Tamar Schlick

List of Publications by Year
in descending order

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255	12,237	25423	43601
papers	citations	59 h-index	95 g-index

320	320	320	10103
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Structure-altering mutations of the SARS-CoV-2 frameshifting RNA element. Biophysical Journal, 2021, 120, 1040-1053.	0.2	43
2	Nucleosome Clutches are Regulated by Chromatin Internal Parameters. Journal of Molecular Biology, 2021, 433, 166701.	2.0	28
3	Histone H1 loss drives lymphoma by disrupting 3D chromatin architecture. Nature, 2021, 589, 299-305.	13.7	155
4	Mesoscale Modeling and Single-Nucleosome Tracking Reveal Remodeling of Clutch Folding and Dynamics in Stem Cell Differentiation. Cell Reports, 2021, 34, 108614.	2.9	47
5	A MULTISCALE VISION-ILLUSTRATIVE APPLICATIONS FROM BIOLOGY TO ENGINEERING. International Journal for Multiscale Computational Engineering, 2021, 19, 39-73.	0.8	10
6	A Fiedler Vector Scoring Approach for Novel RNA Motif Selection. Journal of Physical Chemistry B, 2021, 125, 1144-1155.	1.2	5
7	Biophysicists' outstanding response to Covid-19. Biophysical Journal, 2021, 120, E1-E2.	0.2	2
8	MGO on the go: Multiscale genome symposium - annual biophysical society meeting 2021. Biophysical Reviews, 2021, 13, 309-310.	1.5	2
9	Biomolecular modeling thrives in the age of technology. Nature Computational Science, 2021, 1, 321-331.	3.8	61
10	Biomolecular Modeling and Simulation: A Prospering Multidisciplinary Field. Annual Review of Biophysics, 2021, 50, 267-301.	4.5	27
11	Biophysicistsâ€™ continued outstanding response to COVID-19. Biophysical Journal, 2021, 120, E1.	0.2	2
12	Isabella L. Karle: A Crystallography Pioneer. DNA and Cell Biology, 2021, 40, 843-847.	0.9	0
13	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.	6.6	35
14	Local chromatin fiber folding represses transcription and loop extrusion in quiescent cells. ELife, 2021, 10, .	2.8	18
15	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.	6.2	18
16	RAG-Web: RNA structure prediction/design using RNA-As-Graphs. Bioinformatics, 2020, 36, 647-648.	1.8	7
17	Mesoscale Modeling of Nucleosome-Binding Antibody PL2-6: Mono- versus Bivalent Chromatin Complexes. Biophysical Journal, 2020, 118, 2066-2076.	0.2	3
18	Inverse folding with RNA-As-Graphs produces a large pool of candidate sequences with target topologies. Journal of Structural Biology, 2020, 209, 107438.	1.3	15

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19	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.	3.3	32
20	Cover Image, Volume 10, Issue 2. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1467.	6.2	0
21	Identification of novel RNA design candidates by clustering the extended RNA-As-Graphs library. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129534.	1.1	4
22	Multiscale Genome Organization: Dazzling Subject and Inventive Methods. Biophysical Journal, 2020, 118, E1-E3.	0.2	1
23	ANERGY TO SYNERGY-THE ENERGY FUELING THE RXCOVEA FRAMEWORK. International Journal for Multiscale Computational Engineering, 2020, 18, 329-333.	0.8	1
24	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.	3.3	56
25	Graph-Theoretic Partitioning of RNAs and Classification of Pseudoknots. Lecture Notes in Computer Science, 2019, , 68-79.	1.0	0
26	Scaling molecular dynamics beyond 100,000 processor cores for largeâ€scale biophysical simulations. Journal of Computational Chemistry, 2019, 40, 1919-1930.	1.5	79
27	Sensitive effect of linker histone binding mode and subtype on chromatin condensation. Nucleic Acids Research, 2019, 47, 4948-4957.	6.5	43
28	An extended dual graph library and partitioning algorithm applicable to pseudoknotted RNA structures. Methods, 2019, 162-163, 74-84.	1.9	14
29	Adventures with RNA graphs. Methods, 2018, 143, 16-33.	1.9	35
30	Mesoscale Modeling of Chromatin Fibers. , 2018, , 123-147.		9
31	A pipeline for computational design of novel RNA-like topologies. Nucleic Acids Research, 2018, 46, 7040-7051.	6.5	25
32	Chromatin Fiber Folding Directed by Cooperative Histone Tail Acetylation and Linker Histone Binding. Biophysical Journal, 2018, 114, 2376-2385.	0.2	24
33	Dual Graph Partitioning Highlights a Small Group of Pseudoknot-Containing RNA Submotifs. Genes, 2018, 9, 371.	1.0	12
34	Linking Chromatin Fibers to Gene Folding by Hierarchical Looping. Biophysical Journal, 2017, 112, 434-445.	0.2	46
35	Unraveling Genome Biophysics. Biophysical Journal, 2017, 112, E1-E2.	0.2	1
36	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.	1.2	27

