chemical Calculations?. Journal of Physical Chemistry B, 2010, 114, 1191-1203.	1.2	97
67	Improving the Performance of the Amber RNA Force Field by Tuning the Hydrogen-Bonding Interactions. Journal of Chemical Theory and Computation, 2019, 15, 3288-3305.	2.3	97
68	Interactions of Hydrated Mg2+ Cation with Bases, Base Pairs, and Nucleotides. Electron Topology, Natural Bond Orbital, Electrostatic, and Vibrational Study. Journal of Physical Chemistry B, 2001, 105, 6051-6060.	1.2	95
69	A G-quadruplex-binding compound showing anti-tumour activity in an in vivo model for pancreatic cancer. Scientific Reports, 2015, 5, 11385.	1.6	95
70	Structural Dynamics and Cation Interactions of DNA Quadruplex Molecules Containing Mixed Guanine/Cytosine Quartets Revealed by Large-Scale MD Simulations. Journal of the American Chemical Society, 2001, 123, 3295-3307.	6.6	93
71	Trapped water molecules are essential to structural dynamics and function of a ribozyme. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 13380-13385.	3.3	92
72	Potential Energy Surface of the Cytosine Dimer:Â MP2 Complete Basis Set Limit Interaction Energies, CCSD(T) Correction Term, and Comparison with the AMBER Force Field. Journal of Physical Chemistry B, 2004, 108, 5466-5471.	1.2	91

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73	Hinge-Like Motions in RNA Kink-Turns: The Role of the Second A-Minor Motif and Nominally Unpaired Bases. Biophysical Journal, 2005, 88, 3466-3485.	0.2	91
74	Quantum Chemical Benchmark Study on 46 RNA Backbone Families Using a Dinucleotide Unit. Journal of Chemical Theory and Computation, 2015, 11, 4972-4991.	2.3	90
75	Crystal Structure of d(GGCCAATTGG) Complexed with DAPI Reveals Novel Binding Modeâ€‚â€¡. Biochemistry, 1999, 38, 16443-16451.	1.2	89
76	Folding of guanine quadruplex moleculesâ€“funnel-like mechanism or kinetic partitioning? An overview from MD simulation studies. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 1246-1263.	1.1	89
77	Molecular dynamics simulations of sarcin-ricin rRNA motif. Nucleic Acids Research, 2006, 34, 697-708.	6.5	88
78	Critical Effect of the N2 Amino Group on Structure, Dynamics, and Elasticity of DNA Polypurine Tracts. Biophysical Journal, 2002, 82, 2592-2609.	0.2	84
79	Reference MP2/CBS and CCSD(T) quantum-chemical calculations on stacked adenine dimers. Comparison with DFT-D, MP2.5, SCS(MI)-MP2, M06-2X, CBS(SCS-D) and force field descriptions. Physical Chemistry Chemical Physics, 2010, 12, 3522.	1.3	84
80	Computer Folding of RNA Tetraloops? Are We There Yet?. Journal of Chemical Theory and Computation, 2013, 9, 2115-2125.	2.3	84
81	Theoretical Study of Binding of Hydrated Zn(II) and Mg(II) Cations to 5â€˜-Guanosine Monophosphate. Toward Polarizable Molecular Mechanics for DNA and RNA. Journal of Physical Chemistry B, 2003, 107, 8669-8681.	1.2	82
82	Theoretical studies of RNA catalysis: Hybrid QM/MM methods and their comparison with MD and QM. Methods, 2009, 49, 202-216.	1.9	82
83	Extensive Molecular Dynamics Simulations Showing That Canonical G8 and Protonated A38H⁺ Forms Are Most Consistent with Crystal Structures of Hairpin Ribozyme. Journal of Physical Chemistry B, 2010, 114, 6642-6652.	1.2	81
84	Ion Binding to Quadruplex DNA Stems. Comparison of MM and QM Descriptions Reveals Sizable Polarization Effects Not Included in Contemporary Simulations. Journal of Chemical Theory and Computation, 2014, 10, 1326-1340.	2.3	81
85	Non-Watsonâ^'Crick Base Pairing in RNA. Quantum Chemical Analysis of the cis Watsonâ^'Crick/Sugar Edge Base Pair Family. Journal of Physical Chemistry A, 2005, 109, 2292-2301.	1.1	80
