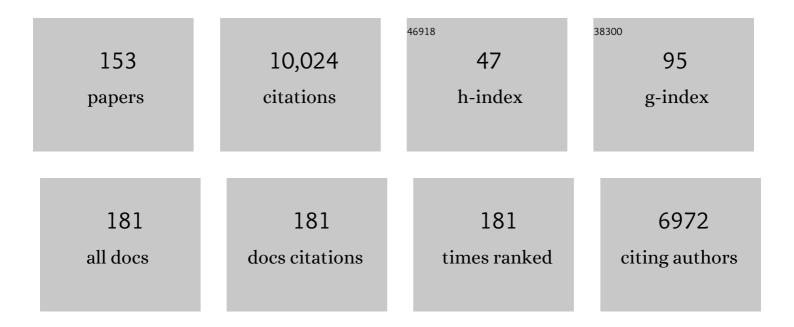
List of Publications by Year in descending order

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RON FIRED

#	Article	IF	CITATIONS
1	fw2.2: A Quantitative Trait Locus Key to the Evolution of Tomato Fruit Size. Science, 2000, 289, 85-88.	6.0	1,290
2	Multiple conformational states of proteins: a molecular dynamics analysis of myoglobin. Science, 1987, 235, 318-321.	6.0	659
3	Computing time scales from reaction coordinates by milestoning. Journal of Chemical Physics, 2004, 120, 10880-10889.	1.2	563
4	Enhanced sampling in molecular dynamics: use of the time-dependent Hartree approximation for a simulation of carbon monoxide diffusion through myoglobin. Journal of the American Chemical Society, 1990, 112, 9161-9175.	6.6	503
5	A method for determining reaction paths in large molecules: Application to myoglobin. Chemical Physics Letters, 1987, 139, 375-380.	1.2	392
6	A new technique to calculate steepest descent paths in flexible polyatomic systems. Journal of Chemical Physics, 1990, 92, 1510-1511.	1.2	264
7	Reaction path study of conformational transitions in flexible systems: Applications to peptides. Journal of Chemical Physics, 1990, 92, 5580-5601.	1.2	254
8	Calculation of classical trajectories with a very large time step: Formalism and numerical examples. Journal of Chemical Physics, 1996, 105, 9299-9315.	1.2	200
9	Modeling side chains in peptides and proteins: Application of the locally enhanced sampling and the simulated annealing methods to find minimum energy conformations. Journal of Chemical Physics, 1991, 95, 9277-9287.	1.2	175
10	Distance-dependent, pair potential for protein folding: Results from linear optimization. Proteins: Structure, Function and Bioinformatics, 2000, 41, 40-46.	1.5	172
11	Extending molecular dynamics time scales with milestoning: Example of complex kinetics in a solvated peptide. Journal of Chemical Physics, 2007, 126, 145104.	1.2	162
12	On the assumptions underlying milestoning. Journal of Chemical Physics, 2008, 129, 174102.	1.2	158
13	MOIL: A program for simulations of macromolecules. Computer Physics Communications, 1995, 91, 159-189.	3.0	154
14	Long-timescale simulation methods. Current Opinion in Structural Biology, 2005, 15, 151-156.	2.6	154
15	Prediction of homoprotein and heteroprotein complexes by protein docking and templateâ€based modeling: A CASPâ€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2016, 84, 323-348.	1.5	148
16	Reaction path study of helix formation in tetrapeptides: Effect of side chains. Journal of Chemical Physics, 1991, 94, 751-760.	1.2	134
17	An atomically detailed study of the folding pathways of protein A with the stochastic difference equation. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 10394-10398.	3.3	125
18	Self-avoiding walk between two fixed points as a tool to calculate reaction paths in large molecular systems. International Journal of Quantum Chemistry, 1990, 38, 167-185.	1.0	123

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19	Linear programming optimization and a double statistical filter for protein threading protocols. Proteins: Structure, Function and Bioinformatics, 2001, 45, 241-261.	1.5	117
20	A Stochastic Algorithm for the Isobaric–Isothermal Ensemble with Ewald Summations for All Long Range Forces. Journal of Chemical Theory and Computation, 2015, 11, 5624-5637.	2.3	114
21	On the design and analysis of protein folding potentials. , 2000, 40, 71-85.		107
22	How Conformational Dynamics of DNA Polymerase Select Correct Substrates: Experiments and Simulations. Structure, 2012, 20, 618-627.	1.6	107
23	Stochastic Path Approach to Compute Atomically Detailed Trajectories:  Application to the Folding of C Peptide. Journal of Physical Chemistry B, 1999, 103, 899-911.	1.2	104
24	Long Time Dynamics of Complex Systems. Accounts of Chemical Research, 2002, 35, 396-403.	7.6	101
