

Thomas E Cheatham

List of Publications by Year in descending order

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127
papers

38,258
citations

25034

57
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17105

122
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131
all docs

131
docs citations

131
times ranked

29024
citing authors

#	ARTICLE	IF	CITATIONS
1	The Amber biomolecular simulation programs. <i>Journal of Computational Chemistry</i> , 2005, 26, 1668-1688.	3.3	7,742
2	PTRAJ and CPPTRAJ: Software for Processing and Analysis of Molecular Dynamics Trajectory Data. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3084-3095.	5.3	4,960
3	Calculating Structures and Free Energies of Complex Molecules: Combining Molecular Mechanics and Continuum Models. <i>Accounts of Chemical Research</i> , 2000, 33, 889-897.	15.6	4,098
4	AMBER, a package of computer programs for applying molecular mechanics, normal mode analysis, molecular dynamics and free energy calculations to simulate the structural and energetic properties of molecules. <i>Computer Physics Communications</i> , 1995, 91, 1-41.	7.5	2,839
5	Determination of Alkali and Halide Monovalent Ion Parameters for Use in Explicitly Solvated Biomolecular Simulations. <i>Journal of Physical Chemistry B</i> , 2008, 112, 9020-9041.	2.6	2,756
6	Refinement of the AMBER Force Field for Nucleic Acids: Improving the Description of λ_{\pm}/λ_3 Conformers. <i>Biophysical Journal</i> , 2007, 92, 3817-3829.	0.5	2,036
7	Continuum Solvent Studies of the Stability of DNA, RNA, and Phosphoramidate-DNA Helices. <i>Journal of the American Chemical Society</i> , 1998, 120, 9401-9409.	13.7	1,442
8	A Modified Version of the Cornell et al. Force Field with Improved Sugar Pucker Phases and Helical Repeat. <i>Journal of Biomolecular Structure and Dynamics</i> , 1999, 16, 845-862.	3.5	882
9	Refinement of the Cornell et al. Nucleic Acids Force Field Based on Reference Quantum Chemical Calculations of Glycosidic Torsion Profiles. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2886-2902.	5.3	873
10	Clustering Molecular Dynamics Trajectories: 1. Characterizing the Performance of Different Clustering Algorithms. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2312-2334.	5.3	721
11	Molecular Dynamics Simulations of the Dynamic and Energetic Properties of Alkali and Halide Ions Using Water-Model-Specific Ion Parameters. <i>Journal of Physical Chemistry B</i> , 2009, 113, 13279-13290.	2.6	476
12	Refinement of the Sugar-Phosphate Backbone Torsion Beta for AMBER Force Fields Improves the Description of Z- and B-DNA. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5723-5736.	5.3	392
13	Assessing the Current State of Amber Force Field Modifications for DNA. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4114-4127.	5.3	351
14	A systematic molecular dynamics study of nearest-neighbor effects on base pair and base pair step conformations and fluctuations in B-DNA. <i>Nucleic Acids Research</i> , 2010, 38, 299-313.	14.5	349
15	The flying ice cube: Velocity rescaling in molecular dynamics leads to violation of energy equipartition. <i>Journal of Computational Chemistry</i> , 1998, 19, 726-740.	3.3	347
16	Performance of Molecular Mechanics Force Fields for RNA Simulations: Stability of UUCG and GNRA Hairpins. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3836-3849.	5.3	339
17	MOLECULAR DYNAMIC SIMULATION OF NUCLEIC ACIDS. <i>Annual Review of Physical Chemistry</i> , 2000, 51, 435-471.	10.8	330
18	Molecular dynamics simulation of nucleic acids: Successes, limitations, and promise. <i>Biopolymers</i> , 2000, 56, 232-256.	2.4	307

