

Ron Elber

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168
papers

8,651
citations

46
h-index

90
g-index

181
ext. papers

9,450
ext. citations

5.1
avg, IF

6.39
L-index

#	Paper	IF	Citations
168	fw2.2: a quantitative trait locus key to the evolution of tomato fruit size. <i>Science</i> , 2000 , 289, 85-8	33.3	1084
167	Multiple conformational states of proteins: a molecular dynamics analysis of myoglobin. <i>Science</i> , 1987 , 235, 318-21	33.3	617
166	Computing time scales from reaction coordinates by milestoning. <i>Journal of Chemical Physics</i> , 2004 , 120, 10880-9	3.9	476
165	Enhanced sampling in molecular dynamics: use of the time-dependent Hartree approximation for a simulation of carbon monoxide diffusion through myoglobin. <i>Journal of the American Chemical Society</i> , 1990 , 112, 9161-9175	16.4	475
164	A method for determining reaction paths in large molecules: Application to myoglobin. <i>Chemical Physics Letters</i> , 1987 , 139, 375-380	2.5	353
163	A new technique to calculate steepest descent paths in flexible polyatomic systems. <i>Journal of Chemical Physics</i> , 1990 , 92, 1510-1511	3.9	242
162	Reaction path study of conformational transitions in flexible systems: Applications to peptides. <i>Journal of Chemical Physics</i> , 1990 , 92, 5580-5601	3.9	234
161	Calculation of classical trajectories with a very large time step: Formalism and numerical examples. <i>Journal of Chemical Physics</i> , 1996 , 105, 9299-9315	3.9	182
160	Modeling side chains in peptides and proteins: Application of the locally enhanced sampling and the simulated annealing methods to find minimum energy conformations. <i>Journal of Chemical Physics</i> , 1991 , 95, 9277-9287	3.9	159
159	Distance-dependent, pair potential for protein folding: Results from linear optimization. <i>Proteins: Structure, Function and Bioinformatics</i> , 2000 , 41, 40-46	4.2	155
158	Long-timescale simulation methods. <i>Current Opinion in Structural Biology</i> , 2005 , 15, 151-6	8.1	145
157	MOIL: A program for simulations of macromolecules. <i>Computer Physics Communications</i> , 1995 , 91, 159-189	4.2	145
156	Extending molecular dynamics time scales with milestoning: example of complex kinetics in a solvated peptide. <i>Journal of Chemical Physics</i> , 2007 , 126, 145104	3.9	140
155	On the assumptions underlying milestoning. <i>Journal of Chemical Physics</i> , 2008 , 129, 174102	3.9	138
154	An atomically detailed study of the folding pathways of protein A with the stochastic difference equation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002 , 99, 10394-8	11.5	119
153	Reaction path study of helix formation in tetrapeptides: Effect of side chains. <i>Journal of Chemical Physics</i> , 1991 , 94, 751-760	3.9	115
152	Self-avoiding walk between two fixed points as a tool to calculate reaction paths in large molecular systems. <i>International Journal of Quantum Chemistry</i> , 1990 , 38, 167-185	2.1	115

151	Linear programming optimization and a double statistical filter for protein threading protocols. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001 , 45, 241-61	4.2	113
150	Prediction of homoprotein and heteroprotein complexes by protein docking and template-based modeling: A CASP-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016 , 84 Suppl 1, 323-48	4.2	111
149	On the design and analysis of protein folding potentials. <i>Proteins: Structure, Function and Bioinformatics</i> , 2000 , 40, 71-85	4.2	100
148	Long time dynamics of complex systems. <i>Accounts of Chemical Research</i> , 2002 , 35, 396-403	24.3	96
147	Stochastic Path Approach to Compute Atomically Detailed Trajectories: Application to the Folding of C Peptide. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 899-911	3.4	96
146	How conformational dynamics of DNA polymerase select correct substrates: experiments and simulations. <i>Structure</i> , 2012 , 20, 618-27	5.2	91
145	Milestoning without a Reaction Coordinate. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 1805-1817	13.7	89
144	A milestoning study of the kinetics of an allosteric transition: atomically detailed simulations of deoxy Scapharca hemoglobin. <i>Biophysical Journal</i> , 2007 , 92, L85-7	2.9	83
143	Exact milestoning. <i>Journal of Chemical Physics</i> , 2015 , 142, 094102	3.9	78
142	Enriching the sequence substitution matrix by structural information. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004 , 54, 41-8	4.2	78
141	RNA and its ionic cloud: solution scattering experiments and atomically detailed simulations. <i>Biophysical Journal</i> , 2012 , 102, 819-28	2.9	75
140	Ligand diffusion in globins: simulations versus experiment. <i>Current Opinion in Structural Biology</i> , 2010 , 20, 162-7	8.1	72
139	Yet another look at the steepest descent path. <i>Computational and Theoretical Chemistry</i> , 1997 , 398-399, 63-71		68
138	SSALN: an alignment algorithm using structure-dependent substitution matrices and gap penalties learned from structurally aligned protein pairs. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006 , 62, 881-91	4.2	68
137	Temperature dependent reaction coordinates. <i>Journal of Chemical Physics</i> , 2000 , 112, 5539-5545	3.9	66
136	Computational studies of ligand diffusion in globins: I. Leghemoglobin. <i>Proteins: Structure, Function and Bioinformatics</i> , 1991 , 10, 70-80	4.2	64
135	Sodium in gramicidin: an example of a permion. <i>Biophysical Journal</i> , 1995 , 68, 906-24	2.9	62
134	Revisiting and computing reaction coordinates with Directional Milestoning. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 6137-48	2.8	61

