

# Klaus Schulten

## List of Publications by Year in descending order

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154  
papers

81,327  
citations

18887

64  
h-index

14386

132  
g-index

158  
all docs

158  
docs citations

158  
times ranked

75560  
citing authors

#	ARTICLE	IF	CITATIONS
1	Scalable molecular dynamics on CPU and GPU architectures with NAMD. <i>Journal of Chemical Physics</i> , 2020, 153, 044130.	1.2	1,548
2	<i>In Situ</i> Conformational Changes of the Escherichia coli Serine Chemoreceptor in Different Signaling States. <i>MBio</i> , 2019, 10, .	1.8	29
3	Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism. <i>Cell</i> , 2019, 179, 1098-1111.e23.	13.5	122
4	Fast pressure-jump all-atom simulations and experiments reveal site-specific protein dehydration-folding dynamics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 5356-5361.	3.3	10
5	NAMD goes quantum: an integrative suite for hybrid simulations. <i>Nature Methods</i> , 2018, 15, 351-354.	9.0	149
6	All-atom molecular dynamics of the HBV capsid reveals insights into biological function and cryo-EM resolution limits. <i>ELife</i> , 2018, 7, .	2.8	92
7	Mechanism for the Regulated Control of Bacterial Transcription Termination by a Universal Adaptor Protein. <i>Molecular Cell</i> , 2018, 71, 911-922.e4.	4.5	65
8	Free-energy simulations reveal molecular mechanism for functional switch of a DNA helicase. <i>ELife</i> , 2018, 7, .	2.8	15
9	Flexible Fitting of Atomic Structures into Electron Microscopy Maps Using Molecular Dynamics. <i>journal of hand surgery Asian-Pacific volume, The</i> , 2018, , 433-443.	0.2	0
10	Structural characterization of mRNA-tRNA translocation intermediates. <i>journal of hand surgery Asian-Pacific volume, The</i> , 2018, , 450-455.	0.2	0
11	Quantitative Characterization of Domain Motions in Molecular Machines. <i>journal of hand surgery Asian-Pacific volume, The</i> , 2018, , 532-541.	0.2	0
12	Computational de novo design of antibodies binding to a peptide with high affinity. <i>Biotechnology and Bioengineering</i> , 2017, 114, 1331-1342.	1.7	25
13	Quantitative Characterization of Domain Motions in Molecular Machines. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3747-3756.	1.2	10
14	Permeability of a Fluid Lipid Bilayer to Short-Chain Alcohols from First Principles. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2523-2532.	2.3	33
15	Lateral Segregation of Photosystem I in Cyanobacterial Thylakoids. <i>Plant Cell</i> , 2017, 29, 1119-1136.	3.1	54
16	Chemomechanical Coupling in Hexameric Proteinâ€“Protein Interfaces Harnesses Energy within V-Type ATPases. <i>Journal of the American Chemical Society</i> , 2017, 139, 293-310.	6.6	44
17	CHARMM-GUI MDFF/xMDFF Utilizer for Molecular Dynamics Flexible Fitting Simulations in Various Environments. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3718-3723.	1.2	24
18	CryoEM structure of MxB reveals a novel oligomerization interface critical for HIV restriction. <i>Science Advances</i> , 2017, 3, e1701264.	4.7	47