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19	Molecular Dynamics Simulations Highlight the Structural Differences among DNA:DNA, RNA:RNA, and DNA:RNA Hybrid Duplexes. <i>Journal of the American Chemical Society</i> , 1997, 119, 4805-4825.	13.7	257
20	Toward Improved Description of DNA Backbone: Revisiting Epsilon and Zeta Torsion Force Field Parameters. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2339-2354.	5.3	255
21	Molecular Dynamics Simulations of the 136 Unique Tetranucleotide Sequences of DNA Oligonucleotides. I. Research Design and Results on d(CpG) Steps. <i>Biophysical Journal</i> , 2004, 87, 3799-3813.	0.5	245
22	DNA Basepair Step Deformability Inferred from Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2003, 85, 2872-2883.	0.5	237
23	Reference Simulations of Noncanonical Nucleic Acids with Different \ddagger Variants of the AMBER Force Field: Quadruplex DNA, Quadruplex RNA, and Z-DNA. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2506-2520.	5.3	231
24	Molecular Dynamics Simulations of the 136 Unique Tetranucleotide Sequences of DNA Oligonucleotides. II: Sequence Context Effects on the Dynamical Structures of the 10 Unique Dinucleotide Steps. <i>Biophysical Journal</i> , 2005, 89, 3721-3740.	0.5	216
25	Simulation and modeling of nucleic acid structure, dynamics and interactions. <i>Current Opinion in Structural Biology</i> , 2004, 14, 360-367.	5.7	212
26	Quantum mechanically derived AMBER-compatible heme parameters for various states of the cytochrome P450 catalytic cycle. <i>Journal of Computational Chemistry</i> , 2012, 33, 119-133.	3.3	210
27	An accurate and simple quantum model for liquid water. <i>Journal of Chemical Physics</i> , 2006, 125, 184507.	3.0	187
28	\ddagger 4ABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. <i>Nucleic Acids Research</i> , 2014, 42, 12272-12283.	14.5	186
29	Molecular Dynamics and Continuum Solvent Studies of the Stability of PolyG-PolyC and PolyA-PolyT DNA Duplexes in Solution. <i>Journal of Biomolecular Structure and Dynamics</i> , 1998, 16, 265-280.	3.5	183
30	Removal of pressure and free energy artifacts in charged periodic systems via net charge corrections to the Ewald potential. <i>Journal of Chemical Physics</i> , 1998, 108, 7070-7084.	3.0	162
31	Spontaneous Formation of KCl Aggregates in Biomolecular Simulations: A Force Field Issue?. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1851-1859.	5.3	159
32	Twenty-five years of nucleic acid simulations. <i>Biopolymers</i> , 2013, 99, 969-977.	2.4	157
33	Molecular Dynamics Simulations and Thermodynamics Analysis of DNA-Drug Complexes. Minor Groove Binding between 4 \ddagger ,6-Diamidino-2-phenylindole and DNA Duplexes in Solution. <i>Journal of the American Chemical Society</i> , 2003, 125, 1759-1769.	13.7	150
34	Intercalation processes of copper complexes in DNA. <i>Nucleic Acids Research</i> , 2015, 43, 5364-5376.	14.5	137
35	Convergence and reproducibility in molecular dynamics simulations of the DNA duplex d(GCACGAACGAACGACGC). <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2015, 1850, 1041-1058.	2.4	136
36	Formation Pathways of a Guanine-Quadruplex DNA Revealed by Molecular Dynamics and Thermodynamic Analysis of the Substates. <i>Biophysical Journal</i> , 2003, 85, 1787-1804.	0.5	128