25	Milestoning without a Reaction Coordinate. Journal of Chemical Theory and Computation, 2010, 6, 1805-1817.	2.3	100
26	Exact milestoning. Journal of Chemical Physics, 2015, 142, 094102.	1.2	100
27	A Milestoning Study of the Kinetics of an Allosteric Transition: Atomically Detailed Simulations of Deoxy Scapharca Hemoglobin. Biophysical Journal, 2007, 92, L85-L87.	0.2	93
28	RNA and Its Ionic Cloud: Solution Scattering Experiments and Atomically Detailed Simulations. Biophysical Journal, 2012, 102, 819-828.	0.2	89
29	Enriching the sequence substitution matrix by structural information. Proteins: Structure, Function and Bioinformatics, 2003, 54, 41-48.	1.5	87
30	SSALN: An alignment algorithm using structure-dependent substitution matrices and gap penalties learned from structurally aligned protein pairs. Proteins: Structure, Function and Bioinformatics, 2005, 62, 881-891.	1.5	79
31	Ligand diffusion in globins: simulations versus experiment. Current Opinion in Structural Biology, 2010, 20, 162-167.	2.6	76
32	Revisiting and Computing Reaction Coordinates with Directional Milestoning. Journal of Physical Chemistry A, 2011, 115, 6137-6148.	1.1	74
33	Yet another look at the steepest descent path. Computational and Theoretical Chemistry, 1997, 398-399, 63-71.	1.5	72
34	Temperature dependent reaction coordinates. Journal of Chemical Physics, 2000, 112, 5539-5545.	1.2	71
35	SHAKE parallelization. European Physical Journal: Special Topics, 2011, 200, 211-223.	1.2	71
36	The Ionic Atmosphere around A-RNA: Poisson-Boltzmann and Molecular Dynamics Simulations. Biophysical Journal, 2012, 102, 829-838.	0.2	68

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37	Sodium in gramicidin: an example of a permion. Biophysical Journal, 1995, 68, 906-924.	0.2	67
38	Calculation of the potential of mean force using molecular dynamics with linear constraints: An application to a conformational transition in a solvated dipeptide. Journal of Chemical Physics, 1990, 93, 4312-4321.	1.2	66
39	Revisiting and parallelizing SHAKE. Journal of Computational Physics, 2005, 209, 193-206.	1.9	66
40	Atomically detailed simulation of the recovery stroke in myosin by Milestoning. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 5001-5005.	3.3	65
41	Computational studies of ligand diffusion in globins: I. Leghemoglobin. Proteins: Structure, Function and Bioinformatics, 1991, 10, 70-80.	1.5	64
42	Distance-dependent, pair potential for protein folding: results from linear optimization. Proteins: Structure, Function and Bioinformatics, 2000, 41, 40-6.	1.5	64
43	Kinetics of Helix Unfolding: Molecular Dynamics Simulations with Milestoning. Journal of Physical Chemistry A, 2009, 113, 7461-7473.	1.1	63
44	Reaction path study of conformational transitions and helix formation in a tetrapeptide Proceedings of the National Academy of Sciences of the United States of America, 1989, 86, 6963-6967.	3.3	60
45	Unassisted Transport of <i>N</i> -Acetyl- <scp>l</scp> -tryptophanamide through Membrane: Experiment and Simulation of Kinetics. Journal of Physical Chemistry B, 2012, 116, 2739-2750.	1.2	59
46	Kinetics of cytochrome C folding: Atomically detailed simulations. Proteins: Structure, Function and Bioinformatics, 2003, 51, 245-257.	1.5	57
47	Improving ranking of models for protein complexes with side chain modeling and atomic potentials. Proteins: Structure, Function and Bioinformatics, 2013, 81, 592-606.	1.5	54
48	Perspective: Computer simulations of long time dynamics. Journal of Chemical Physics, 2016, 144, 060901.	1.2	54
49	PIE—Efficient filters and coarse grained potentials for unbound protein–protein docking. Proteins: Structure, Function and Bioinformatics, 2010, 78, 400-419.	1.5	53
50	Calculating Iso-Committor Surfaces as Optimal Reaction Coordinates with Milestoning. Entropy, 2017, 19, 219.	1.1	51