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37	Cohesin Loss Eliminates All Loop Domains. Cell, 2017, 171, 305-320.e24.	13.5	1,454
38	F-RAG: Generating Atomic Coordinates from RNA Graphs by Fragment Assembly. Journal of Molecular Biology, 2017, 429, 3587-3605.	2.0	36
39	Dependence of the Linker Histone and Chromatin Condensation on the Nucleosome Environment. Journal of Physical Chemistry B, 2017, 121, 7823-7832.	1.2	25
40	RNA Structural Variability and Functional Versatility Challenge RNA Structural Modeling and Design. Biophysical Journal, 2017, 113, E1-E2.	0.2	1
41	Using sequence signatures and kink-turn motifs in knowledge-based statistical potentials for RNA structure prediction. Nucleic Acids Research, 2017, 45, 5414-5422.	6.5	20
42	Partitioning and Classification of RNA Secondary Structures into Pseudonotted and Pseudoknot-free Regions Using a Graph-Theoretical Approach. IAENG International Journal of Computer Science, 2017, 44, 241-246.	0.0	3
43	Computational strategies to address chromatin structure problems. Physical Biology, 2016, 13, 035006.	0.8	14
44	Mesoscale Modeling Reveals Hierarchical Looping of Chromatin Fibers Near Gene Regulatory Elements. Journal of Physical Chemistry B, 2016, 120, 8642-8653.	1.2	40
45	Insertion of oxidized nucleotide triggers rapid DNA polymerase opening. Nucleic Acids Research, 2016, 44, 4409-4424.	6.5	8
46	Correlation among DNA Linker Length, Linker Histone Concentration, and Histone Tails in Chromatin. Biophysical Journal, 2016, 110, 2309-2319.	0.2	29
47	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.	3.3	115
48	Challenges in RNA Structural Modeling and Design. Journal of Molecular Biology, 2016, 428, 733-735.	2.0	17
49	Predicting Large RNA-Like Topologies by a Knowledge-Based Clustering Approach. Journal of Molecular Biology, 2016, 428, 811-821.	2.0	14
50	CHSalign: A Web Server That Builds upon Junction-Explorer and RNAJAG for Pairwise Alignment of RNA Secondary Structures with Coaxial Helical Stacking. PLoS ONE, 2016, 11, e0147097.	1.1	9
51	Molecular Dynamics Simulations. , 2015, , 940-951.		1
52	The chromatin fiber: multiscale problems and approaches. Current Opinion in Structural Biology, 2015, 31, 124-139.	2.6	68
53	Forced unraveling of chromatin fibers with nonuniform linker DNA lengths. Journal of Physics Condensed Matter, 2015, 27, 064113.	0.7	9
54	Computational Prediction of Riboswitch Tertiary Structures Including Pseudoknots by RAGTOP. Methods in Enzymology, 2015, 553, 115-135.	0.4	24