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19	Physical properties of the HIV-1 capsid from all-atom molecular dynamics simulations. Nature Communications, 2017, 8, 15959.	5.8	136
20	Constant-pH Molecular Dynamics Simulations for Large Biomolecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5933-5944.	2.3	139
21	Overall energy conversion efficiency of a photosynthetic vesicle. ELife, 2016, 5, .	2.8	63
22	The Water Permeability and Pore Entrance Structure of Aquaporin-4 Depend on Lipid Bilayer Thickness. Biophysical Journal, 2016, 111, 90-99.	0.2	20
23	Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering. , 2016, 2016, 1048-1057.		22
24	Cyclophilin A stabilizes the HIV-1 capsid through a novel non-canonical binding site. Nature Communications, 2016, 7, 10714.	5.8	126
25	Electrically Tunable Quenching of DNA Fluctuations in Biased Solid-State Nanopores. ACS Nano, 2016, 10, 4482-4488.	7.3	22
26	Contributions of Charged Residues in Structurally Dynamic Capsid Surface Loops to Rous Sarcoma Virus Assembly. Journal of Virology, 2016, 90, 5700-5714.	1.5	12
27	Disulfide Bridges: Bringing Together Frustrated Structure in a Bioactive Peptide. Biophysical Journal, 2016, 110, 1744-1752.	0.2	27
28	All-Atom Molecular Dynamics of Virus Capsids as Drug Targets. Journal of Physical Chemistry Letters, 2016, 7, 1836-1844.	2.1	73
29	Adaptive Multilevel Splitting Method for Molecular Dynamics Calculation of Benzamidine-Trypsin Dissociation Time. Journal of Chemical Theory and Computation, 2016, 12, 2983-2989.	2.3	80
30	Computational Methodologies for Real-Space Structural Refinement of Large Macromolecular Complexes. Annual Review of Biophysics, 2016, 45, 253-278.	4.5	67
31	High Performance Molecular Visualization: In-Situ and Parallel Rendering with EGL. , 2016, 2016, 1014-1023.		6
32	HIV-1 Capsid Function Is Regulated by Dynamics: Quantitative Atomic-Resolution Insights by Integrating Magic-Angle-Spinning NMR, QM/MM, and MD. Journal of the American Chemical Society, 2016, 138, 14066-14075.	6.6	48
33	Mechanism of the Primary Charge Transfer Reaction in the Cytochrome <i>bc<sub>1</sub></i> Complex. Journal of Physical Chemistry B, 2016, 120, 11369-11380.	1.2	30
34	Binding Site Recognition and Docking Dynamics of a Single Electron Transport Protein: Cytochrome <i>c<sub>2</sub></i> . Journal of the American Chemical Society, 2016, 138, 12077-12089.	6.6	15
35	Conserved methionine dictates substrate preference in Nrapm-family divalent metal transporters. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 10310-10315.	3.3	72
36	Crystal Structure and Conformational Change Mechanism of a Bacterial Nrapm-Family Divalent Metal Transporter. Structure, 2016, 24, 2102-2114.	1.6	56

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37	Evaluation of Emerging Energy-Efficient Heterogeneous Computing Platforms for Biomolecular and Cellular Simulation Workloads. , 2016, 2016, 89-100.		23
38	Early Experiences Porting the NAMD and VMD Molecular Simulation and Analysis Software to GPU-Accelerated OpenPOWER Platforms. Lecture Notes in Computer Science, 2016, 9945, 188-206.	1.0	23
39	QwikMDâ€™â€™â€™Integrative Molecular Dynamics Toolkit for Novices and Experts. Scientific Reports, 2016, 6, 26536.	1.6	153
40	Elucidation of Lipid Binding Sites on Lung Surfactant Protein A Using X-ray Crystallography, Mutagenesis, and Molecular Dynamics Simulations. Biochemistry, 2016, 55, 3692-3701.	1.2	25
41	Structure of the human 26S proteasome at a resolution of 3.9 Å.... Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 7816-7821.	3.3	174
42	Advances in the molecular dynamics flexible fitting method for cryo-EM modeling. Methods, 2016, 100, 50-60.	1.9	82
43	Atomic detail visualization of photosynthetic membranes with GPU-accelerated ray tracing. Parallel Computing, 2016, 55, 17-27.	1.3	37
44	Molecular dynamics-based refinement and validation for sub-5 Å... cryo-electron microscopy maps. ELife, 2016, 5, .	2.8	136
45	Structural Refinement of Proteins by Restrained Molecular Dynamics Simulations with Non-interacting Molecular Fragments. PLoS Computational Biology, 2015, 11, e1004368.	1.5	26
46	CryoEM and computer simulations reveal a novel kinase conformational switch in bacterial chemotaxis signaling. ELife, 2015, 4, .	2.8	106
47	Dynamic allostery governs cyclophilin Aâ€™HIV capsid interplay. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 14617-14622.	3.3	76
48	Atomic Modeling of an Immature Retroviral Lattice Using Molecular Dynamics and Mutagenesis. Structure, 2015, 23, 1414-1425.	1.6	35
49	Macromolecular Crystallography for Synthetic Abiological Molecules: Combining xMDFF and PHENIX for Structure Determination of Cyanostar Macrocycles. Journal of the American Chemical Society, 2015, 137, 8810-8818.	6.6	29
50	Molecular dynamics simulations of large macromolecular complexes. Current Opinion in Structural Biology, 2015, 31, 64-74.	2.6	347
51	The ribosome can discriminate the chirality of amino acids within its peptidyl-transferase center. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 6038-6043.	3.3	73
52	Comparative Dynamics and Sequence Dependence of DNA and RNA Binding to Single Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2015, 119, 10048-10058.	1.5	75
53	Dynamic profiling of double-stranded RNA binding proteins. Nucleic Acids Research, 2015, 43, 7566-7576.	6.5	53
54	Mapping Mechanical Force Propagation through Biomolecular Complexes. Nano Letters, 2015, 15, 7370-7376.	4.5	83