51	A new paradigm for atomically detailed simulations of kinetics in biophysical systems. Quarterly Reviews of Biophysics, 2017, 50, e8.	2.4	49
52	Locally enhanced sampling in free energy calculations: Application of mean field approximation to accurate calculation of free energy differences. Journal of Chemical Physics, 1992, 97, 7838-7841.	1.2	47
53	Unit-vector RMS (URMS) as a tool to analyze molecular dynamics trajectories. Proteins: Structure, Function and Bioinformatics, 1999, 37, 554-564.	1.5	47
54	A coarseâ€grained potential for fold recognition and molecular dynamics simulations of proteins. Proteins: Structure, Function and Bioinformatics, 2009, 76, 822-836.	1.5	47

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55	MOIL-opt: Energy-Conserving Molecular Dynamics on a GPU/CPU System. Journal of Chemical Theory and Computation, 2011, 7, 3072-3082.	2.3	47
56	Milestoning: An Efficient Approach for Atomically Detailed Simulations of Kinetics in Biophysics. Annual Review of Biophysics, 2020, 49, 69-85.	4.5	46
57	Membrane Permeation of a Peptide: It Is Better to be Positive. Journal of Physical Chemistry B, 2015, 119, 6412-6420.	1.2	44
58	Atomically detailed potentials to recognize native and approximate protein structures. Proteins: Structure, Function and Bioinformatics, 2005, 61, 44-55.	1.5	43
59	The network of sequence flow between protein structures. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 11627-11632.	3.3	43
60	Simulations of allosteric transitions. Current Opinion in Structural Biology, 2011, 21, 167-172.	2.6	43
61	The thermal equilibrium aspects of the time dependent Hartree and the locally enhanced sampling approximations: Formal properties, a correction, and computational examples for rare gas clusters. Journal of Chemical Physics, 1993, 98, 3380-3388.	1.2	40
62	Revealing the distinct folding phases of an RNA three-helix junction. Nucleic Acids Research, 2018, 46, 7354-7365.	6.5	38
63	Bridging the Gap between Long Time Trajectories and Reaction Pathways. Advances in Chemical Physics, 2003, , 93-129.	0.3	37
64	Computational study of peptide permeation through membrane: searching for hidden slow variables. Molecular Physics, 2013, 111, 3565-3578.	0.8	37
65	Calculations of a list of neighbors in Molecular Dynamics simulations. Journal of Computational Chemistry, 1989, 10, 921-927.	1.5	34
66	Computer determination of peptide conformations in water: different roads to structure Proceedings of the National Academy of Sciences of the United States of America, 1995, 92, 3190-3193.	3.3	34
67	Enzymatic circularization of a malto-octaose linear chain studied by stochastic reaction path calculations on cyclodextrin glycosyltransferase. Proteins: Structure, Function and Bioinformatics, 2001, 43, 327-335.	1.5	34
68	Modeling kinetics and equilibrium of membranes with fields: Milestoning analysis and implication to permeation. Journal of Chemical Physics, 2014, 141, 054101.	1.2	33
69	Toward Quantitative Simulations of Carbon Monoxide Escape Pathways in Myoglobin. Journal of Physical Chemistry B, 2008, 112, 6147-6154.	1.2	32
70	Ligand binding and conformation change in the dimeric hemoglobin of the clam Scapharca inaequivalvis Journal of Biological Chemistry, 1993, 268, 5711-5718.	1.6	32
71	Molecular dynamics study of secondary structure motion in proteins: Application to myohemerythrin. Proteins: Structure, Function and Bioinformatics, 1990, 7, 265-279.	1.5	30
72	The Impact of Protonation on Early Translocation of Anthrax Lethal Factor: Kinetics from Molecular Dynamics Simulations and Milestoning Theory. Journal of the American Chemical Society, 2017, 139, 14837-14840.	6.6	30

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73	Physiological Calcium Concentrations Slow Dynamics at the Lipid-Water Interface. Biophysical Journal, 2018, 115, 1541-1551.	0.2	30
