Ron Elber

List of Publications by Year
in descending order

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153	10,024	46918	38300
papers	citations	47 h-index	95 g-index

181	181	181	6972
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	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
3	Modeling molecular kinetics with Milestoning. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1512.	6.2	10
4	Interfacial Dynamics in Lipid Membranes: The Effects of Headgroup Structures. Journal of Physical Chemistry B, 2021, 125, 1343-1350.	1.2	23
5	A new boundary driven NEMD scheme for heat and particle diffusion in binary mixtures. Molecular Physics, 2021, 119, .	0.8	6
6	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
7	Catalytic Magnesium as a Door Stop for DNA Sliding. Journal of Physical Chemistry B, 2021, 125, 3494-3500.	1.2	3
8	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
9	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
10	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
11	Computer simulations of a heterogeneous membrane with enhanced sampling techniques. Journal of Chemical Physics, 2020, 153, 144110.	1.2	10
12	Dramatic Shape Changes Occur as Cytochrome c Folds. Journal of Physical Chemistry B, 2020, 124, 8240-8248.	1.2	4
13	Value of Temporal Information When Analyzing Reaction Coordinates. Journal of Chemical Theory and Computation, 2020, 16, 6077-6090.	2.3	9
14	Exploring the Reaction Mechanism of HIV Reverse Transcriptase with a Nucleotide Substrate. Journal of Physical Chemistry B, 2020, 124, 4270-4283.	1.2	7
15	Simple and Analytical Model of RNA Collapse. Journal of Physical Chemistry B, 2020, 124, 5149-5155.	1.2	0
16	Milestoning: An Efficient Approach for Atomically Detailed Simulations of Kinetics in Biophysics. Annual Review of Biophysics, 2020, 49, 69-85.	4.5	46
17	Phase Transition in a Heterogeneous Membrane: Atomically Detailed Picture. Journal of Physical Chemistry Letters, 2020, 11, 5263-5267.	2.1	5
18	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

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19	Calcium-Lipid Interactions Observed with Isotope-Edited Infrared Spectroscopy. Biophysical Journal, 2020, 118, 2694-2702.	0.2	9
20	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
21	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
22	Partition of Positively and Negatively Charged Tryptophan Ions in Membranes with Inverted Phospholipid Heads: Simulations and Experiments. Journal of Physical Chemistry B, 2019, 123, 3272-3281.	1.2	5
23	Preferential Equilibrium Partitioning of Positively Charged Tryptophan into Phosphatidylcholine Bilayer Membranes. Journal of Physical Chemistry B, 2019, 123, 170-179.	1.2	13
24	Conformations of an RNA Helix-Junction-Helix Construct Revealed by SAXS Refinement of MD Simulations. Biophysical Journal, 2019, 116, 19-30.	0.2	16
25	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
26	Why Does RNA Collapse? The Importance of Water in a Simulation Study of Helixâ€“Junctionâ€“Helix Systems. Journal of the American Chemical Society, 2018, 140, 16948-16951.	6.6	19
27	Physiological Calcium Concentrations Slow Dynamics at the Lipid-Water Interface. Biophysical Journal, 2018, 115, 1541-1551.	0.2	30
28	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
29	Revealing the distinct folding phases of an RNA three-helix junction. Nucleic Acids Research, 2018, 46, 7354-7365.	6.5	38
30	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
31	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
32	A new paradigm for atomically detailed simulations of kinetics in biophysical systems. Quarterly Reviews of Biophysics, 2017, 50, e8.	2.4	49
33	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
34	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
35	Pyrophosphate Release in the Protein HIV Reverse Transcriptase. Journal of Physical Chemistry B, 2017, 121, 9557-9565.	1.2	15
36	Calculating Iso-Committor Surfaces as Optimal Reaction Coordinates with Milestoning. Entropy, 2017, 19, 219.	1.1	51