133	Calculation of the potential of mean force using molecular dynamics with linear constraints: An application to a conformational transition in a solvated dipeptide. <i>Journal of Chemical Physics</i> , 1990 , 93, 4312-4321	3.9	61
132	Reaction path study of conformational transitions and helix formation in a tetrapeptide. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1989 , 86, 6963-7	11.5	60
131	Atomically detailed simulation of the recovery stroke in myosin by Milestoning. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010 , 107, 5001-5	11.5	58
130	The ionic atmosphere around A-RNA: Poisson-Boltzmann and molecular dynamics simulations. <i>Biophysical Journal</i> , 2012 , 102, 829-38	2.9	57
129	Kinetics of helix unfolding: molecular dynamics simulations with milestoning. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 7461-73	2.8	57
128	Distance-dependent, pair potential for protein folding: results from linear optimization. <i>Proteins: Structure, Function and Bioinformatics</i> , 2000 , 41, 40-6	4.2	57
127	Revisiting and parallelizing SHAKE. <i>Journal of Computational Physics</i> , 2005 , 209, 193-206	4.1	55
126	Kinetics of cytochrome C folding: atomically detailed simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003 , 51, 245-57	4.2	52
125	Unassisted transport of N-acetyl-L-tryptophanamide through membrane: experiment and simulation of kinetics. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 2739-50	3.4	51
124	A Stochastic Algorithm for the Isobaric-Isothermal Ensemble with Ewald Summations for All Long Range Forces. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5624-37	6.4	48
123	Perspective: Computer simulations of long time dynamics. <i>Journal of Chemical Physics</i> , 2016 , 144, 060901	3.9	46
122	Locally enhanced sampling in free energy calculations: Application of mean field approximation to accurate calculation of free energy differences. <i>Journal of Chemical Physics</i> , 1992 , 97, 7838-7841	3.9	44
121	A coarse-grained potential for fold recognition and molecular dynamics simulations of proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009 , 76, 822-36	4.2	43
120	MOIL-opt: Energy-Conserving Molecular Dynamics on a GPU/CPU system. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 3072-3082	6.4	42
119	Unit-vector RMS (URMS) as a tool to analyze molecular dynamics trajectories. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999 , 37, 554-564	4.2	41
118	The network of sequence flow between protein structures. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007 , 104, 11627-32	11.5	40
117	PIE-efficient filters and coarse grained potentials for unbound protein-protein docking. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010 , 78, 400-19	4.2	39
116	Atomically detailed potentials to recognize native and approximate protein structures. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005 , 61, 44-55	4.2	38

