Thomas E Cheatham

List of Publications by Year
in descending order

127	38,258	24978 57	17055 122
papers	citations	h-index	g-index

131	131	131	29024
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Evaluating the accuracy of the AMBER protein force fields in modeling dihydrofolate reductase structures: misbalance in the conformational arrangements of the flexible loop domains. Journal of Biomolecular Structure and Dynamics, 2023, 41, 5946-5960.	2.0	5
2	Backbone Hydrocarbon-Constrained Nucleic Acids Modulate Hybridization Kinetics for RNA. Journal of the American Chemical Society, 2022, 144, 1941-1950.	6.6	5
3	Riboflavin Stabilizes Abasic, Oxidized G-Quadruplex Structures. Biochemistry, 2022, 61, 265-275.	1.2	3
4	Transient Hoogsteen Base Pairs Observed in Unbiased Molecular Dynamics Simulations of DNA. Journal of Physical Chemistry Letters, 2022, 13, 6283-6287.	2.1	2
5	Building the Research Innovation Workforce: Challenges and Recommendations from a Virtual Workshop to Advance the Research Computing Communityâœ±. , 2022, , .		0
6	Ethidium bromide interactions with DNA: an exploration of a classic DNAâ€“ligand complex with unbiased molecular dynamics simulations. Nucleic Acids Research, 2021, 49, 3735-3747.	6.5	55
7	Peptoid Residues Make Diverse, Hyperstable Collagen Triple-Helices. Journal of the American Chemical Society, 2021, 143, 10910-10919.	6.6	28
8	Advancing the Workforce That Supports Computationally and Data Intensive Research. Computing in Science and Engineering, 2021, 23, 19-27.	1.2	8
9	A Research Computing and Data Capabilities Model for Strategic Decision-Making. , 2020, , .		2
10	Ancillary Ligand in Ternary CuII Complexes Guides Binding Selectivity toward Minor-Groove DNA. Journal of Physical Chemistry B, 2020, 124, 11648-11658.	1.2	6
11	Exploring potentially alternative non-canonical DNA duplex structures through simulation. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2201-2210.	2.0	5
12	Lessons learned in atomistic simulation of double-stranded DNA: Solvation and salt concerns [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 1, .	2.2	12
13	Computational Modeling of Stapled Peptides toward a Treatment Strategy for CML and Broader Implications in the Design of Lengthy Peptide Therapeutics. Journal of Physical Chemistry B, 2018, 122, 3864-3875.	1.2	11
14	Consensus Conformations of Dinucleoside Monophosphates Described with Well-Converged Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2018, 14, 1456-1470.	2.3	21
15	Defining a conformational ensemble that directs activation of PPARÎ³. Nature Communications, 2018, 9, 1794.	5.8	53
16	Investigating the ion dependence of the first unfolding step of GTPase-Associating Center ribosomal RNA. Journal of Biomolecular Structure and Dynamics, 2018, 36, 243-253.	2.0	8
17	Computational DNA binding studies of (â€“)-epigallocatechin-3-gallate. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3311-3323.	2.0	15
18	Parallelization of CPPTRAJ enables large scale analysis of molecular dynamics trajectory data. Journal of Computational Chemistry, 2018, 39, 2110-2117.	1.5	97