86	Outer-Shell and Inner-Shell Coordination of Phosphate Group to Hydrated Metal Ions (Mg2+, Cu2+,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 of Physical Chemistry B, 2003, 107, 1913-1923.	1.2	79
87	Large-scale compensation of errors in pairwise-additive empirical force fields: comparison of AMBER intermolecular terms with rigorous DFT-SAPT calculations. Physical Chemistry Chemical Physics, 2010, 12, 10476.	1.3	79
88	Complexes of Pentahydrated Zn2+with Guanine, Adenine, and the Guanineâ^'Cytosine and Adenineâ^'Thymine Base Pairs. Structures and Energies Characterized by Polarizable Molecular Mechanics and ab Initio Calculations. Journal of Physical Chemistry B, 1999, 103, 11415-11427.	1.2	78
89	Global Minimum of the AdenineÂ·Â·Â·Thymine Base Pair Corresponds Neither to Watsonâ^'Crick Nor to Hoogsteen Structures. Molecular Dynamic/Quenching/AMBER and ab Initio beyond Hartreeâ^'Fock Studies. Journal of the American Chemical Society, 2000, 122, 3495-3499.	6.6	78
90	Structure, Stiffness and Substates of the Dickerson-Drew Dodecamer. Journal of Chemical Theory and Computation, 2013, 9, 707-721.	2.3	78

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91	Molecular Dynamics of Hemiprotonated Intercalated Four-Stranded i-DNA:Â Stable Trajectories on a Nanosecond Scale. Journal of the American Chemical Society, 1998, 120, 6147-6151.	6.6	77
92	Molecular Interactions of Nucleic Acid Bases. A Review of Quantum-Chemical Studies. Collection of Czechoslovak Chemical Communications, 2003, 68, 2231-2282.	1.0	77
93	Significant structural deformation of nucleic acid bases in stacked base pairs: an ab initio study beyond Hartreeâ€“Fock. Chemical Physics Letters, 1998, 288, 7-14.	1.2	76
94	The DNA and RNA sugarâ€“phosphate backbone emerges as the key player. An overview of quantum-chemical, structural biology and simulation studies. Physical Chemistry Chemical Physics, 2012, 14, 15257.	1.3	76
95	Principles of RNA Base Pairing:Â Structures and Energies of the Trans Watsonâ€“Crick/Sugar Edge Base Pairs. Journal of Physical Chemistry B, 2005, 109, 11399-11410.	1.2	75
96	Metal ions in non-complementary DNA base pairs: an ab initio study of Cu(I), Ag(I), and Au(I) complexes with the cytosine-adenine base pair. Journal of Biological Inorganic Chemistry, 1999, 4, 537-545.	1.1	73
97	High-Energy Chemistry of Formamide: A Simpler Way for Nucleobase Formation. Journal of Physical Chemistry A, 2014, 118, 719-736.	1.1	73
98	Structure, dynamics, and elasticity of free 16s rRNA helix 44 studied by molecular dynamics simulations. Biopolymers, 2006, 82, 504-520.	1.2	72
99	Triplex intermediates in folding of human telomeric quadruplexes probed by microsecond-scale molecular dynamics simulations. Biochimie, 2014, 105, 22-35.	1.3	72
100	Molecular dynamics of the frame-shifting pseudoknot from beet western yellows virus: the role of non-Watson-Crick base-pairing, ordered hydration, cation binding and base mutations on stability and unfolding 1 1Edited by J. Doudna. Journal of Molecular Biology, 2001, 313, 1073-1091.	2.0	70
101	Conformational dynamics of the human propeller telomeric DNA quadruplex on a microsecond time scale. Nucleic Acids Research, 2013, 41, 2723-2735.	6.5	70
102	Free Energy Landscape of GAGA and UUCG RNA Tetraloops. Journal of Physical Chemistry Letters, 2016, 7, 4032-4038.	2.1	70
103	Unique Tertiary and Neighbor Interactions Determine Conservation Patterns of Cis Watsonâ€“Crick A/G Base-pairs. Journal of Molecular Biology, 2003, 330, 967-978.	2.0	69
104	Molecular basis for AU-rich element recognition and dimerization by the HuR C-terminal RRM. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 2935-2944.	3.3	69