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37	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
38	Simulations of thermodynamics and kinetics on rough energy landscapes with milestoning. Journal of Computational Chemistry, 2016, 37, 602-613.	1.5	11
39	Perspective: Computer simulations of long time dynamics. Journal of Chemical Physics, 2016, 144, 060901.	1.2	54
40	Markovian and Non-Markovian Modeling of Membrane Dynamics with Milestoning. Journal of Physical Chemistry B, 2016, 120, 8208-8216.	1.2	16
41	Comprehensive analysis of sequences of a protein switch. Protein Science, 2016, 25, 135-146.	3.1	20
42	A Mathematical Framework for Exact Milestoning. Multiscale Modeling and Simulation, 2016, 14, 301-322.	0.6	19
43	Exact milestoning. Journal of Chemical Physics, 2015, 142, 094102.	1.2	100
44	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
45	Measurement of the Membrane Dipole Electric Field in DMPC Vesicles Using Vibrational Shifts of p-Cyanophenylalanine and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2015, 119, 2869-2876.	1.2	24
46	Two Is a Pair, Three Is a Network. Biophysical Journal, 2015, 108, 22.	0.2	0
47	From an SNP to a Disease: A Comprehensive Statistical Analysis. Structure, 2015, 23, 1155.	1.6	2
48	Molecular Dynamics Studies of Modular Polyketide Synthase Ketoreductase Stereospecificity. Biochemistry, 2015, 54, 2346-2359.	1.2	15
49	Membrane Permeation of a Peptide: It Is Better to be Positive. Journal of Physical Chemistry B, 2015, 119, 6412-6420.	1.2	44
50	Enzyme Selectivity of HIV Reverse Transcriptase: Conformations, Ligands, and Free Energy Partition. Journal of Physical Chemistry B, 2015, 119, 11513-11526.	1.2	28
51	Extracting the diffusion tensor from molecular dynamics simulation with Milestoning. Journal of Chemical Physics, 2015, 142, 014105.	1.2	14
52	A Stochastic Algorithm for the Isobaricâ€“Isothermal Ensemble with Ewald Summations for All Long Range Forces. Journal of Chemical Theory and Computation, 2015, 11, 5624-5637.	2.3	114
53	Modeling kinetics and equilibrium of membranes with fields: Milestoning analysis and implication to permeation. Journal of Chemical Physics, 2014, 141, 054101.	1.2	33
54	Molecular Dynamics at Extended Timescales. Israel Journal of Chemistry, 2014, 54, 1302-1310.	1.0	1

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55	The energy landscape of a protein switch. Physical Chemistry Chemical Physics, 2014, 16, 6407.	1.3	21
56	DOCK/PIERR: Web Server for Structure Prediction of Proteinâ€“Protein Complexes. Methods in Molecular Biology, 2014, 1137, 199-207.	0.4	26
57	Computational study of peptide permeation through membrane: searching for hidden slow variables. Molecular Physics, 2013, 111, 3565-3578.	0.8	37
58	Coiled-Coil Response to Mechanical Force: Global Stability and Local Cracking. Biophysical Journal, 2013, 105, 951-961.	0.2	20
59	Molecular machines. Current Opinion in Structural Biology, 2013, 23, 206-211.	2.6	11
60	Reaction Paths and Rates. , 2013, , 2186-2191.		0
61	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
62	Catch bond-like kinetics of helix cracking: Network analysis by molecular dynamics and Milestoning. Journal of Chemical Physics, 2013, 139, 121902.	1.2	25
63	Analyzing milestoning networks for molecular kinetics: Definitions, algorithms, and examples. Journal of Chemical Physics, 2013, 139, 174105.	1.2	20
64	9.2 Coarse-Grained Methods: Theory. , 2012, , 2-26.		1
65	Experiments and Comprehensive Simulations of the Formation of a Helical Turn. Journal of Physical Chemistry B, 2012, 116, 6598-6610.	1.2	22
66	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
67	Early Events in Helix Unfolding under External Forces: A Milestoning Analysis. Journal of Physical Chemistry B, 2012, 116, 8662-8691.	1.2	22
68	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
69	The Ionic Atmosphere around A-RNA: Poisson-Boltzmann and Molecular Dynamics Simulations. Biophysical Journal, 2012, 102, 829-838.	0.2	68
70	RNA and Its Ionic Cloud: Solution Scattering Experiments and Atomically Detailed Simulations. Biophysical Journal, 2012, 102, 819-828.	0.2	89
71	Chapter 6. Enhancing the Capacity of Molecular Dynamics Simulations with Trajectory Fragments. RSC Biomolecular Sciences, 2012, , 117-137.	0.4	1
72	Super folds, networks, and barriers. Proteins: Structure, Function and Bioinformatics, 2012, 80, 463-470.	1.5	11