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55	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.	6.6	135
56	RAG-3D: a search tool for RNA 3D substructures. Nucleic Acids Research, 2015, 43, 9474-9488.	6.5	28
57	Uncovering the polymerase-induced cytotoxicity of an oxidized nucleotide. Nature, 2015, 517, 635-639.	13.7	133
58	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.	3.3	131
59	Dynamic condensation of linker histone C-terminal domain regulates chromatin structure. Nucleic Acids Research, 2014, 42, 7553-7560.	6.5	56
60	Optimal and Variant Metal-Ion Routes in DNA Polymerase Î²â€™s Conformational Pathways. Journal of the American Chemical Society, 2014, 136, 3630-3639.	6.6	11
61	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.	3.3	58
62	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.	0.2	12
63	RNA Graph Partitioning for the Discovery of RNA Modularity: A Novel Application of Graph Partition Algorithm to Biology. PLoS ONE, 2014, 9, e106074.	1.1	16
64	How DNA Polymerase X Preferentially Accommodates Incoming dATP Opposite 8-Oxoguanine on the Template. Biophysical Journal, 2013, 105, 2559-2568.	0.2	9
65	Insights into chromatin fibre structure by inÂvitro and in silico single-molecule stretching experiments. Biochemical Society Transactions, 2013, 41, 494-500.	1.6	9
66	Graph Applications to RNA Structure and Function. , 2013, , 23-51.		10
67	â€œGate-keeperâ€•Residues and Active-Site Rearrangements in DNA Polymerase Î¼ Help Discriminate Non-cognate Nucleotides. PLoS Computational Biology, 2013, 9, e1003074.	1.5	9
68	Candidate RNA structures for domain 3 of the foot-and-mouth-disease virus internal ribosome entry site. Nucleic Acids Research, 2013, 41, 1483-1495.	6.5	25
69	Predicting Helical Topologies in RNA Junctions as Tree Graphs. PLoS ONE, 2013, 8, e71947.	1.1	31
70	RNA Structure Analysis and Design, Graph Theory. , 2013, , 1864-1875.		0
71	Models of conformational selection of DNA polymerase X in the presence of oxoG lesions help interpret kinetics data. FASEB Journal, 2013, 27, 758.11.	0.2	0
72	Network Theory Tools for RNA Modeling. WSEAS Transactions on Mathematics, 2013, 9, 941-955.	0.2	20

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73	Dynamic Energy Landscapes of Riboswitches Help Interpret Conformational Rearrangements and Function. PLoS Computational Biology, 2012, 8, e1002368.	1.5	38
74	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.	6.5	40
75	Predicting coaxial helical stacking in RNA junctions. Nucleic Acids Research, 2012, 40, 487-498.	6.5	51
76	Toward Convergence of Experimental Studies and Theoretical Modeling of the Chromatin Fiber. Journal of Biological Chemistry, 2012, 287, 5183-5191.	1.6	87
77	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.	6.6	19
78	A New Toolkit for Modeling RNA from a Pseudo-Torsional Space. Journal of Molecular Biology, 2012, 421, 1-5.	2.0	0
79	Intrinsic Motions of DNA Polymerases Underlie Their Remarkable Specificity and Selectivity and Suggest a Hybrid Substrate Binding Mechanism. RSC Biomolecular Sciences, 2012, , 81-110.	0.4	2
80	Perspective: pre-chemistry conformational changes in DNA polymerase mechanisms. Theoretical Chemistry Accounts, 2012, 131, 1287.	0.5	34
81	Analysis of Junctions in RNA with Coaxial Stacked Helices. FASEB Journal, 2012, 26, 948.1.	0.2	0
82	Molecular dynamics studies of polymerase X/DNA complexes in the presence of OxoG on the templating strand. FASEB Journal, 2012, 26, 539.8.	0.2	0
83	DNA Polymerases: Structure, Function, and Modeling. , 2011, , 49-66.		0
84	The Effect of Linker Histone's Nucleosome Binding Affinity on Chromatin Unfolding Mechanisms. Biophysical Journal, 2011, 101, 1670-1680.	0.2	31
85	Biomolecular modeling and simulation: a field coming of age. Quarterly Reviews of Biophysics, 2011, 44, 191-228.	2.4	136
86	Computational approaches to RNA structure prediction, analysis, and design. Current Opinion in Structural Biology, 2011, 21, 306-318.	2.6	139
87	RAG: An update to the RNA-As-Graphs resource. BMC Bioinformatics, 2011, 12, 219.	1.2	46
88	Computational approaches to 3D modeling of RNA. Journal of Physics Condensed Matter, 2010, 22, 283101.	0.7	98
89	Computational generation and screening of RNA motifs in large nucleotide sequence pools. Nucleic Acids Research, 2010, 38, e139-e139.	6.5	34
90	Biomolecular Structure and Modeling: Historical Perspective. Interdisciplinary Applied Mathematics, 2010, , 1-40.	0.2	0

