Tamar Schlick

List of Publications by Year
in descending order

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255 papers	12,237 citations	22153 59 h-index	38395 95 g-index
320 all docs	320 docs citations	320 times ranked	8853 citing authors

#	Article	IF	Citations
1	Cohesin Loss Eliminates All Loop Domains. Cell, 2017, 171, 305-320.e24.	28.9	1,454
2	Molecular Modeling and Simulation. Interdisciplinary Applied Mathematics, 2002, , .	0.3	416
3	Molecular Modeling and Simulation: An Interdisciplinary Guide. Interdisciplinary Applied Mathematics, 2010, , .	0.3	297
4	Evidence for heteromorphic chromatin fibers from analysis of nucleosome interactions. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 13317-13322.	7.1	240
5	Optimized particle-mesh Ewald/multiple-time step integration for molecular dynamics simulations. Journal of Chemical Physics, 2001, 115, 4003-4018.	3.0	194
6	Algorithmic Challenges in Computational Molecular Biophysics. Journal of Computational Physics, 1999, 151, 9-48.	3.8	176
7	Role of histone tails in chromatin folding revealed by a mesoscopic oligonucleosome model. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 16236-16241.	7.1	167
8	Histone H1 loss drives lymphoma by disrupting 3D chromatin architecture. Nature, 2021, 589, 299-305.	27.8	155
9	Modeling superhelical DNA: recent analytical and dynamic approaches. Current Opinion in Structural Biology, 1995, 5, 245-262.	5.7	146
10	Orchestration of cooperative events in DNA synthesis and repair mechanism unraveled by transition path sampling of DNA polymerase Â's closing. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 5970-5975.	7.1	146
11	A Tale of Tails: How Histone Tails Mediate Chromatin Compaction in Different Salt and Linker Histone Environments. Journal of Physical Chemistry A, 2009, 113, 4045-4059.	2.5	144
12	Supercoiled DNA energetics and dynamics by computer simulation. Journal of Molecular Biology, 1992, 223, 1089-1119.	4.2	141
13	Exploring the repertoire of RNA secondary motifs using graph theory; implications for RNA design. Nucleic Acids Research, 2003, 31, 2926-2943.	14.5	139
14	Computational approaches to RNA structure prediction, analysis, and design. Current Opinion in Structural Biology, 2011, 21, 306-318.	5.7	139
15	Biomolecular modeling and simulation: a field coming of age. Quarterly Reviews of Biophysics, 2011, 44, 191-228.	5.7	136
16	Chromatin Unfolding by Epigenetic Modifications Explained by Dramatic Impairment of Internucleosome Interactions: A Multiscale Computational Study. Journal of the American Chemical Society, 2015, 137, 10205-10215.	13.7	135
17	Uncovering the polymerase-induced cytotoxicity of an oxidized nucleotide. Nature, 2015, 517, 635-639.	27.8	133
18	Chromatin fiber polymorphism triggered by variations of DNA linker lengths. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 8061-8066.	7.1	131

#	Article	IF	Citations
19	A-tract bending: insights into experimental structures by computational models 1 1Edited by Dr I. Tinoco. Journal of Molecular Biology, 2000, 301, 643-663.	4.2	127
20	Critical Role of Magnesium Ions in DNA Polymerase Î²'s Closing and Active Site Assembly. Journal of the American Chemical Society, 2004, 126, 8441-8453.	13.7	127
21	The influence of salt on the structure and energetics of supercoiled DNA. Biophysical Journal, 1994, 67, 2146-2166.	0.5	124
22	A Combined Wormlike-Chain and Bead Model for Dynamic Simulations of Long Linear DNA. Journal of Computational Physics, 1997, 136, 168-179.	3.8	123