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55	Intrinsic Stepwise Translocation of Stretched ssDNA in Graphene Nanopores. <i>Nano Letters</i> , 2015, 15, 8322-8330.	4.5	47
56	Multilevel Summation Method for Electrostatic Force Evaluation. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 766-779.	2.3	46
57	Structure, function, and quantum dynamics of pigment-protein complexes. , 2014, , 123-143.		3
58	Ultrastable cellulosome-adhesion complex tightens under load. <i>Nature Communications</i> , 2014, 5, 5635.	5.8	92
59	Molecular insights into the membrane-associated phosphatidylinositol 4-kinase III $\beta$ . <i>Nature Communications</i> , 2014, 5, 3552.	5.8	52
60	Assembly of Nsp1 Nucleoporins Provides Insight into Nuclear Pore Complex Gating. <i>PLoS Computational Biology</i> , 2014, 10, e1003488.	1.5	42
61	Petascale Tcl with NAMD, VMD, and Swift/T. , 2014, , .		9
62	Multiple-Replica Strategies for Free-Energy Calculations in NAMD: Multiple-Walker Adaptive Biasing Force and Walker Selection Rules. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5276-5285.	2.3	66
63	Integration of energy and electron transfer processes in the photosynthetic membrane of <i>Rhodobacter sphaeroides</i> . <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2014, 1837, 1769-1780.	0.5	99
64	Structural mechanism of voltage-dependent gating in an isolated voltage-sensing domain. <i>Nature Structural and Molecular Biology</i> , 2014, 21, 244-252.	3.6	228
65	A Highly Tilted Membrane Configuration for the Prefusion State of Synaptobrevin. <i>Biophysical Journal</i> , 2014, 107, 2112-2121.	0.2	34
66	GPU-accelerated analysis and visualization of large structures solved by molecular dynamics flexible fitting. <i>Faraday Discussions</i> , 2014, 169, 265-283.	1.6	37
67	xMDFF: molecular dynamics flexible fitting of low-resolution X-ray structures. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 2344-2355.	2.5	50
68	Calculation of Lipid-Bilayer Permeabilities Using an Average Force. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 554-564.	2.3	57
69	Synaptotagmin's Role in Neurotransmitter Release Likely Involves Ca <sup>2+</sup> -induced Conformational Transition. <i>Biophysical Journal</i> , 2014, 107, 1156-1166.	0.2	42
70	Generalized scalable multiple copy algorithms for molecular dynamics simulations in NAMD. <i>Computer Physics Communications</i> , 2014, 185, 908-916.	3.0	115
71	Macrolide antibiotics allosterically predispose the ribosome for translation arrest. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 9804-9809.	3.3	99
72	Diffusive Models of Membrane Permeation with Explicit Orientational Freedom. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2710-2718.	2.3	43