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91	Biomolecular Structure and Modeling: Problem and Application Perspective. Interdisciplinary Applied Mathematics, 2010, , 41-75.	0.2	0
92	Protein Structure Hierarchy. Interdisciplinary Applied Mathematics, 2010, , 105-128.	0.2	1
93	Nucleic Acids Structure Minitutorial. Interdisciplinary Applied Mathematics, 2010, , 129-162.	0.2	1
94	Topics in Nucleic Acids Structure: DNA Interactions and Folding. Interdisciplinary Applied Mathematics, 2010, , 163-204.	0.2	1
95	Topics in Nucleic Acids Structure: Noncanonical Helices and RNA Structure. Interdisciplinary Applied Mathematics, 2010, , 205-236.	0.2	2
96	Theoretical and Computational Approaches to Biomolecular Structure. Interdisciplinary Applied Mathematics, 2010, , 237-264.	0.2	0
97	Force Fields. Interdisciplinary Applied Mathematics, 2010, , 265-298.	0.2	0
98	Nonbonded Computations. Interdisciplinary Applied Mathematics, 2010, , 299-344.	0.2	1
99	Multivariate Minimization in Computational Chemistry. Interdisciplinary Applied Mathematics, 2010, , 345-384.	0.2	1
100	Monte Carlo Techniques. Interdisciplinary Applied Mathematics, 2010, , 385-423.	0.2	1
101	Molecular Dynamics: Basics. Interdisciplinary Applied Mathematics, 2010, , 425-461.	0.2	9
102	Molecular Dynamics: Further Topics. Interdisciplinary Applied Mathematics, 2010, , 463-517.	0.2	1
103	Similarity and Diversity in Chemical Design. Interdisciplinary Applied Mathematics, 2010, , 519-553.	0.2	1
104	Chromatin Ionic Atmosphere Analyzed by a Mesoscale Electrostatic Approach. Biophysical Journal, 2010, 99, 2587-2596.	0.2	23
105	Modeling DNA Polymerase Î¼ Motions: Subtle Transitions before Chemistry. Biophysical Journal, 2010, 99, 3463-3472.	0.2	23
106	DNA Pol Î»Ëˆs Extraordinary Ability To Stabilize Misaligned DNA. Journal of the American Chemical Society, 2010, 132, 13403-13416.	6.6	15
107	Modeling Studies of Chromatin Fiber Structure as a Function of DNA Linker Length. Journal of Molecular Biology, 2010, 403, 777-802.	2.0	98
108	Molecular Modeling and Simulation: An Interdisciplinary Guide. Interdisciplinary Applied Mathematics, 2010, , .	0.2	297

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109	Mathematical and Biological Scientists Assess the State of the Art in RNA Science at an IMA Workshop, RNA in Biology, Bioengineering, and Biotechnology. International Journal for Multiscale Computational Engineering, 2010, 8, 369-378.	0.8	5
110	Structural insights into DNA polymerase X from African swine fever virus in the presence of oxoG lesions. FASEB Journal, 2010, 24, 876.15.	0.2	0
111	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.	3.3	240
112	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.	1.1	144
113	Mesoscale simulations of two nucleosome-repeat length oligonucleosomes. Physical Chemistry Chemical Physics, 2009, 11, 10729.	1.3	45
114	Analysis of Four-Way Junctions in RNA Structures. Journal of Molecular Biology, 2009, 390, 547-559.	2.0	94
115	Tertiary Motifs Revealed in Analyses of Higher-Order RNA Junctions. Journal of Molecular Biology, 2009, 393, 67-82.	2.0	42
116	Analysis of Riboswitch Structure and Function by an Energy Landscape Framework. Journal of Molecular Biology, 2009, 393, 993-1003.	2.0	27
117	Relationship Between Conformational Changes in Pol Î»â€™s Active Site Upon Binding Incorrect Nucleotides and Mismatch Incorporation Rates. Journal of Physical Chemistry B, 2009, 113, 13035-13047.	1.2	8
118	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
119	From Macroscopic to Mesoscopic Models of Chromatin Folding. , 2009, , 514-535.		2
120	Monte Carlo, harmonic approximation, and coarse-graining approaches for enhanced sampling of biomolecular structure. F1000 Biology Reports, 2009, 1, 48.	4.0	12
121	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.	2.6	15
122	Substrateâ€induced DNA strand misalignment during catalytic cycling by DNA polymerase Î». EMBO Reports, 2008, 9, 459-464.	2.0	36
123	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.	6.6	43
124	Mismatched Base-Pair Simulations for ASFV Pol X/DNA Complexes Help Interpret Frequent Gâ€¢G Misincorporation. Journal of Molecular Biology, 2008, 384, 1086-1097.	2.0	20
125	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.	6.6	20
126	Annotation of tertiary interactions in RNA structures reveals variations and correlations. Rna, 2008, 14, 2465-2477.	1.6	63