23	BIOMOLECULAR DYNAMICS AT LONG TIMESTEPS:Bridging the Timescale Gap Between Simulation and Experimentation. Annual Review of Biophysics and Biomolecular Structure, 1997, 26, 181-222.	18.3	117
24	Hierarchical looping of zigzag nucleosome chains in metaphase chromosomes. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 1238-1243.	7.1	115
25	Numerical Experience with Limited-Memory Quasi-Newton and Truncated Newton Methods. SIAM Journal on Optimization, 1993, 3, 582-608.	2.0	112
26	Electrostatic mechanism of nucleosomal array folding revealed by computer simulation. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 8180-8185.	7.1	104
27	Flexible Histone Tails in a New Mesoscopic Oligonucleosome Model. Biophysical Journal, 2006, 91, 133-150.	0.5	104
28	Trefoil Knotting Revealed by Molecular Dynamics Simulations of Supercoiled DNA. Science, 1992, 257, 1110-1115.	12.6	103
29	TNPACKâ€"A truncated Newton minimization package for large-scale problems. ACM Transactions on Mathematical Software, 1992, 18, 46-70.	2.9	103
30	Computational approaches to 3D modeling of RNA. Journal of Physics Condensed Matter, 2010, 22, 283101.	1.8	98
31	Modeling Studies of Chromatin Fiber Structure as a Function of DNA Linker Length. Journal of Molecular Biology, 2010, 403, 777-802.	4.2	98
32	Dynamics of site juxtaposition in supercoiled DNA. Proceedings of the National Academy of Sciences of the United States of America, 2001, 98, 968-973.	7.1	97
33	Computational Modeling Predicts the Structure and Dynamics of Chromatin Fiber. Structure, 2001, 9, 105-114.	3.3	96
34	Internal motion of supercoiled DNA: brownian dynamics simulations of site juxtaposition 1 1Edited by I. Tinoco. Journal of Molecular Biology, 1998, 284, 287-296.	4.2	95
35	A Family of Symplectic Integrators: Stability, Accuracy, and Molecular Dynamics Applications. SIAM Journal of Scientific Computing, 1997, 18, 203-222.	2.8	94
36	Analysis of Four-Way Junctions in RNA Structures. Journal of Molecular Biology, 2009, 390, 547-559.	4.2	94

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37	Overcoming stability limitations in biomolecular dynamics. I. Combining force splitting via extrapolation with Langevin dynamics in LN. Journal of Chemical Physics, 1998, 109, 1617-1632.	3.0	93
38	A powerful truncated Newton method for potential energy minimization. Journal of Computational Chemistry, 1987, 8, 1025-1039.	3.3	90
39	Modeling saltâ€mediated electrostatics of macromolecules: The discrete surface charge optimization algorithm and its application to the nucleosome. Biopolymers, 2001, 58, 106-115.	2.4	90
40	Polymerase Î² simulations suggest that Arg258 rotation is a slow step rather than large subdomain motions per se 1 1Edited by B. Honig. Journal of Molecular Biology, 2002, 317, 651-671.	4.2	87
41	Toward Convergence of Experimental Studies and Theoretical Modeling of the Chromatin Fiber. Journal of Biological Chemistry, 2012, 287, 5183-5191.	3.4	87
42	Nonlinear Resonance Artifacts in Molecular Dynamics Simulations. Journal of Computational Physics, 1998, 140, 1-29.	3.8	86
43	The Loop Opening/Closing Motion of the Enzyme Triosephosphate Isomerase. Biophysical Journal, 1998, 74, 72-81.	0.5	79
44	Scaling molecular dynamics beyond 100,000 processor cores for largeâ€scale biophysical simulations. Journal of Computational Chemistry, 2019, 40, 1919-1930.	3.3	79