115	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. <i>Journal of Chemical Physics</i> , 1993 , 98, 3380-3388	3.9	38
114	A new paradigm for atomically detailed simulations of kinetics in biophysical systems. <i>Quarterly Reviews of Biophysics</i> , 2017 , 50, e8	7	37
113	Improving ranking of models for protein complexes with side chain modeling and atomic potentials. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013 , 81, 592-606	4.2	37
112	SHAKE parallelization. <i>European Physical Journal: Special Topics</i> , 2011 , 200, 211-223	2.3	36
111	Simulations of allosteric transitions. <i>Current Opinion in Structural Biology</i> , 2011 , 21, 167-72	8.1	35
110	Membrane permeation of a peptide: it is better to be positive. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 6412-20	3.4	32
109	Toward quantitative simulations of carbon monoxide escape pathways in myoglobin. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 6147-54	3.4	32
108	Computational study of peptide permeation through membrane: Searching for hidden slow variables. <i>Molecular Physics</i> , 2013 , 111, 3565-3578	1.7	31
107	Enzymatic circularization of a malto-octaose linear chain studied by stochastic reaction path calculations on cyclodextrin glycosyltransferase. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001 , 43, 327-35	4.2	31
106	Computer determination of peptide conformations in water: different roads to structure. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1995 , 92, 3190-3	11.5	31
105	Calculating Iso-Committer Surfaces as Optimal Reaction Coordinates with Milestoning. <i>Entropy</i> , 2017 , 19,	2.8	30
104	Modeling kinetics and equilibrium of membranes with fields: milestoning analysis and implication to permeation. <i>Journal of Chemical Physics</i> , 2014 , 141, 054101	3.9	30
103	Calculations of a list of neighbors in Molecular Dynamics simulations. <i>Journal of Computational Chemistry</i> , 1989 , 10, 921-927	3.5	29
102	Molecular dynamics study of secondary structure motions in proteins: application to myohemerythrin. <i>Proteins: Structure, Function and Bioinformatics</i> , 1990 , 7, 265-79	4.2	28
101	Ligand binding and conformation change in the dimeric hemoglobin of the clam <i>Scapharca inaequalis</i> . <i>Journal of Biological Chemistry</i> , 1993 , 268, 5711-5718	5.4	28
100	Bridging the Gap between Long Time Trajectories and Reaction Pathways. <i>Advances in Chemical Physics</i> , 2003 , 93-129		27
99	Lifetimes of rotational resonances in molecule-surface scattering. <i>Molecular Physics</i> , 1985 , 55, 1369-1381.	1.7	26
98	DOCK/PIERR: web server for structure prediction of protein-protein complexes. <i>Methods in Molecular Biology</i> , 2014 , 1137, 199-207	1.4	26

97	Ligand binding and conformation change in the dimeric hemoglobin of the clam <i>Scapharca inaequalvis</i> . <i>Journal of Biological Chemistry</i> , 1993 , 268, 5711-8	5.4	25
96	Enzyme Selectivity of HIV Reverse Transcriptase: Conformations, Ligands, and Free Energy Partition. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 11513-26	3.4	24
95	Catch bond-like kinetics of helix cracking: network analysis by molecular dynamics and milestoning. <i>Journal of Chemical Physics</i> , 2013 , 139, 121902	3.9	23
94	Building and assessing atomic models of proteins from structural templates: learning and benchmarks. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009 , 76, 930-45	4.2	23
93	Revealing the distinct folding phases of an RNA three-helix junction. <i>Nucleic Acids Research</i> , 2018 , 46, 7354-7365	20.1	23
92	The Impact of Protonation on Early Translocation of Anthrax Lethal Factor: Kinetics from Molecular Dynamics Simulations and Milestoning Theory. <i>Journal of the American Chemical Society</i> , 2017 , 139, 14837-14840	16.4	22
91	Measurement of the membrane dipole electric field in DMPC vesicles using vibrational shifts of p-cyanophenylalanine and molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 2869-76	3.4	22
90	Maximum feasibility guideline in the design and analysis of protein folding potentials. <i>Journal of Computational Chemistry</i> , 2002 , 23, 111-8	3.5	21
89	Experiments and comprehensive simulations of the formation of a helical turn. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 6598-610	3.4	20
88	Chemical Development of Latent Fingerprints: Computational Design of Ninhydrin Analogues. <i>Journal of Forensic Sciences</i> , 2000 , 45, 14767J	1.8	20
87	Early events in helix unfolding under external forces: a milestoning analysis. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 8662-91	3.4	19
86	Computational exploration of the network of sequence flow between protein structures. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010 , 78, 985-1003	4.2	19
85	Calculation of Point-to-Point Short-Time and Rare Trajectories with Boundary Value Formulation. <i>Journal of Chemical Theory and Computation</i> , 2006 , 2, 484-94	6.4	19
84	Revisiting Molecular Dynamics on a CPU/GPU system: Water Kernel and SHAKE Parallelization. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 4624-4636	6.4	18
83	Analyzing milestoning networks for molecular kinetics: definitions, algorithms, and examples. <i>Journal of Chemical Physics</i> , 2013 , 139, 174105	3.9	17
82	A template-finding algorithm and a comprehensive benchmark for homology modeling of proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008 , 72, 910-28	4.2	17
81	Large-scale linear programming techniques for the design of protein folding potentials. <i>Mathematical Programming</i> , 2004 , 101, 301	2.1	17
80	Coiled-coil response to mechanical force: global stability and local cracking. <i>Biophysical Journal</i> , 2013 , 105, 951-61	2.9	16