74	Enzyme Selectivity of HIV Reverse Transcriptase: Conformations, Ligands, and Free Energy Partition. Journal of Physical Chemistry B, 2015, 119, 11513-11526.	1.2	28
75	Lifetimes of rotational resonances in molecule-surface scattering. Molecular Physics, 1985, 55, 1369-1381.	0.8	26
76	The transition between active and inactive conformations of Abl kinase studied by rock climbing and Milestoning. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129508.	1.1	26
77	DOCK/PIERR: Web Server for Structure Prediction of Protein–Protein Complexes. Methods in Molecular Biology, 2014, 1137, 199-207.	0.4	26
78	Building and assessing atomic models of proteins from structural templates: Learning and benchmarks. Proteins: Structure, Function and Bioinformatics, 2009, 76, 930-945.	1.5	25
79	Revisiting Molecular Dynamics on a CPU/GPU System: Water Kernel and SHAKE Parallelization. Journal of Chemical Theory and Computation, 2012, 8, 4624-4636.	2.3	25
80	Catch bond-like kinetics of helix cracking: Network analysis by molecular dynamics and Milestoning. Journal of Chemical Physics, 2013, 139, 121902.	1.2	25
81	Ligand binding and conformation change in the dimeric hemoglobin of the clam Scapharca inaequivalvis. Journal of Biological Chemistry, 1993, 268, 5711-8.	1.6	25
82	Maximum feasibility guideline in the design and analysis of protein folding potentials. Journal of Computational Chemistry, 2002, 23, 111-118.	1.5	24
83	Measurement of the Membrane Dipole Electric Field in DMPC Vesicles Using Vibrational Shifts of <i>p</i> -Cyanophenylalanine and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2015, 119, 2869-2876.	1.2	24
84	Ion Permeation through a Phospholipid Membrane: Transition State, Path Splitting, and Calculation of Permeability. Journal of Chemical Theory and Computation, 2019, 15, 720-730.	2.3	24
85	Interfacial Dynamics in Lipid Membranes: The Effects of Headgroup Structures. Journal of Physical Chemistry B, 2021, 125, 1343-1350.	1.2	23
86	Computational exploration of the network of sequence flow between protein structures. Proteins: Structure, Function and Bioinformatics, 2010, 78, 985-1003.	1.5	22
87	Experiments and Comprehensive Simulations of the Formation of a Helical Turn. Journal of Physical Chemistry B, 2012, 116, 6598-6610.	1.2	22
88	Early Events in Helix Unfolding under External Forces: A Milestoning Analysis. Journal of Physical Chemistry B, 2012, 116, 8662-8691.	1.2	22
89	Chemical Development of Latent Fingerprints: Computational Design of Ninhydrin Analogues. Journal of Forensic Sciences, 2000, 45, 757-760.	0.9	22
90	Large-scale linear programming techniques for the design of protein folding potentials. Mathematical Programming, 2004, 101, 301.	1.6	21

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91	The energy landscape of a protein switch. Physical Chemistry Chemical Physics, 2014, 16, 6407.	1.3	21
92	Calculation of Point-to-Point Short-Time and Rare Trajectories with Boundary Value Formulation. Journal of Chemical Theory and Computation, 2006, 2, 484-494.	2.3	20
93	Coiled-Coil Response to Mechanical Force: Global Stability and Local Cracking. Biophysical Journal, 2013, 105, 951-961.	0.2	20
94	Analyzing milestoning networks for molecular kinetics: Definitions, algorithms, and examples. Journal of Chemical Physics, 2013, 139, 174105.	1.2	20
95	Comprehensive analysis of sequences of a protein switch. Protein Science, 2016, 25, 135-146.	3.1	20
96	Computer Simulations of the Dissociation Mechanism of Gleevec from Abl Kinase with Milestoning. Journal of Physical Chemistry B, 2021, 125, 5706-5715.	1.2	20
97	A Mathematical Framework for Exact Milestoning. Multiscale Modeling and Simulation, 2016, 14, 301-322.	0.6	19
98	Why Does RNA Collapse? The Importance of Water in a Simulation Study of Helix–Junction–Helix Systems. Journal of the American Chemical Society, 2018, 140, 16948-16951.	6.6	19