45	Engineering Teams Up with Computer-Simulation and Visualization Tools to Probe Biomolecular Mechanisms. Biophysical Journal, 2003, 85, 1-4.	0.5	77
46	In vitro RNA random pools are not structurally diverse: A computational analysis. Rna, 2005, 11, 853-863.	3.5	76
47	RAG: RNA-As-Graphs database--concepts, analysis, and features. Bioinformatics, 2004, 20, 1285-1291.	4.1	74
48	A Hoogsteen base pair embedded in undistorted B-DNA. Nucleic Acids Research, 2002, 30, 5244-5252.	14.5	71
49	Analysis of Protein Sequence/Structure Similarity Relationships. Biophysical Journal, 2002, 83, 2781-2791.	0.5	70
50	Fidelity Discrimination in DNA Polymerase Î²:Â Differing Closing Profiles for a Mismatched (G:A) versus Matched (G:C) Base Pair. Journal of the American Chemical Society, 2005, 127, 13245-13252.	13.7	69
51	Translational and vibrational energy dependence of the cross section for H + C2H4 .fwdarw. C2H5*. The Journal of Physical Chemistry, 1981, 85, 958-968.	2.9	68
52	The chromatin fiber: multiscale problems and approaches. Current Opinion in Structural Biology, 2015, 31, 124-139.	5.7	68
53	Regulation of DNA Repair Fidelity by Molecular Checkpoints:Â â€œGatesâ€• in DNA Polymerase Î²'s Substrate Selectionâ€. Biochemistry, 2006, 45, 15142-15156.	2.5	66
54	LIN: A new algorithm to simulate the dynamics of biomolecules by combining implicit-integration and normal mode techniques. Journal of Computational Chemistry, 1993, 14, 1212-1233.	3.3	65

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55	Extrapolation versus impulse in multiple-timestepping schemes. II. Linear analysis and applications to Newtonian and Langevin dynamics. Journal of Chemical Physics, 1998, 109, 1633-1642.	3.0	65
56	DNA Polymerase Î² Catalysis:Â Are Different Mechanisms Possible?. Journal of the American Chemical Society, 2007, 129, 11100-11110.	13.7	65
57	Resonance in the dynamics of chemical systems simulated by the implicit midpoint scheme. Chemical Physics Letters, 1995, 237, 525-535.	2.6	63
58	Annotation of tertiary interactions in RNA structures reveals variations and correlations. Rna, 2008, 14, 2465-2477.	3.5	63
59	Molecular dynamics by the Backward-Euler method. Communications on Pure and Applied Mathematics, 1989, 42, 1001-1031.	3.1	62
60	Biomolecular free energy profiles by a shooting/umbrella sampling protocol, â€œBOLASâ€• Journal of Chemical Physics, 2004, 121, 2436-2444.	3.0	62
61	Biomolecular modeling thrives in the age of technology. Nature Computational Science, 2021, 1, 321-331.	8.0	61
62	Graph-based sampling for approximating global helical topologies of RNA. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 4079-4084.	7.1	58
63	Mismatch-Induced Conformational Distortions in Polymerase Î² Support an Induced-Fit Mechanism for Fidelityâ€. Biochemistry, 2005, 44, 13328-13341.	2.5	57
64	RAG: RNA-As-Graphs web resource. BMC Bioinformatics, 2004, 5, 88.	2.6	56
65	Dynamic condensation of linker histone C-terminal domain regulates chromatin structure. Nucleic Acids Research, 2014, 42, 7553-7560.	14.5	56
66	Mesoscale modeling reveals formation of an epigenetically driven HOXC gene hub. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 4955-4962.	7.1	56
67	Local Deformations Revealed by Dynamics Simulations of DNA Polymerase Î² with DNA Mismatches at the Primer Terminus. Journal of Molecular Biology, 2002, 321, 459-478.	4.2	54
68	Constructing irregular surfaces to enclose macromolecular complexes for mesoscale modeling using the discrete surface charge optimization (DISCO) algorithm. Journal of Computational Chemistry, 2003, 24, 2063-2074.	3.3	54