79	Physiological Calcium Concentrations Slow Dynamics at the Lipid-Water Interface. <i>Biophysical Journal</i> , 2018 , 115, 1541-1551	2.9	16
78	Milestoning: An Efficient Approach for Atomically Detailed Simulations of Kinetics in Biophysics. <i>Annual Review of Biophysics</i> , 2020 , 49, 69-85	21.1	15
77	2020 ,		15
76	Computational analysis of sequence selection mechanisms. <i>Structure</i> , 2004 , 12, 547-57	5.2	15
75	Molecular dynamics studies of modular polyketide synthase ketoreductase stereospecificity. <i>Biochemistry</i> , 2015 , 54, 2346-59	3.2	14
74	Ion Permeation through a Phospholipid Membrane: Transition State, Path Splitting, and Calculation of Permeability. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 720-730	6.4	14
73	A MATHEMATICAL FRAMEWORK FOR EXACT MILESTONING. <i>Multiscale Modeling and Simulation</i> , 2016 , 14, 301-322	1.8	13
72	Homology as a Tool in Optimization Problems: Structure Determination of 2D Heteropolymers. <i>The Journal of Physical Chemistry</i> , 1995 , 99, 11550-11556		13
71	Why Does RNA Collapse? The Importance of Water in a Simulation Study of Helix-Junction-Helix Systems. <i>Journal of the American Chemical Society</i> , 2018 , 140, 16948-16951	16.4	13
70	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. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 3424-3436	3.4	12
69	Extracting the diffusion tensor from molecular dynamics simulation with Milestoning. <i>Journal of Chemical Physics</i> , 2015 , 142, 014105	3.9	12
68	The energy landscape of a protein switch. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 6407-21	3.6	12
67	Energy design for protein-protein interactions. <i>Journal of Chemical Physics</i> , 2011 , 135, 065102	3.9	12
66	Markovian and Non-Markovian Modeling of Membrane Dynamics with Milestoning. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 8208-16	3.4	12
65	Pyrophosphate Release in the Protein HIV Reverse Transcriptase. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 9557-9565	3.4	11
64	Extension of a protein docking algorithm to membranes and applications to amyloid precursor protein dimerization. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015 , 83, 2170-85	4.2	11
63	Super folds, networks, and barriers. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012 , 80, 463-70	4.2	11
62	The transition between active and inactive conformations of Abl kinase studied by rock climbing and Milestoning. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2020 , 1864, 129508	4	11

61	Comprehensive analysis of sequences of a protein switch. <i>Protein Science</i> , 2016 , 25, 135-46	6.3	11
60	Simulations of thermodynamics and kinetics on rough energy landscapes with milestoning. <i>Journal of Computational Chemistry</i> , 2016 , 37, 602-13	3.5	9
59	Conformations of an RNA Helix-Junction-Helix Construct Revealed by SAXS Refinement of MD Simulations. <i>Biophysical Journal</i> , 2019 , 116, 19-30	2.9	9
58	A mixed alchemical and equilibrium dynamics to simulate heterogeneous dense fluids: Illustrations for Lennard-Jones mixtures and phospholipid membranes. <i>Journal of Chemical Physics</i> , 2018 , 149, 072323-9	3.9	9
57	Molecular machines. <i>Current Opinion in Structural Biology</i> , 2013 , 23, 206-11	8.1	8
56	Computer Simulations of the Dissociation Mechanism of Gleevec from Abl Kinase with Milestoning. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 5706-5715	3.4	8
55	Rock climbing: A local-global algorithm to compute minimum energy and minimum free energy pathways. <i>Journal of Chemical Physics</i> , 2017 , 147, 152718	3.9	7
54	Thermodynamic Cycle Without Turning Off Self-Interactions: Formal Discussion and a Numerical Example. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 3022-3033	6.4	7
53	REACTION PATH STUDIES OF BIOLOGICAL MOLECULES. <i>Advanced Series in Physical Chemistry</i> , 1996 , 65-136		7
52	Preferential Equilibrium Partitioning of Positively Charged Tryptophan into Phosphatidylcholine Bilayer Membranes. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 170-179	3.4	7
51	Interfacial Dynamics in Lipid Membranes: The Effects of Headgroup Structures. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 1343-1350	3.4	7
50	Long-time methods for molecular dynamics simulations: Markov State Models and Milestoning. <i>Progress in Molecular Biology and Translational Science</i> , 2020 , 170, 215-237	4	6
49	The evolutionary capacity of protein structures 2004 ,		6
48	Exploring the Reaction Mechanism of HIV Reverse Transcriptase with a Nucleotide Substrate. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 4270-4283	3.4	5
47	Calcium-Lipid Interactions Observed with Isotope-Edited Infrared Spectroscopy. <i>Biophysical Journal</i> , 2020 , 118, 2694-2702	2.9	5
46	Computer simulations of a heterogeneous membrane with enhanced sampling techniques. <i>Journal of Chemical Physics</i> , 2020 , 153, 144110	3.9	5
45	Protein Recognition by Sequence-to-Structure Fitness: Bridging Efficiency and Capacity of Threading Models. <i>Advances in Chemical Physics</i> , 2002 , 77-130		4
44	Probing Translocation in Mutants of the Anthrax Channel: Atomically Detailed Simulations with Milestoning. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 10296-10305	3.4	4