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73	Unassisted Transport of N-Acetyl-<scp>l</scp>-tryptophanamide through Membrane: Experiment and Simulation of Kinetics. Journal of Physical Chemistry B, 2012, 116, 2739-2750.	1.2	59
74	How Conformational Dynamics of DNA Polymerase Select Correct Substrates: Experiments and Simulations. Structure, 2012, 20, 618-627.	1.6	107
75	Dynamics of inducedâ€fit in HIV reverse transcriptase specificity and resistance. FASEB Journal, 2012, 26, 964.5.	0.2	0
76	Revisiting and Computing Reaction Coordinates with Directional Milestoning. Journal of Physical Chemistry A, 2011, 115, 6137-6148.	1.1	74
77	MOIL-opt: Energy-Conserving Molecular Dynamics on a GPU/CPU System. Journal of Chemical Theory and Computation, 2011, 7, 3072-3082.	2.3	47
78	Progress at Last. Structure, 2011, 19, 1725.	1.6	1
79	Simulations of allosteric transitions. Current Opinion in Structural Biology, 2011, 21, 167-172.	2.6	43
80	SHAKE parallelization. European Physical Journal: Special Topics, 2011, 200, 211-223.	1.2	71
81	Energy design for protein-protein interactions. Journal of Chemical Physics, 2011, 135, 065102.	1.2	13
82	Ligand diffusion in globins: simulations versus experiment. Current Opinion in Structural Biology, 2010, 20, 162-167.	2.6	76
83	Watching Biomolecular Machines in Action. Structure, 2010, 18, 415-416.	1.6	1
84	PIEâ€"Efficient filters and coarse grained potentials for unbound proteinâ€"protein docking. Proteins: Structure, Function and Bioinformatics, 2010, 78, 400-419.	1.5	53
85	Computational exploration of the network of sequence flow between protein structures. Proteins: Structure, Function and Bioinformatics, 2010, 78, 985-1003.	1.5	22
86	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
87	Milestoning without a Reaction Coordinate. Journal of Chemical Theory and Computation, 2010, 6, 1805-1817.	2.3	100
88	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
89	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
90	Kinetics of Helix Unfolding: Molecular Dynamics Simulations with Milestoning. Journal of Physical Chemistry A, 2009, 113, 7461-7473.	1.1	63

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91	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
92	Toward Quantitative Simulations of Carbon Monoxide Escape Pathways in Myoglobin. Journal of Physical Chemistry B, 2008, 112, 6147-6154.	1.2	32
93	On the assumptions underlying milestoning. Journal of Chemical Physics, 2008, 129, 174102.	1.2	158
94	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
95	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
96	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
97	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
98	Revisiting and parallelizing SHAKE. Journal of Computational Physics, 2005, 209, 193-206.	1.9	66
99	Long-timescale simulation methods. Current Opinion in Structural Biology, 2005, 15, 151-156.	2.6	154
100	Atomically detailed potentials to recognize native and approximate protein structures. Proteins: Structure, Function and Bioinformatics, 2005, 61, 44-55.	1.5	43
101	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
102	Computing time scales from reaction coordinates by milestoning. Journal of Chemical Physics, 2004, 120, 10880-10889.	1.2	563
103	The evolutionary capacity of protein structures. , 2004, , .		6
104	Computational Analysis of Sequence Selection Mechanisms. Structure, 2004, 12, 547-557.	1.6	15
105	Large-scale linear programming techniques for the design of protein folding potentials. Mathematical Programming, 2004, 101, 301.	1.6	21
106	Kinetics of cytochrome C folding: Atomically detailed simulations. Proteins: Structure, Function and Bioinformatics, 2003, 51, 245-257.	1.5	57
107	Enriching the sequence substitution matrix by structural information. Proteins: Structure, Function and Bioinformatics, 2003, 54, 41-48.	1.5	87
108	Bridging the Gap between Long Time Trajectories and Reaction Pathways. Advances in Chemical Physics, 2003, , 93-129.	0.3	37