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37	Improved Force Field Parameters Lead to a Better Description of RNA Structure. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3969-3972.	5.3	126
38	Highly sampled tetranucleotide and tetraloop motifs enable evaluation of common RNA force fields. <i>Rna</i> , 2015, 21, 1578-1590.	3.5	123
39	Single Stranded Loops of Quadruplex DNA As Key Benchmark for Testing Nucleic Acids Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2514-2530.	5.3	121
40	Multidimensional Replica Exchange Molecular Dynamics Yields a Converged Ensemble of an RNA Tetranucleotide. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 492-499.	5.3	120
41	Explaining the varied glycosidic conformational, G-tract length and sequence preferences for anti-parallel G-quadruplexes. <i>Nucleic Acids Research</i> , 2011, 39, 4499-4512.	14.5	119
42	Molecular Dynamics Simulations of Guanine Quadruplex Loops: Advances and Force Field Limitations. <i>Biophysical Journal</i> , 2004, 87, 227-242.	0.5	116
43	Molecular dynamics simulations of G-DNA and perspectives on the simulation of nucleic acid structures. <i>Methods</i> , 2012, 57, 25-39.	3.8	111
44	Structural dynamics of possible late-stage intermediates in folding of quadruplex DNA studied by molecular simulations. <i>Nucleic Acids Research</i> , 2013, 41, 7128-7143.	14.5	111
45	Relative Stability of Different DNA Guanine Quadruplex Stem Topologies Derived Using Large-Scale Quantum-Chemical Computations. <i>Journal of the American Chemical Society</i> , 2013, 135, 9785-9796.	13.7	108
46	Dynamically Amorphous Character of Electronic States in Poly(dA) ⁿ Poly(dT) DNA. <i>Journal of Physical Chemistry B</i> , 2003, 107, 2581-2587.	2.6	106
47	Insight into the stabilization of A-DNA by specific ion association: spontaneous B-DNA to A-DNA transitions observed in molecular dynamics simulations of d[ACCCGCGGT] ₂ in the presence of hexaamminecobalt(III). <i>Structure</i> , 1997, 5, 1297-1311.	3.3	104
48	Adventures in Improving the Scaling and Accuracy of a Parallel Molecular Dynamics Program. <i>Journal of Supercomputing</i> , 1997, 11, 255-278.	3.6	99
49	Parallelization of CPPTRAJ enables large scale analysis of molecular dynamics trajectory data. <i>Journal of Computational Chemistry</i> , 2018, 39, 2110-2117.	3.3	97
50	Antifreeze Proteins at the Ice/Water Interface: Three Calculated Discriminating Properties for Orientation of Type I Proteins. <i>Biophysical Journal</i> , 2007, 93, 1442-1451.	0.5	90
51	Evaluation of Enhanced Sampling Provided by Accelerated Molecular Dynamics with Hamiltonian Replica Exchange Methods. <i>Journal of Physical Chemistry B</i> , 2014, 118, 3543-3552.	2.6	86
52	Critical Effect of the N2 Amino Group on Structure, Dynamics, and Elasticity of DNA Polypurine Tracts. <i>Biophysical Journal</i> , 2002, 82, 2592-2609.	0.5	84
53	A Coarse-Grained Model of DNA with Explicit Solvation by Water and Ions. <i>Journal of Physical Chemistry B</i> , 2011, 115, 132-142.	2.6	78
54	Triplex intermediates in folding of human telomeric quadruplexes probed by microsecond-scale molecular dynamics simulations. <i>Biochimie</i> , 2014, 105, 22-35.	2.6	72