43	Defect-Assisted Permeation Through a Phospholipid Membrane: Experimental and Computational Study of the Peptide WKW. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 6792-6798	3.4	3
42	Probing the role of local propensity in peptide turn formation. <i>International Journal of Quantum Chemistry</i> , 2000 , 80, 1125-1128	2.1	3
41	Value of Temporal Information When Analyzing Reaction Coordinates. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 6077-6090	6.4	3
40	Partition of Positively and Negatively Charged Tryptophan Ions in Membranes with Inverted Phospholipid Heads: Simulations and Experiments. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 3272-3281	3.4	2
39	Phase Transition in a Heterogeneous Membrane: Atomically Detailed Picture. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 5263-5267	6.4	2
38	Milestoning with wind: Exploring the impact of a biasing potential in exact calculation of kinetics. <i>Journal of Chemical Physics</i> , 2020 , 152, 224105	3.9	2
37	ScMile: A Script to Investigate Kinetics with Short Time Molecular Dynamics Trajectories and the Milestoning Theory. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 860-874	6.4	2
36	Dramatic Shape Changes Occur as Cytochrome Folds. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 8240-8248	3.4	2
35	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. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 9547-9556	3.4	2
34	From an SNP to a Disease: A Comprehensive Statistical Analysis. <i>Structure</i> , 2015 , 23, 1155	5.2	1
33	Molecular Dynamics at Extended Timescales. <i>Israel Journal of Chemistry</i> , 2014 , 54, 1302-1310	3.4	1
32	9.2 Coarse-Grained Methods: Theory 2012 , 2-26		1
31	Chapter 6: Enhancing the Capacity of Molecular Dynamics Simulations with Trajectory Fragments. <i>RSC Biomolecular Sciences</i> , 2012 , 117-137		1
30	Progress at last. <i>Structure</i> , 2011 , 19, 1725	5.2	1
29	Modeling molecular kinetics with Milestoning. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021 , 11, e1512	7.9	1
28	Unit-vector RMS (URMS) as a tool to analyze molecular dynamics trajectories 1999 , 37, 554		1
27	Unit-vector RMS (URMS) as a tool to analyze molecular dynamics trajectories 1999 , 37, 554		1
26	Chemical development of latent fingerprints: computational design of ninhydrin analogues. <i>Journal of Forensic Sciences</i> , 2000 , 45, 757-60	1.8	1

- 25 Watching biomolecular machines in action. *Structure*, **2010**, 18, 415-6 5.2 ○
- 24 A new boundary driven NEMD scheme for heat and particle diffusion in binary mixtures. *Molecular Physics*, e1892849 1.7 ○
- 23 Catalytic Magnesium as a Door Stop for DNA Sliding. *Journal of Physical Chemistry B*, **2021**, 125, 3494-3504 3.0 ○
- 22 Simple and Analytical Model of RNA Collapse. *Journal of Physical Chemistry B*, **2020**, 124, 5149-5155 3.4
- 21 Two is a pair, three is a network. *Biophysical Journal*, **2015**, 108, 22 2.9
- 20 The Schrödinger Representation **2020**, 41-47
- 19 A Simple Numerical Example of Rate Calculations **2020**, 223-231
- 18 Path Integrals **2020**, 63-67
- 17 Rare Events and Reaction Coordinates **2020**, 233-240
- 16 The Master Equation as a Model for Transitions Between Macrostates **2020**, 203-212
- 15 Barrier Crossing **2020**, 69-87
- 14 An Example of the Use of Cells **2020**, 255-257
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- 8 Discrete Systems **2020**, 49-61

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6 Celling **2020**, 241-253

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4 The Langevin Equation and Stochastic Processes **2020**, 1-27

3 Diffusive Dynamics on a Multidimensional Energy Landscape **2020**, 157-171

2 Sampling Transition Paths **2020**, 89-115

1 Dynamics of induced-fit in HIV reverse transcriptase specificity and resistance. *FASEB Journal*, **2012**, 26, 964.5

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