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73	Light Harvesting by Lamellar Chromatophores in <i>Rhodospirillum rubrum</i> . <i>Biophysical Journal</i> , 2014, 106, 2503-2510.	0.2	48
74	Separation of photo-induced radical pair in cryptochrome to a functionally critical distance. <i>Scientific Reports</i> , 2014, 4, 3845.	1.6	65
75	A structural model of the active ribosome-bound membrane protein insertase YidC. <i>ELife</i> , 2014, 3, e03035.	2.8	69
76	Mature HIV-1 capsid structure by cryo-electron microscopy and all-atom molecular dynamics. <i>Nature</i> , 2013, 497, 643-646.	13.7	712
77	Early experiences scaling VMD molecular visualization and analysis jobs on blue waters. , 2013, , .		17
78	Excited state dynamics in photosynthetic reaction center and light harvesting complex 1. <i>Journal of Chemical Physics</i> , 2012, 137, 065101.	1.2	46
79	GPU/CPU Algorithm for Generalized Born/Solvent-Accessible Surface Area Implicit Solvent Calculations. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2521-2530.	2.3	49
80	Open Quantum Dynamics Calculations with the Hierarchy Equations of Motion on Parallel Computers. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2808-2816.	2.3	157
81	Parallel Generalized Born Implicit Solvent Calculations with NAMD. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3635-3642.	2.3	137
82	Implementation of accelerated molecular dynamics in NAMD. <i>Computational Science &amp; Discovery</i> , 2011, 4, 015002.	1.5	124
83	The Light-Harvesting Apparatus in Purple Photosynthetic Bacteria: Introduction to a Quantum Biological Device. , 2011, , 19-48.		3
84	The effect of correlated bath fluctuations on exciton transfer. <i>Journal of Chemical Physics</i> , 2011, 134, 095102.	1.2	88
85	Applications of the molecular dynamics flexible fitting method. <i>Journal of Structural Biology</i> , 2011, 173, 420-427.	1.3	44
86	High-Performance Scalable Molecular Dynamics Simulations of a Polarizable Force Field Based on Classical Drude Oscillators in NAMD. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 87-92.	2.1	233
87	Cryo-EM structure of the ribosome-â€œSecYE complex in the membrane environment. <i>Nature Structural and Molecular Biology</i> , 2011, 18, 614-621.	3.6	264
88	Symmetry-Restrained Flexible Fitting for Symmetric EM Maps. <i>Structure</i> , 2011, 19, 1211-1218.	1.6	66
89	Stereochemical errors and their implications for molecular dynamics simulations. <i>BMC Bioinformatics</i> , 2011, 12, 190.	1.2	50
90	Förster Energy Transfer Theory as Reflected in the Structures of Photosynthetic Light-Harvesting Systems. <i>ChemPhysChem</i> , 2011, 12, 518-531.	1.0	142

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91	Viewing the Mechanisms of Translation through the Computational Microscope. , 2011, , 142-157.		3
92	GPU-accelerated molecular modeling coming of age. Journal of Molecular Graphics and Modelling, 2010, 29, 116-125.	1.3	336
93	Self-Assembly of Photosynthetic Membranes. ChemPhysChem, 2010, 11, 1154-1159.	1.0	23
94	Challenges in protein-folding simulations. Nature Physics, 2010, 6, 751-758.	6.5	310
95	Energy transfer dynamics in an RC-LH1-PufX tubular photosynthetic membrane. New Journal of Physics, 2010, 12, 085005.	1.2	23
96	Photosynthetic Vesicle Architecture and Constraints on Efficient Energy Harvesting. Biophysical Journal, 2010, 99, 67-75.	0.2	60
97	Ribosome-induced changes in elongation factor Tu conformation control GTP hydrolysis. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 1063-1068.	3.3	219
98	Discovery Through the Computational Microscope. Structure, 2009, 17, 1295-1306.	1.6	302
99	Modeling transport through synthetic nanopores. IEEE Nanotechnology Magazine, 2009, 3, 20-28.	0.9	43
100	Structural model and excitonic properties of the dimeric RC-LH1-PufX complex from Rhodospira rubra. Chemical Physics, 2009, 357, 188-197.	0.9	48
101	Molecular dynamics flexible fitting: A practical guide to combine cryo-electron microscopy and X-ray crystallography. Methods, 2009, 49, 174-180.	1.9	305
102	Protein-Induced Membrane Curvature Investigated through Molecular Dynamics Flexible Fitting. Biophysical Journal, 2009, 97, 321-329.	0.2	68
103	Elucidating the Mechanism behind Irreversible Deformation of Viral Capsids. Biophysical Journal, 2009, 97, 2061-2069.	0.2	94
104	Membrane Curvature Induced by Aggregates of LH2s and Monomeric LH1s. Biophysical Journal, 2009, 97, 2978-2984.	0.2	28
105	Light harvesting complex II B850 excitation dynamics. Journal of Chemical Physics, 2009, 131, 225101.	1.2	136
106	From Atomic-Level Structure to Supramolecular Organization in the Photosynthetic Unit of Purple Bacteria. Advances in Photosynthesis and Respiration, 2009, , 275-294.	1.0	15
107	Flexible Fitting of Atomic Structures into Electron Microscopy Maps Using Molecular Dynamics. Structure, 2008, 16, 673-683.	1.6	833
108	Atomic-level structural and functional model of a bacterial photosynthetic membrane vesicle. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 15723-15728.	3.3	166