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109	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
110	Long Time Dynamics of Complex Systems. Accounts of Chemical Research, 2002, 35, 396-403.	7.6	101
111	Protein Recognition by Sequence-to-Structure Fitness: Bridging Efficiency and Capacity of Threading Models. Advances in Chemical Physics, 2002, , 77-130.	0.3	10
112	Maximum feasibility guideline in the design and analysis of protein folding potentials. Journal of Computational Chemistry, 2002, 23, 111-118.	1.5	24
113	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
114	Linear programming optimization and a double statistical filter for protein threading protocols. Proteins: Structure, Function and Bioinformatics, 2001, 45, 241-261.	1.5	117
115	On the design and analysis of protein folding potentials. , 2000, 40, 71-85.		107
116	Distance-dependent, pair potential for protein folding: Results from linear optimization. Proteins: Structure, Function and Bioinformatics, 2000, 41, 40-46.	1.5	172
117	Probing the role of local propensity in peptide turn formation. International Journal of Quantum Chemistry, 2000, 80, 1125-1128.	1.0	3
118	Temperature dependent reaction coordinates. Journal of Chemical Physics, 2000, 112, 5539-5545.	1.2	71
119	fw2.2: A Quantitative Trait Locus Key to the Evolution of Tomato Fruit Size. Science, 2000, 289, 85-88.	6.0	1,290
120	Chemical Development of Latent Fingerprints: Computational Design of Ninhydrin Analogues. Journal of Forensic Sciences, 2000, 45, 757-760.	0.9	22
121	Chemical development of latent fingerprints: computational design of ninhydrin analogues. Journal of Forensic Sciences, 2000, 45, 757-60.	0.9	2
122	Distance-dependent, pair potential for protein folding: results from linear optimization. Proteins: Structure, Function and Bioinformatics, 2000, 41, 40-6.	1.5	64
123	Unit-vector RMS (URMS) as a tool to analyze molecular dynamics trajectories. Proteins: Structure, Function and Bioinformatics, 1999, 37, 554-564.	1.5	47
124	Stochastic Path Approach to Compute Atomically Detailed Trajectories:â€‰ Application to the Folding of C Peptide. Journal of Physical Chemistry B, 1999, 103, 899-911.	1.2	104
125	Unit-vector RMS (URMS) as a tool to analyze molecular dynamics trajectories. , 1999, 37, 554.		1
126	Unit-vector RMS (URMS) as a tool to analyze molecular dynamics trajectories. , 1999, 37, 554.		1

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127	Dynamics of peptide folding. , 1998, , .		0
128	Yet another look at the steepest descent path. Computational and Theoretical Chemistry, 1997, 398-399, 63-71.	1.5	72
129	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
130	REACTION PATH STUDIES OF BIOLOGICAL MOLECULES. Advanced Series in Physical Chemistry, 1996, , 65-136.	1.5	9
131	MOIL: A program for simulations of macromolecules. Computer Physics Communications, 1995, 91, 159-189.	3.0	154
132	Homology as a Tool in Optimization Problems: Structure Determination of 2D Heteropolymers. The Journal of Physical Chemistry, 1995, 99, 11550-11556.	2.9	14
133	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
134	Sodium in gramicidin: an example of a permion. Biophysical Journal, 1995, 68, 906-924.	0.2	67
135	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
136	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
137	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
138	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
139	Conformational Transitions. AIP Conference Proceedings, 1991, , .	0.3	2
140	Computational studies of ligand diffusion in globins: I. Leghemoglobin. Proteins: Structure, Function and Bioinformatics, 1991, 10, 70-80.	1.5	64
141	Reaction path study of helix formation in tetrapeptides: Effect of side chains. Journal of Chemical Physics, 1991, 94, 751-760.	1.2	134
142	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
143	Molecular dynamics study of secondary structure motion in proteins: Application to myohemerythrin. Proteins: Structure, Function and Bioinformatics, 1990, 7, 265-279.	1.5	30
144	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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145	A new technique to calculate steepest descent paths in flexible polyatomic systems. Journal of Chemical Physics, 1990, 92, 1510-1511.	1.2	264
146	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
147	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
148	Reaction path study of conformational transitions in flexible systems: Applications to peptides. Journal of Chemical Physics, 1990, 92, 5580-5601.	1.2	254
149	Calculations of a list of neighbors in Molecular Dynamics simulations. Journal of Computational Chemistry, 1989, 10, 921-927.	1.5	34
150	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
151	A method for determining reaction paths in large molecules: Application to myoglobin. Chemical Physics Letters, 1987, 139, 375-380.	1.2	392
152	Multiple conformational states of proteins: a molecular dynamics analysis of myoglobin. Science, 1987, 235, 318-321.	6.0	659
153	Lifetimes of rotational resonances in molecule-surface scattering. Molecular Physics, 1985, 55, 1369-1381.	0.8	26