69	A truncated Newton minimizer adapted for CHARMM and biomolecular applications. Journal of Computational Chemistry, 1994, 15, 532-552.	3.3	52
70	In Silico Evidence for DNA Polymerase-Î²â€™s Substrate-Induced Conformational Change. Biophysical Journal, 2004, 87, 3088-3099.	0.5	52
71	Correct and incorrect nucleotide incorporation pathways in DNA polymerase Î². Biochemical and Biophysical Research Communications, 2006, 350, 521-529.	2.1	52
72	Molecular dynamics-based approaches for enhanced sampling of long-time, large-scale conformational changes in biomolecules. F1000 Biology Reports, 2009, 1, 51.	4.0	52

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73	Candidates for Novel RNA Topologies. Journal of Molecular Biology, 2004, 341, 1129-1144.	4.2	51
74	Predicting coaxial helical stacking in RNA junctions. Nucleic Acids Research, 2012, 40, 487-498.	14.5	51
75	Efficient multiple-time-step integrators with distance-based force splitting for particle-mesh-Ewald molecular dynamics simulations. Journal of Chemical Physics, 2002, 116, 5971-5983.	3.0	49
76	The Langevin/implicitâ€Euler/normalâ€mode scheme for molecular dynamics at large time steps. Journal of Chemical Physics, 1994, 101, 4995-5012.	3.0	48
77	Highly Organized but Pliant Active Site of DNA Polymerase Î²: Compensatory Mechanisms in Mutant Enzymes Revealed by Dynamics Simulations and Energy Analyses. Biophysical Journal, 2004, 86, 3392-3408.	0.5	47
78	A computational proposal for designing structured RNA pools for in vitro selection of RNAs. Rna, 2007, 13, 478-492.	3.5	47
79	Mesoscale Modeling and Single-Nucleosome Tracking Reveal Remodeling of Clutch Folding and Dynamics in Stem Cell Differentiation. Cell Reports, 2021, 34, 108614.	6.4	47
80	RAG: An update to the RNA-As-Graphs resource. BMC Bioinformatics, 2011, 12, 219.	2.6	46
81	Linking Chromatin Fibers to Gene Folding by Hierarchical Looping. Biophysical Journal, 2017, 112, 434-445.	0.5	46
82	TNPACKâ€”a truncated Newton minimization package for large-scale problems. ACM Transactions on Mathematical Software, 1992, 18, 71-111.	2.9	45
83	Mesoscale simulations of two nucleosome-repeat length oligonucleosomes. Physical Chemistry Chemical Physics, 2009, 11, 10729.	2.8	45
84	Lattice protein folding with two and four-body statistical potentials. Proteins: Structure, Function and Bioinformatics, 2001, 43, 161-174.	2.6	44
85	Quantum Mechanics/Molecular Mechanics Investigation of the Chemical Reaction in Dpo4 Reveals Water-Dependent Pathways and Requirements for Active Site Reorganization. Journal of the American Chemical Society, 2008, 130, 13240-13250.	13.7	43
86	Sensitive effect of linker histone binding mode and subtype on chromatin condensation. Nucleic Acids Research, 2019, 47, 4948-4957.	14.5	43
87	Structure-altering mutations of the SARS-CoV-2 frameshifting RNA element. Biophysical Journal, 2021, 120, 1040-1053.	0.5	43
88	Tertiary Motifs Revealed in Analyses of Higher-Order RNA Junctions. Journal of Molecular Biology, 2009, 393, 67-82.	4.2	42
89	On higher buckling transitions in supercoiled DNA. Biopolymers, 1994, 34, 565-597.	2.4	40
90	A Quantum Mechanical Investigation of Possible Mechanisms for the Nucleotidyl Transfer Reaction Catalyzed by DNA Polymerase Î². Journal of Physical Chemistry B, 2007, 111, 11244-11252.	2.6	40