105	Can We Accurately Describe the Structure of Adenine Tracts in B-DNA? Reference Quantum-Chemical Computations Reveal Overstabilization of Stacking by Molecular Mechanics. Journal of Chemical Theory and Computation, 2012, 8, 2448-2460.	2.3	67
106	Dependence of A-RNA simulations on the choice of the force field and salt strength. Physical Chemistry Chemical Physics, 2009, 11, 10701.	1.3	66
107	Intramolecular flexibility of DNA bases in adenineâ€“thymine and guanineâ€“cytosine Watsonâ€“Crick base pairs. Journal of Molecular Structure, 1999, 477, 15-21.	1.8	65
108	Molecular dynamics simulations of RNA kissing-loop motifs reveal structural dynamics and formation of cation-binding pockets. Nucleic Acids Research, 2003, 31, 6942-6952.	6.5	65

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109	Structural Dynamics of Precursor and Product of the RNA Enzyme from the Hepatitis Delta Virus as Revealed by Molecular Dynamics Simulations. Journal of Molecular Biology, 2005, 351, 731-748.	2.0	65
110	Emergence of the First Catalytic Oligonucleotides in a Formamideâ€Based Origin Scenario. Chemistry - A European Journal, 2016, 22, 3572-3586.	1.7	65
111	Cation binding to 15-TBA quadruplex DNA is a multiple-pathway cation-dependent process. Nucleic Acids Research, 2011, 39, 9789-9802.	6.5	64
112	Simulations of A-RNA Duplexes. The Effect of Sequence, Solute Force Field, Water Model, and Salt Concentration. Journal of Physical Chemistry B, 2012, 116, 9899-9916.	1.2	64
113	Reverse Watsonâ^'Crick Isocytosineâ^'Cytosine and Guanineâ^'Cytosine Base Pairs Stabilized by the Formation of the Minor Tautomers of Bases. An ab Initio Study in the Gas Phase and in a Water Cluster. Journal of Physical Chemistry A, 1998, 102, 10374-10379.	1.1	62
114	Insights into Stability and Folding of GNRA and UNCG Tetraloops Revealed by Microsecond Molecular Dynamics and Well-Tempered Metadynamics. Journal of Chemical Theory and Computation, 2015, 11, 3866-3877.	2.3	60
115	Mechanical properties of symmetric and asymmetric DNA A-tracts: implications for looping and nucleosome positioning. Nucleic Acids Research, 2014, 42, 7383-7394.	6.5	59
116	Anharmonic and harmonic intermolecular vibrational modes of the DNA base pairs. Journal of Chemical Physics, 1997, 106, 1472-1479.	1.2	58
117	Insight into G-DNA Structural Polymorphism and Folding from Sequence and Loop Connectivity through Free Energy Analysis. Journal of the American Chemical Society, 2011, 133, 14270-14279.	6.6	58
118	On the Road from Formamide Ices to Nucleobases: IR-Spectroscopic Observation of a Direct Reaction between Cyano Radicals and Formamide in a High-Energy Impact Event. Journal of the American Chemical Society, 2012, 134, 20788-20796.	6.6	58
119	Quantum Chemical Studies of Nucleic Acids: Can We Construct a Bridge to the RNA Structural Biology and Bioinformatics Communities?. Journal of Physical Chemistry B, 2010, 114, 15723-15741.	1.2	57
120	Sugar Edge/Sugar Edge Base Pairs in RNA:Â Stabilities and Structures from Quantum Chemical Calculations. Journal of Physical Chemistry B, 2005, 109, 18680-18689.	1.2	56
121	Comparison of ab Initio, DFT, and Semiempirical QM/MM Approaches for Description of Catalytic Mechanism of Hairpin Ribozyme. Journal of Chemical Theory and Computation, 2014, 10, 1608-1622.	2.3	56
122	Theoretical Study on the Structure, Stability, and Electronic Properties of the Guanineâ^'Znâ^'Cytosine Base Pair in M-DNA. Journal of Physical Chemistry B, 2007, 111, 870-879.	1.2	55
123	Trans Hoogsteen/Sugar Edge Base Pairing in RNA. Structures, Energies, and Stabilities from Quantum Chemical Calculations. Journal of Physical Chemistry B, 2009, 113, 1743-1755.	1.2	55