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55	On the absence of intrahelical DNA dynamics on the $\hat{1}/4$ s to ms timescale. <i>Nature Communications</i> , 2014, 5, 5152.	12.8	70
56	Self-Tensioning Aquatic Caddisfly Silk: Ca ²⁺ -Dependent Structure, Strength, and Load Cycle Hysteresis. <i>Biomacromolecules</i> , 2013, 14, 3668-3681.	5.4	64
57	Unrestrained Molecular Dynamics of Photodamaged DNA in Aqueous Solution. <i>Journal of the American Chemical Society</i> , 1997, 119, 7095-7104.	13.7	62
58	Recent advances in molecular dynamics simulation towards the realistic representation of biomolecules in solution. <i>Theoretical Chemistry Accounts</i> , 1998, 99, 279-288.	1.4	61
59	Reliable Oligonucleotide Conformational Ensemble Generation in Explicit Solvent for Force Field Assessment Using Reservoir Replica Exchange Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2013, 117, 4014-4027.	2.6	60
60	Insight into G-DNA Structural Polymorphism and Folding from Sequence and Loop Connectivity through Free Energy Analysis. <i>Journal of the American Chemical Society</i> , 2011, 133, 14270-14279.	13.7	58
61	The ABCs of molecular dynamics simulations on B-DNA, circa 2012. <i>Journal of Biosciences</i> , 2012, 37, 379-397.	1.1	55
62	Ethidium bromide interactions with DNA: an exploration of a classic DNA-ligand complex with unbiased molecular dynamics simulations. <i>Nucleic Acids Research</i> , 2021, 49, 3735-3747.	14.5	55
63	Defining a conformational ensemble that directs activation of PPAR $\hat{3}$. <i>Nature Communications</i> , 2018, 9, 1794.	12.8	53
64	Geometrical and Electronic Structure Variability of the Sugar-phosphate Backbone in Nucleic Acids. <i>Journal of Physical Chemistry B</i> , 2008, 112, 8188-8197.	2.6	52
65	Inhibitor-induced structural change in the HCV IRES domain IIa RNA. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 7263-7268.	7.1	52
66	Divalent Ion Dependent Conformational Changes in an RNA Stem-Loop Observed by Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3382-3389.	5.3	48
67	Molecular basis for the broad substrate selectivity of a peptide prenyltransferase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 14037-14042.	7.1	45
68	Proton Transfer Studied Using a Combined Ab Initio Reactive Potential Energy Surface with Quantum Path Integral Methodology. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2566-2580.	5.3	44
69	DNA Deformability at the Base Pair Level. <i>Journal of the American Chemical Society</i> , 2004, 126, 4124-4125.	13.7	41
70	Structure-Activity Relationship of Capsaicin Analogs and Transient Receptor Potential Vanilloid 1-Mediated Human Lung Epithelial Cell Toxicity. <i>Journal of Pharmacology and Experimental Therapeutics</i> , 2011, 337, 400-410.	2.5	40
71	Efficient treatment of induced dipoles. <i>Journal of Chemical Physics</i> , 2015, 143, 074115.	3.0	38
72	Transitions of Double-Stranded DNA Between the A- and B-Forms. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8449-8456.	2.6	38

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73	Araiosamines A ^D : Tris-bromoindole Cyclic Guanidine Alkaloids from the Marine Sponge <i>Clathria (Thalysias) araiosa</i> . <i>Journal of Organic Chemistry</i> , 2011, 76, 5515-5523.	3.2	36
74	Application of Thiol ^{ene} /Thiol ^{ene} Reactions for Peptide and Protein Macrocyclizations. <i>Chemistry - A European Journal</i> , 2017, 23, 7087-7092.	3.3	36
75	Restrained molecular dynamics of solvated duplex DNA using the particle mesh Ewald method. <i>Journal of Biomolecular NMR</i> , 1999, 13, 119-131.	2.8	33
76	Oxazinin A, a Pseudodimeric Natural Product of Mixed Biosynthetic Origin from a Filamentous Fungus. <i>Organic Letters</i> , 2014, 16, 4774-4777.	4.6	32
77	Influence of BII Backbone Substates on DNA Twist: A Unified View and Comparison of Simulation and Experiment for All 136 Distinct Tetranucleotide Sequences. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 275-287.	5.4	31
78	Totopotensamides, Polyketide ^{Cyclic Peptide Hybrids} from a Mollusk-Associated Bacterium <i>Streptomyces</i> sp.. <i>Journal of Natural Products</i> , 2012, 75, 644-649.	3.0	30
79	Molecular dynamics simulations and coupled nucleotide substitution experiments indicate the nature of A ^A base pairing and a putative structure of the coralyne-induced homo-adenine duplex. <i>Nucleic Acids Research</i> , 2009, 37, 7715-7727.	14.5	28
80	Disruption of Bcr-Abl Coiled Coil Oligomerization by Design. <i>Journal of Biological Chemistry</i> , 2011, 286, 27751-27760.	3.4	28
81	Dissociative reactions of benzonorbadienes with tetrazines: scope of leaving groups and mechanistic insights. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 9855-9865.	2.8	28
82	Peptoid Residues Make Diverse, Hyperstable Collagen Triple-Helices. <i>Journal of the American Chemical Society</i> , 2021, 143, 10910-10919.	13.7	28
83	Molecular dynamics re-refinement of two different small RNA loop structures using the original NMR data suggest a common structure. <i>Journal of Biomolecular NMR</i> , 2012, 53, 321-339.	2.8	26
84	Conformational dynamics of CYP3A4 demonstrate the important role of Arg212 coupled with the opening of ingress, egress and solvent channels to dehydrogenation of 4-hydroxy-tamoxifen. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2012, 1820, 1605-1617.	2.4	24
85	Molecular dynamics guided study of salt bridge length dependence in both fluorinated and non ^{fluorinated} parallel dimeric coiled ^{coils} . <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 74, 612-629.	2.6	23
86	Improved Cytochrome P450 3A4 Molecular Models Accurately Predict the Phe215 Requirement for Raloxifene Dehydrogenation Selectivity. <i>Biochemistry</i> , 2010, 49, 9011-9019.	2.5	23
87	Improved Coiled-Coil Design Enhances Interaction with Bcr-Abl and Induces Apoptosis. <i>Molecular Pharmaceutics</i> , 2012, 9, 187-195.	4.6	23
88	Stem-Loop V of Varkud Satellite RNA Exhibits Characteristics of the Mg ²⁺ Bound Structure in the Presence of Monovalent Ions. <i>Journal of Physical Chemistry B</i> , 2015, 119, 12355-12364.	2.6	22
89	Consensus Conformations of Dinucleoside Monophosphates Described with Well-Converged Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1456-1470.	5.3	21
90	Computational Science and Engineering Online (CSE-Online): A Cyber-Infrastructure for Scientific Computing. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 971-984.	5.4	20