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91	Crucial role of dynamic linker histone binding and divalent ions for DNA accessibility and gene regulation revealed by mesoscale modeling of oligonucleosomes. Nucleic Acids Research, 2012, 40, 8803-8817.	14.5	40
92	Mesoscale Modeling Reveals Hierarchical Looping of Chromatin Fibers Near Gene Regulatory Elements. Journal of Physical Chemistry B, 2016, 120, 8642-8653.	2.6	40
93	Masking Resonance Artifacts in Force-Splitting Methods for Biomolecular Simulations by Extrapolative Langevin Dynamics. Journal of Computational Physics, 1999, 151, 74-113.	3.8	39
94	Efficient Implementation of the Truncated-Newton Algorithm for Large-Scale Chemistry Applications. SIAM Journal on Optimization, 1999, 10, 132-154.	2.0	39
95	Dynamic Energy Landscapes of Riboswitches Help Interpret Conformational Rearrangements and Function. PLoS Computational Biology, 2012, 8, e1002368.	3.2	38
96	Inertial stochastic dynamics. I. Long-time-step methods for Langevin dynamics. Journal of Chemical Physics, 2000, 112, 7313-7322.	3.0	36
97	Time-Trimming Tricks for Dynamic Simulations. Structure, 2001, 9, R45-R53.	3.3	36
98	Unbiased Rotational Moves for Rigid-Body Dynamics. Biophysical Journal, 2003, 85, 2973-2976.	0.5	36
99	Substrateâ€induced DNA strand misalignment during catalytic cycling by DNA polymerase Î». EMBO Reports, 2008, 9, 459-464.	4.5	36
100	F-RAG: Generating Atomic Coordinates from RNA Graphs by Fragment Assembly. Journal of Molecular Biology, 2017, 429, 3587-3605.	4.2	36
101	Adventures with RNA graphs. Methods, 2018, 143, 16-33.	3.8	35
102	To Knot or Not to Knot: Multiple Conformations of the SARS-CoV-2 Frameshifting RNA Element. Journal of the American Chemical Society, 2021, 143, 11404-11422.	13.7	35
103	Macroscopic modeling and simulations of supercoiled DNA with bound proteins. Journal of Chemical Physics, 2002, 117, 8573-8586.	3.0	34
104	Computational generation and screening of RNA motifs in large nucleotide sequence pools. Nucleic Acids Research, 2010, 38, e139-e139.	14.5	34
105	Perspective: pre-chemistry conformational changes in DNA polymerase mechanisms. Theoretical Chemistry Accounts, 2012, 131, 1287.	1.4	34
106	Deoxyadenosine sugar puckering pathway simulated by the stochastic difference equation algorithm. Chemical Physics Letters, 2003, 378, 1-8.	2.6	33
107	In Silico Studies of the African Swine Fever Virus DNA Polymerase X Support an Induced-Fit Mechanism. Biophysical Journal, 2006, 90, 42-56.	0.5	32
108	Emergence of chromatin hierarchical loops from protein disorder and nucleosome asymmetry. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 7216-7224.	7.1	32

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109	Can classical equations simulate quantum-mechanical behavior? a molecular dynamics investigation of a diatomic molecule with a morse potential. Communications on Pure and Applied Mathematics, 1989, 42, 1141-1163.	3.1	31
110	Conformational Transition Pathway of Polymerase Î²/DNA upon Binding Correct Incoming Substrate. Journal of Physical Chemistry B, 2005, 109, 5358-5367.	2.6	31
111	Optimization Methods in Computational Chemistry. Reviews in Computational Chemistry, 2007, , 1-71.	1.5	31
112	The Effect of Linker Histone's Nucleosome Binding Affinity on Chromatin Unfolding Mechanisms. Biophysical Journal, 2011, 101, 1670-1680.	0.5	31
113	Predicting Helical Topologies in RNA Junctions as Tree Graphs. PLoS ONE, 2013, 8, e71947.	2.5	31