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109	Modeling Induction Phenomena in Intermolecular Interactions with an Ab Initio Force Field. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1914-1926.	2.3	34
110	Accelerating molecular modeling applications with graphics processors. <i>Journal of Computational Chemistry</i> , 2007, 28, 2618-2640.	1.5	619
111	Imaging the Migration Pathways for O <sub>2</sub> , CO, NO, and Xe Inside Myoglobin. <i>Biophysical Journal</i> , 2006, 91, 1844-1857.	0.2	258
112	Molecular Dynamics Simulations of the Complete Satellite Tobacco Mosaic Virus. <i>Structure</i> , 2006, 14, 437-449.	1.6	390
113	Scalable molecular dynamics with NAMD. <i>Journal of Computational Chemistry</i> , 2005, 26, 1781-1802.	1.5	15,208
114	Structural dynamics of the lac repressor-DNA complex revealed by a multiscale simulation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 6783-6788.	3.3	135
115	Imaging $\hat{I}_{\pm}$ -Hemolysin with Molecular Dynamics: Ionic Conductance, Osmotic Permeability, and the Electrostatic Potential Map. <i>Biophysical Journal</i> , 2005, 88, 3745-3761.	0.2	620
116	Free energy calculation from steered molecular dynamics simulations using Jarzynski's equality. <i>Journal of Chemical Physics</i> , 2003, 119, 3559-3566.	1.2	712
117	Mechanisms of Selectivity in Channels and Enzymes Studied with Interactive Molecular Dynamics. <i>Biophysical Journal</i> , 2003, 85, 36-48.	0.2	88
118	Reaction paths based on mean first-passage times. <i>Journal of Chemical Physics</i> , 2003, 119, 1313-1319.	1.2	72
119	Robustness and Optimality of Light Harvesting in Cyanobacterial Photosystem I. <i>Journal of Physical Chemistry B</i> , 2002, 106, 7948-7960.	1.2	134
120	General random matrix approach to account for the effect of static disorder on the spectral properties of light harvesting systems. <i>Physical Review E</i> , 2002, 65, 031916.	0.8	62
121	Photosynthetic apparatus of purple bacteria. <i>Quarterly Reviews of Biophysics</i> , 2002, 35, 1-62.	2.4	353
122	Excitons in a photosynthetic light-harvesting system: A combined molecular dynamics, quantum chemistry, and polaron model study. <i>Physical Review E</i> , 2002, 65, 031919.	0.8	261
123	Kinetics of Excitation Migration and Trapping in the Photosynthetic Unit of Purple Bacteria. <i>Journal of Physical Chemistry B</i> , 2001, 105, 8259-8267.	1.2	128
124	Phylogenetic Analysis of Metabolic Pathways. <i>Journal of Molecular Evolution</i> , 2001, 52, 471-489.	0.8	83
125	A system for interactive molecular dynamics simulation. , 2001, , .		108
126	Physik der Photosynthese: Wie Bakterien die Quantenphysik ausnutzen, um effizient Photosynthese zu betreiben. <i>Physik Journal</i> , 2001, 57, 49-53.	0.1	4