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19	Influence of BII Backbone Substates on DNA Twist: A Unified View and Comparison of Simulation and Experiment for All 136 Distinct Tetranucleotide Sequences. Journal of Chemical Information and Modeling, 2017, 57, 275-287.	2.5	31
20	Application of Thiolâ€“yne/Thiolâ€“ene Reactions for Peptide and Protein Macrocyclizations. Chemistry - A European Journal, 2017, 23, 7087-7092.	1.7	36
21	Computational Assessment of Potassium and Magnesium Ion Binding to a Buried Pocket in GTPase-Associating Center RNA. Journal of Physical Chemistry B, 2017, 121, 451-462.	1.2	15
22	Mg2+ Binding Promotes SLV as a Scaffold in Varkud Satellite Ribozyme SLI-SLV Kissing Loop Junction. Biophysical Journal, 2017, 113, 313-320.	0.2	13
23	Dissociative reactions of benzonorbornadienes with tetrazines: scope of leaving groups and mechanistic insights. Organic and Biomolecular Chemistry, 2017, 15, 9855-9865.	1.5	28
24	Transitions of Double-Stranded DNA Between the A- and B-Forms. Journal of Physical Chemistry B, 2016, 120, 8449-8456.	1.2	38
25	Molecular basis for the broad substrate selectivity of a peptide prenyltransferase. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 14037-14042.	3.3	45
26	Divalent Ion Dependent Conformational Changes in an RNA Stem-Loop Observed by Molecular Dynamics. Journal of Chemical Theory and Computation, 2016, 12, 3382-3389.	2.3	48
27	Assessing the Current State of Amber Force Field Modifications for DNA. Journal of Chemical Theory and Computation, 2016, 12, 4114-4127.	2.3	351
28	Using Wavelet Analysis To Assist in Identification of Significant Events in Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2016, 56, 1282-1291.	2.5	17
29	Probing the influence of hypermodified residues within the tRNA3Lys anticodon stem loop interacting with the A-loop primer sequence from HIV-1. Biochimica Et Biophysica Acta - General Subjects, 2016, 1860, 607-617.	1.1	5
30	Efficient treatment of induced dipoles. Journal of Chemical Physics, 2015, 143, 074115.	1.2	38
31	Convergence and reproducibility in molecular dynamics simulations of the DNA duplex d(GCACGAACGAACGAACGC). Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 1041-1058.	1.1	136
32	Intercalation processes of copper complexes in DNA. Nucleic Acids Research, 2015, 43, 5364-5376.	6.5	137
33	Highly sampled tetranucleotide and tetraloop motifs enable evaluation of common RNA force fields. Rna, 2015, 21, 1578-1590.	1.6	123
34	Improved Force Field Parameters Lead to a Better Description of RNA Structure. Journal of Chemical Theory and Computation, 2015, 11, 3969-3972.	2.3	126
35	Stem-Loop V of Varkud Satellite RNA Exhibits Characteristics of the Mg²⁺ Bound Structure in the Presence of Monovalent Ions. Journal of Physical Chemistry B, 2015, 119, 12355-12364.	1.2	22
36	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

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37	DNA Backbone BI/BII Distribution and Dynamics in E2 Protein-Bound Environment Determined by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2015, 119, 14111-14119.	1.2	13
38	Î¼ABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. Nucleic Acids Research, 2014, 42, 12272-12283.	6.5	186
39	Triplex intermediates in folding of human telomeric quadruplexes probed by microsecond-scale molecular dynamics simulations. Biochimie, 2014, 105, 22-35.	1.3	72
40	On the absence of intrahelical DNA dynamics on the Î¼s to ms timescale. Nature Communications, 2014, 5, 5152.	5.8	70
41	DNA Binding Dynamics and Energetics of Cobalt, Nickel, and Copper Metallopeptides. ChemMedChem, 2014, 9, 1252-1259.	1.6	17
42	Molecular Modeling of Nucleic Acid Structure: Setup and Analysis. Current Protocols in Nucleic Acid Chemistry, 2014, 56, 7.10.1-21.	0.5	4
43	Re-Engineered p53 Chimera with Enhanced Homo-Oligomerization That Maintains Tumor Suppressor Activity. Molecular Pharmaceutics, 2014, 11, 2442-2452.	2.3	7
44	Oxazinin A, a Pseudodimeric Natural Product of Mixed Biosynthetic Origin from a Filamentous Fungus. Organic Letters, 2014, 16, 4774-4777.	2.4	32
45	Evaluation of Enhanced Sampling Provided by Accelerated Molecular Dynamics with Hamiltonian Replica Exchange Methods. Journal of Physical Chemistry B, 2014, 118, 3543-3552.	1.2	86
46	Multidimensional Replica Exchange Molecular Dynamics Yields a Converged Ensemble of an RNA Tetranucleotide. Journal of Chemical Theory and Computation, 2014, 10, 492-499.	2.3	120
47	Structural and Energetic Analysis of 2-Aminobenzimidazole Inhibitors in Complex with the Hepatitis C Virus IRES RNA Using Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2014, 54, 1758-1772.	2.5	12
48	iBIOMES Lite: Summarizing Biomolecular Simulation Data in Limited Settings. Journal of Chemical Information and Modeling, 2014, 54, 1810-1819.	2.5	8
49	Twentyâ€five years of nucleic acid simulations. Biopolymers, 2013, 99, 969-977.	1.2	157
50	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
51	PTRAJ and CPPTRAJ: Software for Processing and Analysis of Molecular Dynamics Trajectory Data. Journal of Chemical Theory and Computation, 2013, 9, 3084-3095.	2.3	4,960
52	Self-Tensioning Aquatic Caddisfly Silk: Ca²⁺-Dependent Structure, Strength, and Load Cycle Hysteresis. Biomacromolecules, 2013, 14, 3668-3681.	2.6	64
53	iBIOMES: Managing and Sharing Biomolecular Simulation Data in a Distributed Environment. Journal of Chemical Information and Modeling, 2013, 53, 726-736.	2.5	18
54	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