114	An Efficient Projection Protocol for Chemical Databases:â€‰ Singular Value Decomposition Combined with Truncated-Newton Minimization. Journal of Chemical Information and Computer Sciences, 2000, 40, 167-177.	2.8	30
115	An analysis of the structural and energetic properties of deoxyribose by potential energy methods. Journal of Computational Chemistry, 1987, 8, 1199-1224.	3.3	29
116	A molecular dynamics simulation of a water droplet by the implicitâ€Euler/Langevin scheme. Journal of Chemical Physics, 1991, 94, 2118-2129.	3.0	29
117	Solvent effects on supercoiled DNA dynamics explored by Langevin dynamics simulations. Physical Review E, 1995, 51, 6188-6203.	2.1	29
118	Dynamic simulations of 13 TATA variants refine kinetic hypotheses of sequence/activity relationships 1 1Edited by B. Honig. Journal of Molecular Biology, 2001, 308, 681-703.	4.2	29
119	Correlation among DNA Linker Length, Linker Histone Concentration, and Histone Tails in Chromatin. Biophysical Journal, 2016, 110, 2309-2319.	0.5	29
120	Implicit discretization schemes for Langevin dynamics. Molecular Physics, 1995, 84, 1077-1098.	1.7	28
121	Title is missing!. Journal of Mathematical Imaging and Vision, 2003, 19, 33-48.	1.3	28
122	Inherent speedup limitations in multiple time step/particle mesh Ewald algorithms. Journal of Computational Chemistry, 2003, 24, 77-88.	3.3	28
123	RAG-3D: a search tool for RNA 3D substructures. Nucleic Acids Research, 2015, 43, 9474-9488.	14.5	28
124	Nucleosome Clutches are Regulated by Chromatin Internal Parameters. Journal of Molecular Biology, 2021, 433, 166701.	4.2	28
125	Inertial stochastic dynamics. II. Influence of inertia on slow kinetic processes of supercoiled DNA. Journal of Chemical Physics, 2000, 112, 7323-7338.	3.0	27
126	RAGPOOLS: RNA-As-Graph-Pools a web server for assisting the design of structured RNA pools for in vitro selection. Bioinformatics, 2007, 23, 2959-2960.	4.1	27

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127	Analysis of Riboswitch Structure and Function by an Energy Landscape Framework. Journal of Molecular Biology, 2009, 393, 993-1003.	4.2	27
128	Kilobase Pair Chromatin Fiber Contacts Promoted by Living-System-Like DNA Linker Length Distributions and Nucleosome Depletion. Journal of Physical Chemistry B, 2017, 121, 3882-3894.	2.6	27
129	Biomolecular Modeling and Simulation: A Prospering Multidisciplinary Field. Annual Review of Biophysics, 2021, 50, 267-301.	10.0	27
130	Modular RNA architecture revealed by computational analysis of existing pseudoknots and ribosomal RNAs. Nucleic Acids Research, 2005, 33, 1384-1398.	14.5	26
131	Modified Cholesky Factorizations for Sparse Preconditioners. SIAM Journal of Scientific Computing, 1993, 14, 424-445.	2.8	25
132	The notion of error in Langevin dynamics. I. Linear analysis. Journal of Chemical Physics, 1996, 105, 299-318.	3.0	25
133	Special stability advantages of position-Verlet over velocity-Verlet in multiple-time step integration. Journal of Chemical Physics, 2001, 115, 4019-4029.	3.0	25
134	Candidate RNA structures for domain 3 of the foot-and-mouth-disease virus internal ribosome entry site. Nucleic Acids Research, 2013, 41, 1483-1495.	14.5	25
135	Dependence of the Linker Histone and Chromatin Condensation on the Nucleosome Environment. Journal of Physical Chemistry B, 2017, 121, 7823-7832.	2.6	25
136	A pipeline for computational design of novel RNA-like topologies. Nucleic Acids Research, 2018, 46, 7040-7051.	14.5	25