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91	iBIOMES: Managing and Sharing Biomolecular Simulation Data in a Distributed Environment. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 726-736.	5.4	18
92	DNA Binding Dynamics and Energetics of Cobalt, Nickel, and Copper Metallopeptides. <i>ChemMedChem</i> , 2014, 9, 1252-1259.	3.2	17
93	Using Wavelet Analysis To Assist in Identification of Significant Events in Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1282-1291.	5.4	17
94	Explicitly Solvated Ligand Contribution to Continuum Solvation Models for Binding Free Energies: Selectivity of Theophylline Binding to an RNA Aptamer. <i>Journal of Physical Chemistry B</i> , 2010, 114, 2227-2237.	2.6	15
95	Computational Assessment of Potassium and Magnesium Ion Binding to a Buried Pocket in GTPase-Associating Center RNA. <i>Journal of Physical Chemistry B</i> , 2017, 121, 451-462.	2.6	15
96	Computational DNA binding studies of (â€“) -epigallocatechin-3-gallate. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018, 36, 3311-3323.	3.5	15
97	DNA Backbone BI/BII Distribution and Dynamics in E2 Protein-Bound Environment Determined by Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2015, 119, 14111-14119.	2.6	13
98	Mg ²⁺ Binding Promotes SLV as a Scaffold in Varkud Satellite Ribozyme SLI-SLV Kissing Loop Junction. <i>Biophysical Journal</i> , 2017, 113, 313-320.	0.5	13
99	Structural and Energetic Analysis of 2-Aminobenzimidazole Inhibitors in Complex with the Hepatitis C Virus IRES RNA Using Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1758-1772.	5.4	12
100	Lessons learned in atomistic simulation of double-stranded DNA: Solvation and salt concerns [Article v1.0]. <i>Living Journal of Computational Molecular Science</i> , 2019, 1, .	6.4	12
101	Computational Modeling of Stapled Peptides toward a Treatment Strategy for CML and Broader Implications in the Design of Lengthy Peptide Therapeutics. <i>Journal of Physical Chemistry B</i> , 2018, 122, 3864-3875.	2.6	11
102	Molecular Modeling of Nucleic Acid Structure. <i>Current Protocols in Nucleic Acid Chemistry</i> , 2013, 54, 7.5.1-7.5.13.	0.5	10
103	iBIOMES Lite: Summarizing Biomolecular Simulation Data in Limited Settings. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1810-1819.	5.4	8
104	Investigating the ion dependence of the first unfolding step of GTPase-Associating Center ribosomal RNA. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018, 36, 243-253.	3.5	8
105	Advancing the Workforce That Supports Computationally and Data Intensive Research. <i>Computing in Science and Engineering</i> , 2021, 23, 19-27.	1.2	8
106	Re-Engineered p53 Chimera with Enhanced Homo-Oligomerization That Maintains Tumor Suppressor Activity. <i>Molecular Pharmaceutics</i> , 2014, 11, 2442-2452.	4.6	7
107	Molecular Modeling of Nucleic Acid Structure: Setup and Analysis. <i>Current Protocols in Nucleic Acid Chemistry</i> , 2001, 6, Unit 7.10.	0.5	6
108	Ancillary Ligand in Ternary Cull Complexes Guides Binding Selectivity toward Minor-Groove DNA. <i>Journal of Physical Chemistry B</i> , 2020, 124, 11648-11658.	2.6	6