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127	Estimating the Fraction of Non-Coding RNAs in Mammalian Transcriptomes. Bioinformatics and Biology Insights, 2008, 2, BBI.S443.	1.0	0
128	Studies of African Swine Fever Virus Polymerase X/DNA complexes in the presence of mismatched base pairs. FASEB Journal, 2008, 22, 990.2.	0.2	0
129	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.	1.8	27
130	Efficient global biopolymer sampling with end-transfer configurational bias Monte Carlo. Journal of Chemical Physics, 2007, 126, 044107.	1.2	20
131	Optimization Methods in Computational Chemistry. Reviews in Computational Chemistry, 2007, , 1-71.	1.5	31
132	A computational proposal for designing structured RNA pools for in vitro selection of RNAs. Rna, 2007, 13, 478-492.	1.6	47
133	DNA Polymerase Î² Catalysis:Â Are Different Mechanisms Possible?. Journal of the American Chemical Society, 2007, 129, 11100-11110.	6.6	65
134	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.	1.2	40
135	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.	0.2	23
136	Distinct energetics and closing pathways for DNA polymerase beta with 8-oxoG template and different incoming nucleotides. , 2007, 7, 7.		22
137	Regulation of DNA Repair Fidelity by Molecular Checkpoints:Â â€œGatesâ€•in DNA Polymerase Î²'s Substrate Selectionâ€. Biochemistry, 2006, 45, 15142-15156.	1.2	66
138	In Silico Studies of the African Swine Fever Virus DNA Polymerase X Support an Induced-Fit Mechanism. Biophysical Journal, 2006, 90, 42-56.	0.2	32
139	Stereochemistry and Position-Dependent Effects of Carcinogens on TATA/TBP Binding. Biophysical Journal, 2006, 90, 1865-1877.	0.2	17
140	Flexible Histone Tails in a New Mesoscopic Oligonucleosome Model. Biophysical Journal, 2006, 91, 133-150.	0.2	104
141	Sequential Side-Chain Residue Motions Transform the Binary into the Ternary State of DNA Polymerase Î». Biophysical Journal, 2006, 91, 3182-3195.	0.2	17
142	Correct and incorrect nucleotide incorporation pathways in DNA polymerase Î². Biochemical and Biophysical Research Communications, 2006, 350, 521-529.	1.0	52
143	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.	3.1	19
144	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.	3.3	167