124	Investigations of Stacked DNA Base-Pair Steps: Highly Accurate Stacking Interaction Energies, Energy Decomposition, and Many-Body Stacking Effects. Journal of Chemical Theory and Computation, 2019, 15, 95-115.	2.3	55
125	Molecular Dynamics of DNA Quadruplex Molecules Containing Inosine, 6-Thioguanine and 6-Thiopurine. Biophysical Journal, 2001, 80, 455-468.	0.2	54
126	RNA Kink-Turns as Molecular Elbows: Hydration, Cation Binding, and Large-Scale Dynamics. Structure, 2006, 14, 825-835.	1.6	54

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127	Conformations of Flanking Bases in HIV-1 RNA DIS Kissing Complexes Studied by Molecular Dynamics. Biophysical Journal, 2007, 93, 3932-3949.	0.2	54
128	Protonation States of the Key Active Site Residues and Structural Dynamics of the glmS Riboswitch As Revealed by Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 8701-8712.	1.2	54
129	Chemical Shifts in Nucleic Acids Studied by Density Functional Theory Calculations and Comparison with Experiment. Chemistry - A European Journal, 2012, 18, 12372-12387.	1.7	54
130	How to understand atomistic molecular dynamics simulations of <scp>RNA</scp> and proteinâ€“<scp>RNA</scp> complexes?. Wiley Interdisciplinary Reviews RNA, 2017, 8, e1405.	3.2	54
131	How Proximal Nucleobases Regulate the Catalytic Activity of G-Quadruplex/Hemin DNAzymes. ACS Catalysis, 2018, 8, 11352-11361.	5.5	54
132	Fitting Corrections to an RNA Force Field Using Experimental Data. Journal of Chemical Theory and Computation, 2019, 15, 3425-3431.	2.3	54
133	A Systematic ab Initio Study of the Hydration of Selected Palladium Square-Planar Complexes. A Comparison with Platinum Analogues. Journal of Physical Chemistry A, 2001, 105, 8086-8092.	1.1	53
134	Theoretical Study of the Guanine â† 6-Thioguanine Substitution in Duplexes, Triplexes, and Tetraplexes. Journal of the American Chemical Society, 2004, 126, 14642-14650.	6.6	52
135	Geometrical and Electronic Structure Variability of the Sugarâ”phosphate Backbone in Nucleic Acids. Journal of Physical Chemistry B, 2008, 112, 8188-8197.	1.2	52
136	Balance of Attraction and Repulsion in Nucleic-Acid Base Stacking: CCSD(T)/Complete-Basis-Set-Limit Calculations on Uracil Dimer and a Comparison with the Force-Field Description. Journal of Chemical Theory and Computation, 2009, 5, 1524-1544.	2.3	51
137	Structure of a Stable G-Hairpin. Journal of the American Chemical Society, 2017, 139, 3591-3594.	6.6	51
138	Protonation of Platinated Adenine Nucleobases. Gas Phase vs Condensed Phase Picture. Inorganic Chemistry, 2001, 40, 3269-3278.	1.9	50
139	The Influence of the Thymine C5 Methyl Group on Spontaneous Base Pair Breathing in DNA. Journal of Biological Chemistry, 2002, 277, 28491-28497.	1.6	50
140	Coarse-Grained Simulations Complemented by Atomistic Molecular Dynamics Provide New Insights into Folding and Unfolding of Human Telomeric G-Quadruplexes. Journal of Chemical Theory and Computation, 2016, 12, 6077-6097.	2.3	50
141	Effect of Monovalent Ion Parameters on Molecular Dynamics Simulations of G-Quadruplexes. Journal of Chemical Theory and Computation, 2017, 13, 3911-3926.	2.3	50
142	Synthesis of (<scp>d</scp>)-erythrose from glycolaldehyde aqueous solutions under electric field. Chemical Communications, 2018, 54, 3211-3214.	2.2	50
143	The Influence of N7Guanine Modifications on the Strength of Watsonâ”Crick Base Pairing and Guanine N1Acidity:Â Comparison of Gas-Phase and Condensed-Phase Trends. Journal of Physical Chemistry B, 2003, 107, 5349-5356.	1.2	49
144	Structural and evolutionary classification of G/U wobble basepairs in the ribosome. Nucleic Acids Research, 2006, 34, 1326-1341.	6.5	49

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