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55	Reliable Oligonucleotide Conformational Ensemble Generation in Explicit Solvent for Force Field Assessment Using Reservoir Replica Exchange Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2013, 117, 4014-4027.	1.2	60
56	Molecular Modeling of Nucleic Acid Structure. Current Protocols in Nucleic Acid Chemistry, 2013, 54, 7.5.1-7.5.13.	0.5	10
57	Molecular Modeling of Nucleic Acid Structure: Electrostatics and Solvation. Current Protocols in Nucleic Acid Chemistry, 2013, 55, 7.9.1-27.	0.5	5
58	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
59	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
60	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
61	Molecular dynamics re-refinement of two different small RNA loop structures using the original NMR data suggest a common structure. Journal of Biomolecular NMR, 2012, 53, 321-339.	1.6	26
62	Molecular dynamics simulations of G-DNA and perspectives on the simulation of nucleic acid structures. Methods, 2012, 57, 25-39.	1.9	111
63	Totopotensamides, Polyketideâ€“Cyclic Peptide Hybrids from a Mollusk-Associated Bacterium Streptomyces sp.. Journal of Natural Products, 2012, 75, 644-649.	1.5	30
64	Improved Coiled-Coil Design Enhances Interaction with Bcr-Abl and Induces Apoptosis. Molecular Pharmaceutics, 2012, 9, 187-195.	2.3	23
65	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. Biochimica Et Biophysica Acta - General Subjects, 2012, 1820, 1605-1617.	1.1	24
66	The ABCs of molecular dynamics simulations on B-DNA, circa 2012. Journal of Biosciences, 2012, 37, 379-397.	0.5	55
67	Quantum mechanically derived AMBERâ€compatible heme parameters for various states of the cytochrome P450 catalytic cycle. Journal of Computational Chemistry, 2012, 33, 119-133.	1.5	210
68	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
69	A Coarse-Grained Model of DNA with Explicit Solvation by Water and Ions. Journal of Physical Chemistry B, 2011, 115, 132-142.	1.2	78
70	Araiosamines Aâ€“D: Tris-bromoindole Cyclic Guanidine Alkaloids from the Marine Sponge Clathria (Thalysias) araiosa. Journal of Organic Chemistry, 2011, 76, 5515-5523.	1.7	36
71	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
72	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