99	A templateâ€finding algorithm and a comprehensive benchmark for homology modeling of proteins. Proteins: Structure, Function and Bioinformatics, 2008, 72, 910-928.	1.5	18
100	Peptide Permeation across a Phosphocholine Membrane: An Atomically Detailed Mechanism Determined through Simulations and Supported by Experimentation. Journal of Physical Chemistry B, 2022, 126, 2834-2849.	1.2	17
101	Markovian and Non-Markovian Modeling of Membrane Dynamics with Milestoning. Journal of Physical Chemistry B, 2016, 120, 8208-8216.	1.2	16
102	Conformations of an RNA Helix-Junction-Helix Construct Revealed by SAXS Refinement of MD Simulations. Biophysical Journal, 2019, 116, 19-30.	0.2	16
103	Computational Analysis of Sequence Selection Mechanisms. Structure, 2004, 12, 547-557.	1.6	15
104	Extension of a protein docking algorithm to membranes and applications to amyloid precursor protein dimerization. Proteins: Structure, Function and Bioinformatics, 2015, 83, 2170-2185.	1.5	15
105	Molecular Dynamics Studies of Modular Polyketide Synthase Ketoreductase Stereospecificity. Biochemistry, 2015, 54, 2346-2359.	1.2	15
106	Direct Measurement of the Effect of Cholesterol and 6-Ketocholestanol on the Membrane Dipole Electric Field Using Vibrational Stark Effect Spectroscopy Coupled with Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2017, 121, 3424-3436.	1.2	15
107	Pyrophosphate Release in the Protein HIV Reverse Transcriptase. Journal of Physical Chemistry B, 2017, 121, 9557-9565.	1.2	15
108	A mixed alchemical and equilibrium dynamics to simulate heterogeneous dense fluids: Illustrations for Lennard-Jones mixtures and phospholipid membranes. Journal of Chemical Physics, 2018, 149, 072325.	1.2	15

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109	Homology as a Tool in Optimization Problems: Structure Determination of 2D Heteropolymers. The Journal of Physical Chemistry, 1995, 99, 11550-11556.	2.9	14
110	Extracting the diffusion tensor from molecular dynamics simulation with Milestoning. Journal of Chemical Physics, 2015, 142, 014105.	1.2	14
111	Energy design for protein-protein interactions. Journal of Chemical Physics, 2011, 135, 065102.	1.2	13
112	Preferential Equilibrium Partitioning of Positively Charged Tryptophan into Phosphatidylcholine Bilayer Membranes. Journal of Physical Chemistry B, 2019, 123, 170-179.	1.2	13
113	Super folds, networks, and barriers. Proteins: Structure, Function and Bioinformatics, 2012, 80, 463-470.	1.5	11
114	Molecular machines. Current Opinion in Structural Biology, 2013, 23, 206-211.	2.6	11
115	Simulations of thermodynamics and kinetics on rough energy landscapes with milestoning. Journal of Computational Chemistry, 2016, 37, 602-613.	1.5	11
116	Rock climbing: A local-global algorithm to compute minimum energy and minimum free energy pathways. Journal of Chemical Physics, 2017, 147, 152718.	1.2	11
117	A peptide-derived strategy for specifically targeting the mitochondria and ER of cancer cells: a new approach in fighting cancer. Chemical Science, 2022, 13, 6929-6941.	3.7	11
118	Protein Recognition by Sequence-to-Structure Fitness: Bridging Efficiency and Capacity of Threading Models. Advances in Chemical Physics, 2002, , 77-130.	0.3	10
119	Defect-Assisted Permeation Through a Phospholipid Membrane: Experimental and Computational Study of the Peptide WKW. Journal of Physical Chemistry B, 2019, 123, 6792-6798.	1.2	10
120	Computer simulations of a heterogeneous membrane with enhanced sampling techniques. Journal of Chemical Physics, 2020, 153, 144110.	1.2	10
121	Modeling molecular kinetics with Milestoning. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1512.	6.2	10
122	Value of Temporal Information When Analyzing Reaction Coordinates. Journal of Chemical Theory and Computation, 2020, 16, 6077-6090.	2.3	9