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145	Special Section On Multiscale Modeling In Biology. Multiscale Modeling and Simulation, 2006, 5, 1174-1174.	0.6	4
146	RNA: The Cousin Left Behind Becomes a Star. , 2006, , 259-281.		2
147	Exploring the Connection Between Synthetic and Natural RNAs in Genomes: A Novel Computational Approach. , 2006, , 35-56.		0
148	Predicting candidate genomic sequences that correspond to synthetic functional RNA motifs. Nucleic Acids Research, 2005, 33, 6057-6069.	6.5	23
149	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.	3.3	104
150	The Critical Collaboration between Art and Science: An Experiment on a Bird in the Air Pump and the Ramifications of Genomics for Society. Leonardo, 2005, 38, 323-329.	0.2	2
151	Modular RNA architecture revealed by computational analysis of existing pseudoknots and ribosomal RNAs. Nucleic Acids Research, 2005, 33, 1384-1398.	6.5	26
152	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.	6.6	69
153	Conformational Transition Pathway of Polymerase Î²/DNA upon Binding Correct Incoming Substrate. Journal of Physical Chemistry B, 2005, 109, 5358-5367.	1.2	31
154	Mismatch-Induced Conformational Distortions in Polymerase Î² Support an Induced-Fit Mechanism for Fidelityâ€. Biochemistry, 2005, 44, 13328-13341.	1.2	57
155	In vitro RNA random pools are not structurally diverse: A computational analysis. Rna, 2005, 11, 853-863.	1.6	76
156	Searching for 2D RNA geometries in bacterial genomes. , 2004, , .		6
157	RAG: RNA-As-Graphs database--concepts, analysis, and features. Bioinformatics, 2004, 20, 1285-1291.	1.8	74
158	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.	3.3	146
159	RAG: RNA-As-Graphs web resource. BMC Bioinformatics, 2004, 5, 88.	1.2	56
160	Structural motifs in ribosomal RNAs: Implications for RNA design and genomics. Biopolymers, 2004, 73, 340-347.	1.2	11
161	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.	6.6	127
162	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.	0.2	47

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163	In Silico Evidence for DNA Polymerase-Î²â€™s Substrate-Induced Conformational Change. Biophysical Journal, 2004, 87, 3088-3099.	0.2	52
164	Biomolecular free energy profiles by a shooting/umbrella sampling protocol, â€œBOLASâ€• Journal of Chemical Physics, 2004, 121, 2436-2444.	1.2	62
165	Candidates for Novel RNA Topologies. Journal of Molecular Biology, 2004, 341, 1129-1144.	2.0	51
166	Deformations of promoter DNA bound to carcinogens help interpret effects on TATA-element structure and activity. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2004, 362, 1479-1496.	1.6	7
167	Title is missing!. Journal of Mathematical Imaging and Vision, 2003, 19, 33-48.	0.8	28
168	Principal component analysis combined with truncated-Newton minimization for dimensionality reduction of chemical databases. Mathematical Programming, 2003, 95, 161-185.	1.6	6
169	Inherent speedup limitations in multiple time step/particle mesh Ewald algorithms. Journal of Computational Chemistry, 2003, 24, 77-88.	1.5	28
170	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.	1.5	54
171	Sequence-dependent solution structure and motions of 13 TATA/TBP (TATA-box binding protein) complexes. Biopolymers, 2003, 69, 216-243.	1.2	16
172	Deoxyadenosine sugar puckering pathway simulated by the stochastic difference equation algorithm. Chemical Physics Letters, 2003, 378, 1-8.	1.2	33
173	Engineering Teams Up with Computer-Simulation and Visualization Tools to Probe Biomolecular Mechanisms. Biophysical Journal, 2003, 85, 1-4.	0.2	77
174	Effect of DNA Superhelicity and Bound Proteins on Mechanistic Aspects of the Hin-Mediated and Fis-Enhanced Inversion. Biophysical Journal, 2003, 85, 804-817.	0.2	6
175	Unbiased Rotational Moves for Rigid-Body Dynamics. Biophysical Journal, 2003, 85, 2973-2976.	0.2	36
176	Exploring the repertoire of RNA secondary motifs using graph theory; implications for RNA design. Nucleic Acids Research, 2003, 31, 2926-2943.	6.5	139
177	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.	1.2	49
178	Macroscopic modeling and simulations of supercoiled DNA with bound proteins. Journal of Chemical Physics, 2002, 117, 8573-8586.	1.2	34
179	A More Lenient Stopping Rule for Line Search Algorithms. Optimization Methods and Software, 2002, 17, 683-700.	1.6	10
180	A Hoogsteen base pair embedded in undistorted B-DNA. Nucleic Acids Research, 2002, 30, 5244-5252.	6.5	71

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181	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.	2.0	87
182	Molecular Modeling and Simulation. Interdisciplinary Applied Mathematics, 2002, , .	0.2	416
183	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.	2.0	54
184	Analysis of Protein Sequence/Structure Similarity Relationships. Biophysical Journal, 2002, 83, 2781-2791.	0.2	70
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