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73	Disruption of Bcr-Abl Coiled Coil Oligomerization by Design. Journal of Biological Chemistry, 2011, 286, 27751-27760.	1.6	28
74	Structure-Activity Relationship of Capsaicin Analogs and Transient Receptor Potential Vanilloid 1-Mediated Human Lung Epithelial Cell Toxicity. Journal of Pharmacology and Experimental Therapeutics, 2011, 337, 400-410.	1.3	40
75	Inhibitor-induced structural change in the HCV IRES domain IIa RNA. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 7263-7268.	3.3	52
76	Improved Cytochrome P450 3A4 Molecular Models Accurately Predict the Phe215 Requirement for Raloxifene Dehydrogenation Selectivity. Biochemistry, 2010, 49, 9011-9019.	1.2	23
77	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
78	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
79	Proton Transfer Studied Using a Combined Ab Initio Reactive Potential Energy Surface with Quantum Path Integral Methodology. Journal of Chemical Theory and Computation, 2010, 6, 2566-2580.	2.3	44
80	Explicitly Solvated Ligand Contribution to Continuum Solvation Models for Binding Free Energies: Selectivity of Theophylline Binding to an RNA Aptamer. Journal of Physical Chemistry B, 2010, 114, 2227-2237.	1.2	15
81	Molecular dynamics simulations and coupled nucleotide substitution experiments indicate the nature of AÂ·A base pairing and a putative structure of the coralyne-induced homo-adenine duplex. Nucleic Acids Research, 2009, 37, 7715-7727.	6.5	28
82	Molecular dynamics guided study of salt bridge length dependence in both fluorinated and nonâ€fluorinated parallel dimeric coiledâ€coils. Proteins: Structure, Function and Bioinformatics, 2009, 74, 612-629.	1.5	23
83	Molecular Dynamics Simulations of the Dynamic and Energetic Properties of Alkali and Halide Ions Using Water-Model-Specific Ion Parameters. Journal of Physical Chemistry B, 2009, 113, 13279-13290.	1.2	476
84	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
85	Differential electronic states observed during Aâ€“B DNA duplex conformational transitions. Soft Matter, 2009, 5, 685-690.	1.2	3
86	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
87	Determination of Alkali and Halide Monovalent Ion Parameters for Use in Explicitly Solvated Biomolecular Simulations. Journal of Physical Chemistry B, 2008, 112, 9020-9041.	1.2	2,756
88	A combined theoretical and experimental study of dehydrogenation selectivity by hepatic P450 enzymes during tamoxifen metabolism. FASEB Journal, 2008, 22, 919.1.	0.2	0
89	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.	0.2	0
90	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

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91	Spontaneous Formation of KCl Aggregates in Biomolecular Simulations: A Force Field Issue?. Journal of Chemical Theory and Computation, 2007, 3, 1851-1859.	2.3	159
92	Antifreeze Proteins at the Ice/Water Interface: Three Calculated Discriminating Properties for Orientation of Type I Proteins. Biophysical Journal, 2007, 93, 1442-1451.	0.2	90
93	Clustering Molecular Dynamics Trajectories: 1. Characterizing the Performance of Different Clustering Algorithms. Journal of Chemical Theory and Computation, 2007, 3, 2312-2334.	2.3	721
94	Computational Science and Engineering Online (CSE-Online):Â A Cyber-Infrastructure for Scientific Computing. Journal of Chemical Information and Modeling, 2006, 46, 971-984.	2.5	20
95	An accurate and simple quantum model for liquid water. Journal of Chemical Physics, 2006, 125, 184507.	1.2	187
96	The Amber biomolecular simulation programs. Journal of Computational Chemistry, 2005, 26, 1668-1688.	1.5	7,742
97	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. Biophysical Journal, 2005, 89, 3721-3740.	0.2	216
98	Simulation and modeling of nucleic acid structure, dynamics and interactions. Current Opinion in Structural Biology, 2004, 14, 360-367.	2.6	212
99	DNA Deformability at the Base Pair Level. Journal of the American Chemical Society, 2004, 126, 4124-4125.	6.6	41
100	Molecular Dynamics Simulations of Guanine Quadruplex Loops: Advances and Force Field Limitations. Biophysical Journal, 2004, 87, 227-242.	0.2	116
101	Molecular Dynamics Simulations of the 136 Unique Tetranucleotide Sequences of DNA Oligonucleotides. I. Research Design and Results on d(CpG) Steps. Biophysical Journal, 2004, 87, 3799-3813.	0.2	245
102	Molecular Dynamics Simulations and Thermodynamics Analysis of DNAâ˜'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
103	Dynamically Amorphous Character of Electronic States in Poly(dA)â˜'Poly(dT) DNA. Journal of Physical Chemistry B, 2003, 107, 2581-2587.	1.2	106
104	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
105	DNA Basepair Step Deformability Inferred from Molecular Dynamics Simulations. Biophysical Journal, 2003, 85, 2872-2883.	0.2	237
106	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
107	Molecular Modeling of Nucleic Acid Structure: Electrostatics and Solvation. Current Protocols in Nucleic Acid Chemistry, 2001, 5, Unit 7.9.	0.5	3
108	Molecular Modeling of Nucleic Acid Structure: Setup and Analysis. Current Protocols in Nucleic Acid Chemistry, 2001, 6, Unit 7.10.	0.5	6