123	Calcium-Lipid Interactions Observed with Isotope-Edited Infrared Spectroscopy. Biophysical Journal, 2020, 118, 2694-2702.	0.2	9
124	Impact of the Protonation State of Phosphatidylinositol 4,5-Bisphosphate (PIP2) on the Binding Kinetics and Thermodynamics to Transient Receptor Potential Vanilloid (TRPV5): A Milestoning Study. Journal of Physical Chemistry B, 2021, 125, 9547-9556.	1.2	9
125	REACTION PATH STUDIES OF BIOLOGICAL MOLECULES. Advanced Series in Physical Chemistry, 1996, , 65-136.	1.5	9
126	Long-time methods for molecular dynamics simulations: Markov State Models and Milestoning. Progress in Molecular Biology and Translational Science, 2020, 170, 215-237.	0.9	8

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127	Thermodynamic Cycle without Turning Off Self-Interactions: Formal Discussion and a Numerical Example. Journal of Chemical Theory and Computation, 2012, 8, 3022-3033.	2.3	7
128	ScMile: A Script to Investigate Kinetics with Short Time Molecular Dynamics Trajectories and the Milestoning Theory. Journal of Chemical Theory and Computation, 2020, 16, 860-874.	2.3	7
129	Exploring the Reaction Mechanism of HIV Reverse Transcriptase with a Nucleotide Substrate. Journal of Physical Chemistry B, 2020, 124, 4270-4283.	1.2	7
130	Milestoning with wind: Exploring the impact of a biasing potential in exact calculation of kinetics. Journal of Chemical Physics, 2020, 152, 224105.	1.2	7
131	The evolutionary capacity of protein structures. , 2004, , .		6
132	Probing Translocation in Mutants of the Anthrax Channel: Atomically Detailed Simulations with Milestoning. Journal of Physical Chemistry B, 2018, 122, 10296-10305.	1.2	6
133	A new boundary driven NEMD scheme for heat and particle diffusion in binary mixtures. Molecular Physics, 2021, 119, .	0.8	6
134	Partition of Positively and Negatively Charged Tryptophan lons in Membranes with Inverted Phospholipid Heads: Simulations and Experiments. Journal of Physical Chemistry B, 2019, 123, 3272-3281.	1.2	5
135	Phase Transition in a Heterogeneous Membrane: Atomically Detailed Picture. Journal of Physical Chemistry Letters, 2020, 11, 5263-5267.	2.1	5
136	Dramatic Shape Changes Occur as Cytochrome <i>c</i> Folds. Journal of Physical Chemistry B, 2020, 124, 8240-8248.	1.2	4
137	Probing the role of local propensity in peptide turn formation. International Journal of Quantum Chemistry, 2000, 80, 1125-1128.	1.0	3
138	Catalytic Magnesium as a Door Stop for DNA Sliding. Journal of Physical Chemistry B, 2021, 125, 3494-3500.	1.2	3
139	Conformational Transitions. AIP Conference Proceedings, 1991, , .	0.3	2
140	From an SNP to a Disease: A Comprehensive Statistical Analysis. Structure, 2015, 23, 1155.	1.6	2
141	Chemical development of latent fingerprints: computational design of ninhydrin analogues. Journal of Forensic Sciences, 2000, 45, 757-60.	0.9	2
142	Watching Biomolecular Machines in Action. Structure, 2010, 18, 415-416.	1.6	1
143	Progress at Last. Structure, 2011, 19, 1725.	1.6	1

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145	Chapter 6. Enhancing the Capacity of Molecular Dynamics Simulations with Trajectory Fragments. RSC Biomolecular Sciences, 2012, , 117-137.	0.4	1
146	Molecular Dynamics at Extended Timescales. Israel Journal of Chemistry, 2014, 54, 1302-1310.	1.0	1
147	Unit-vector RMS (URMS) as a tool to analyze molecular dynamics trajectories. , 1999, 37, 554.		1
148	Unit-vector RMS (URMS) as a tool to analyze molecular dynamics trajectories. , 1999, 37, 554.		1
149	Dynamics of peptide folding. , 1998, , .		0
150	Reaction Paths and Rates. , 2013, , 2186-2191.		0
151	Two Is a Pair, Three Is a Network. Biophysical Journal, 2015, 108, 22.	0.2	0
152	Simple and Analytical Model of RNA Collapse. Journal of Physical Chemistry B, 2020, 124, 5149-5155.	1.2	0
153	Dynamics of inducedâ€fit in HIV reverse transcriptase specificity and resistance. FASEB Journal, 2012, 26, 964.5.	0.2	0