137	Increasing the time step in molecular dynamics. Chemical Physics Letters, 1992, 198, 538-546.	2.6	24
138	Long timestep dynamics of peptides by the dynamics driver approach. Proteins: Structure, Function and Bioinformatics, 1995, 21, 282-302.	2.6	24
139	Computational Prediction of Riboswitch Tertiary Structures Including Pseudoknots by RAGTOP. Methods in Enzymology, 2015, 553, 115-135.	1.0	24
140	Chromatin Fiber Folding Directed by Cooperative Histone Tail Acetylation and Linker Histone Binding. Biophysical Journal, 2018, 114, 2376-2385.	0.5	24
141	Predicting candidate genomic sequences that correspond to synthetic functional RNA motifs. Nucleic Acids Research, 2005, 33, 6057-6069.	14.5	23
142	Differing Conformational Pathways Before and After Chemistry for Insertion of dATP versus dCTP Opposite 8-OxoG in DNA Polymerase Î². Biophysical Journal, 2007, 92, 3063-3070.	0.5	23
143	Chromatin Ionic Atmosphere Analyzed by a Mesoscale Electrostatic Approach. Biophysical Journal, 2010, 99, 2587-2596.	0.5	23
144	Modeling DNA Polymerase Î¼ Motions: Subtle Transitions before Chemistry. Biophysical Journal, 2010, 99, 3463-3472.	0.5	23

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145	Distinct energetics and closing pathways for DNA polymerase beta with 8-oxoG template and different incoming nucleotides. , 2007, 7, 7.		22
146	Remark on Algorithm 702â€"the updated truncated Newton minimization package. ACM Transactions on Mathematical Software, 1999, 25, 108-122.	2.9	21
147	A new program for optimizing periodic boundary models of solvated biomolecules (PBCAID). Journal of Computational Chemistry, 2001, 22, 1843-1850.	3.3	21
148	A recipe for evaluating and differentiating cos ? expressions. Journal of Computational Chemistry, 1989, 10, 951-956.	3.3	20
149	Modeling biomolecules: larger scales, longer durations. IEEE Computational Science and Engineering, 1994, 1, 19-30.	0.6	20
150	Computational Molecular Biophysics Today: A Confluence of Methodological Advances and Complex Biomolecular Applications. Journal of Computational Physics, 1999, 151, 1-8.	3.8	20
151	Efficient global biopolymer sampling with end-transfer configurational bias Monte Carlo. Journal of Chemical Physics, 2007, 126, 044107.	3.0	20
152	Mismatched Base-Pair Simulations for ASFV Pol X/DNA Complexes Help Interpret Frequent Gâ€¢G Misincorporation. Journal of Molecular Biology, 2008, 384, 1086-1097.	4.2	20
153	Simulations of DNA Pol Î» R517 Mutants Indicate 517's Crucial Role in Ternary Complex Stability and Suggest DNA Slippage Origin. Journal of the American Chemical Society, 2008, 130, 3967-3977.	13.7	20
154	Using sequence signatures and kink-turn motifs in knowledge-based statistical potentials for RNA structure prediction. Nucleic Acids Research, 2017, 45, 5414-5422.	14.5	20
155	Network Theory Tools for RNA Modeling. WSEAS Transactions on Mathematics, 2013, 9, 941-955.	0.5	20
156	New splitting formulations for lattice summations. Journal of Chemical Physics, 2001, 115, 8312-8326.	3.0	19
157	Subtle but variable conformational rearrangements in the replication cycle of Sulfolobus solfataricus P2 DNA polymerase IV (Dpo4) may accommodate lesion bypass. Protein Science, 2006, 15, 135-151.	7.6	19
158	Unfavorable Electrostatic and Steric Interactions in DNA Polymerase Î² E295K Mutant Interfere with the Enzymeâ€™s Pathway. Journal of the American Chemical Society, 2012, 134, 9999-10010.	13.7	19