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109	Molecular dynamics simulation of nucleic acids: Successes, limitations, and promise. Biopolymers, 2000, 56, 232-256.	1.2	307
110	Calculating Structures and Free Energies of Complex Molecules:â€‰ Combining Molecular Mechanics and Continuum Models. Accounts of Chemical Research, 2000, 33, 889-897.	7.6	4,098
111	MOLECULARDYNAMICSSIMULATION OFNUCLEICACIDS. Annual Review of Physical Chemistry, 2000, 51, 435-471.	4.8	330
112	Molecular dynamics simulation of nucleic acids: Successes, limitations, and promise*. , 2000, 56, 232.		3
113	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.	1.2	5
114	Restrained molecular dynamics of solvated duplex DNA using the particle mesh Ewald method. Journal of Biomolecular NMR, 1999, 13, 119-131.	1.6	33
115	A Modified Version of the Cornellet al.Force Field with Improved Sugar Pucker Phases and Helical Repeat. Journal of Biomolecular Structure and Dynamics, 1999, 16, 845-862.	2.0	882
116	The flying ice cube: Velocity rescaling in molecular dynamics leads to violation of energy equipartition. Journal of Computational Chemistry, 1998, 19, 726-740.	1.5	347
117	Recent advances in molecular dynamics simulation towards the realistic representation of biomolecules in solution. Theoretical Chemistry Accounts, 1998, 99, 279-288.	0.5	61
118	Molecular Dynamics and Continuum Solvent Studies of the Stability of PolyG-PolyC and PolyA-PolyT DNA Duplexes in Solution. Journal of Biomolecular Structure and Dynamics, 1998, 16, 265-280.	2.0	183
119	Continuum Solvent Studies of the Stability of DNA, RNA, and Phosphoramidateâ^'DNA Helices. Journal of the American Chemical Society, 1998, 120, 9401-9409.	6.6	1,442
120	Removal of pressure and free energy artifacts in charged periodic systems via net charge corrections to the Ewald potential. Journal of Chemical Physics, 1998, 108, 7070-7084.	1.2	162
121	The flying ice cube: Velocity rescaling in molecular dynamics leads to violation of energy equipartition. , 1998, 19, 726.		1
122	The flying ice cube: Velocity rescaling in molecular dynamics leads to violation of energy equipartition. , 1998, 19, 726.		4
123	Unrestrained Molecular Dynamics of Photodamaged DNA in Aqueous Solution. Journal of the American Chemical Society, 1997, 119, 7095-7104.	6.6	62
124	Molecular Dynamics Simulations Highlight the Structural Differences among DNA:DNA, RNA:RNA, and DNA:RNA Hybrid Duplexes. Journal of the American Chemical Society, 1997, 119, 4805-4825.	6.6	257
125	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[ACCCGCGGGT]2 in the presence of hexaamminecobalt(III). Structure, 1997, 5, 1297-1311.	1.6	104
126	Adventures in Improving the Scaling and Accuracy of a Parallel Molecular Dynamics Program. Journal of Supercomputing, 1997, 11, 255-278.	2.4	99

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127	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. Computer Physics Communications, 1995, 91, 1-41.	3.0	2,839