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127	Excitation energy trapping by the reaction center of Rhodobacter Sphaeroides. International Journal of Quantum Chemistry, 2000, 77, 139-151.	1.0	52
128	Efficient light harvesting through carotenoids. Photosynthesis Research, 2000, 66, 125-144.	1.6	157
129	A Model for Photoreceptor-Based Magnetoreception in Birds. Biophysical Journal, 2000, 78, 707-718.	0.2	955
130	Contributory presentations/posters. Journal of Biosciences, 1999, 24, 33-198.	0.5	0
131	Investigating a back door mechanism of actin phosphate release by steered molecular dynamics. , 1999, 35, 262-273.		106
132	Steered molecular dynamics simulations of force-induced protein domain unfolding. , 1999, 35, 453-463.		246
133	Energy transfer between carotenoids and bacteriochlorophylls in light-harvesting complex II of purple bacteria. Physical Review E, 1999, 59, 3293-3311.	0.8	161
134	Expansion method for stationary states of quantum billiards. American Journal of Physics, 1999, 67, 133-141.	0.3	44
135	Investigating a back door mechanism of actin phosphate release by steered molecular dynamics. , 1999, 35, 262.		1
136	Steered molecular dynamics simulations of force-induced protein domain unfolding. , 1999, 35, 453.		1
137	Steered molecular dynamics simulations of force-induced protein domain unfolding. Proteins: Structure, Function and Bioinformatics, 1999, 35, 453-463.	1.5	8
138	Structure prediction of a complex between the chromosomal protein HMG-D and DNA. , 1998, 30, 113-135.		30
139	Excitons and excitation transfer in the photosynthetic unit of purple bacteria. Journal of Luminescence, 1998, 76-77, 310-321.	1.5	43
140	Electronic Excitations in Aggregates of Bacteriochlorophylls. Journal of Physical Chemistry B, 1998, 102, 7640-7650.	1.2	119
141	Pigment Organization and Transfer of Electronic Excitation in the Photosynthetic Unit of Purple Bacteria. Journal of Physical Chemistry B, 1997, 101, 3854-3871.	1.2	282
142	Theory of heterogeneous relaxation in compartmentalized tissues. Magnetic Resonance in Medicine, 1997, 37, 666-675.	1.9	15
143	Protein domain movements: detection of rigid domains and visualization of hinges in comparisons of atomic coordinates. Proteins: Structure, Function and Bioinformatics, 1997, 29, 1-14.	1.5	230
144	Protein domain movements: detection of rigid domains and visualization of hinges in comparisons of atomic coordinates. , 1997, 29, 1.		5

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145	NEURONAL OSCILLATIONS AND STOCHASTIC LIMIT CYCLES. International Journal of Neural Systems, 1996, 07, 399-402.	3.2	2
146	Introduction to the diffusion Monte Carlo method. American Journal of Physics, 1996, 64, 633-644.	0.3	98
147	The crystal structure of the light-harvesting complex II (B800â€“850) from Rhodospirillum molischianum. Structure, 1996, 4, 581-597.	1.6	1,056
148	Molecular dynamics study of phospholipase A2 on a membrane surface. , 1996, 25, 12-27.		65
149	VMD: Visual molecular dynamics. Journal of Molecular Graphics, 1996, 14, 33-38.	1.7	46,937
150	Molecular Dynamics Studies of Bacteriorhodopsin's Photocycles. Israel Journal of Chemistry, 1995, 35, 447-464.	1.0	58
151	Predicting the structure of the light-harvesting complex II of <i>rhodospirillum molischianum</i> . Protein Science, 1995, 4, 1670-1682.	3.1	43
152	Velocity reassignment echoes in proteins. Journal of Chemical Physics, 1995, 103, 3124-3139.	1.2	12
153	Understanding Structure and Function of Membrane Proteins Using Free Energy Calculations. , 0, , 187-211.		0
154	Towards an Understanding of Membrane Channels. , 0, , 153-190.		3