159	Bridging chromatin structure and function over a range of experimental spatial and temporal scales by molecular modeling. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1434.	14.6	18
160	Pursuing Laplaceâ€™s Vision on Modern Computers. The IMA Volumes in Mathematics and Its Applications, 1996, , 219-247.	0.5	18
161	Local chromatin fiber folding represses transcription and loop extrusion in quiescent cells. ELife, 2021, 10, .	6.0	18
162	Stereochemistry and Position-Dependent Effects of Carcinogens on TATA/TBP Binding. Biophysical Journal, 2006, 90, 1865-1877.	0.5	17

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163	Sequential Side-Chain Residue Motions Transform the Binary into the Ternary State of DNA Polymerase Î». Biophysical Journal, 2006, 91, 3182-3195.	0.5	17
164	Challenges in RNA Structural Modeling and Design. Journal of Molecular Biology, 2016, 428, 733-735.	4.2	17
165	A transitionâ€rate investigation by molecular dynamics with the Langevin/implicitâ€Euler scheme. Journal of Chemical Physics, 1991, 95, 4986-4996.	3.0	16
166	Sequence-dependent solution structure and motions of 13 TATA/TBP (TATA-box binding protein) complexes. Biopolymers, 2003, 69, 216-243.	2.4	16
167	RNA Graph Partitioning for the Discovery of RNA Modularity: A Novel Application of Graph Partition Algorithm to Biology. PLoS ONE, 2014, 9, e106074.	2.5	16
168	A computational screen for C/D box snoRNAs in the human genomic region associated with Prader-Willi and Angelman syndromes. Journal of Biomedical Science, 2008, 15, 697-705.	7.0	15
169	DNA Pol Î»Ë†s Extraordinary Ability To Stabilize Misaligned DNA. Journal of the American Chemical Society, 2010, 132, 13403-13416.	13.7	15
170	Inverse folding with RNA-As-Graphs produces a large pool of candidate sequences with target topologies. Journal of Structural Biology, 2020, 209, 107438.	2.8	15
171	Computational strategies to address chromatin structure problems. Physical Biology, 2016, 13, 035006.	1.8	14
172	Predicting Large RNA-Like Topologies by a Knowledge-Based Clustering Approach. Journal of Molecular Biology, 2016, 428, 811-821.	4.2	14
173	An extended dual graph library and partitioning algorithm applicable to pseudoknotted RNA structures. Methods, 2019, 162-163, 74-84.	3.8	14
174	Generating folded protein structures with a lattice chain growth algorithm. Journal of Chemical Physics, 2000, 113, 5511.	3.0	13
175	Interconversion between Parallel and Antiparallel Conformations of a 4H RNA junction in Domain 3 of Foot-and-Mouth Disease Virus IRES Captured by Dynamics Simulations. Biophysical Journal, 2014, 106, 447-458.	0.5	12
176	Dual Graph Partitioning Highlights a Small Group of Pseudoknot-Containing RNA Submotifs. Genes, 2018, 9, 371.	2.4	12
177	Monte Carlo, harmonic approximation, and coarse-graining approaches for enhanced sampling of biomolecular structure. F1000 Biology Reports, 2009, 1, 48.	4.0	12
178	RAG: RNA-As-Graphs databaseâ€"concepts, analysis, and features. Nutrition and Health, 1987, 5, 1285-1291.	1.5	11
179	Buckling transitions in superhelical DNA: Dependence on the elastic constants and DNA size. , 1997, 41, 5-25.		11
180	Structural motifs in ribosomal RNAs: Implications for RNA design and genomics. Biopolymers, 2004, 73, 340-347.	2.4	11

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181	Optimal and Variant Metal-Ion Routes in DNA Polymerase Î²â€™s Conformational Pathways. Journal of the American Chemical Society, 2014, 136, 3630-3639.	13.7	11
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