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109	Molecular Modeling of Nucleic Acid Structure: Electrostatics and Solvation. Current Protocols in Nucleic Acid Chemistry, 2013, 55, 7.9.1-27.	0.5	5
110	Probing the influence of hypermodified residues within the tRNA ³ Lys anticodon stem loop interacting with the A-loop primer sequence from HIV-1. Biochimica Et Biophysica Acta - General Subjects, 2016, 1860, 607-617.	2.4	5
111	Exploring potentially alternative non-canonical DNA duplex structures through simulation. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2201-2210.	3.5	5
112	Molecular dynamics simulation of nucleic acids: Successes, limitations, and promise* We would like to dedicate this article to Peter Kollman, a friend, collaborator, mentor, and all around good guy. Peter was very enthusiastic about DNA simulation; he will be sorely missed.. Biopolymers, 2000, 56, 232.	2.4	5
113	Backbone Hydrocarbon-Constrained Nucleic Acids Modulate Hybridization Kinetics for RNA. Journal of the American Chemical Society, 2022, 144, 1941-1950.	13.7	5
114	Evaluating the accuracy of the AMBER protein force fields in modeling dihydrofolate reductase structures: imbalance in the conformational arrangements of the flexible loop domains. Journal of Biomolecular Structure and Dynamics, 2023, 41, 5946-5960.	3.5	5
115	Molecular Modeling of Nucleic Acid Structure: Setup and Analysis. Current Protocols in Nucleic Acid Chemistry, 2014, 56, 7.10.1-21.	0.5	4
116	The flying ice cube: Velocity rescaling in molecular dynamics leads to violation of energy equipartition. , 1998, 19, 726.		4
117	Molecular Modeling of Nucleic Acid Structure: Electrostatics and Solvation. Current Protocols in Nucleic Acid Chemistry, 2001, 5, Unit 7.9.	0.5	3
118	Differential electronic states observed during Aâ€“B DNA duplex conformational transitions. Soft Matter, 2009, 5, 685-690.	2.7	3
119	Molecular dynamics simulation of nucleic acids: Successes, limitations, and promise* . , 2000, 56, 232.		3
120	Riboflavin Stabilizes Abasic, Oxidized G-Quadruplex Structures. Biochemistry, 2022, 61, 265-275.	2.5	3
121	Molecular Modeling of Nucleic Acid Structure: Energy and Sampling. Current Protocols in Nucleic Acid Chemistry, 2013, 54, 7.8.1-7.8.21.	0.5	2
122	A Research Computing and Data Capabilities Model for Strategic Decision-Making. , 2020, , .		2
123	Transient Hoogsteen Base Pairs Observed in Unbiased Molecular Dynamics Simulations of DNA. Journal of Physical Chemistry Letters, 2022, 13, 6283-6287.	4.6	2
124	The flying ice cube: Velocity rescaling in molecular dynamics leads to violation of energy equipartition. , 1998, 19, 726.		1
125	A combined theoretical and experimental study of dehydrogenation selectivity by hepatic P450 enzymes during tamoxifen metabolism. FASEB Journal, 2008, 22, 919.1.	0.5	0
126	Probing the influence of ligand binding on cytochrome P450 enzyme remodeling and dynamics: Using molecular dynamics simulation to give insight into multiple cytochrome 2B4 structures. FASEB Journal, 2008, 22, 633.7.	0.5	0

#	ARTICLE	IF	CITATIONS
127	Building the Research Innovation Workforce: Challenges and Recommendations from a Virtual Workshop to Advance the Research Computing Community. , 2022, , .		0