Klaus Schulten

List of Publications by Year
in descending order

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154 papers	81,327 citations	16451 64 h-index	11607 135 g-index
158 all docs	158 docs citations	158 times ranked	67392 citing authors

#	Article	IF	Citations
1	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	3.0	1,548
2	In Situ Conformational Changes of the Escherichia coli Serine Chemoreceptor in Different Signaling States. MBio, 2019, 10, .	4.1	29
3	Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism. Cell, 2019, 179, 1098-1111.e23.	28.9	122
4	Fast pressure-jump all-atom simulations and experiments reveal site-specific protein dehydration-folding dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 5356-5361.	7.1	10
5	NAMD goes quantum: an integrative suite for hybrid simulations. Nature Methods, 2018, 15, 351-354.	19.0	149
6	All-atom molecular dynamics of the HBV capsid reveals insights into biological function and cryo-EM resolution limits. ELife, 2018, 7, .	6.0	92
7	Mechanism for the Regulated Control of Bacterial Transcription Termination by a Universal Adaptor Protein. Molecular Cell, 2018, 71, 911-922.e4.	9.7	65
8	Free-energy simulations reveal molecular mechanism for functional switch of a DNA helicase. ELife, 2018, 7, .	6.0	15
9	Flexible Fitting of Atomic Structures into Electron Microscopy Maps Using Molecular Dynamics. journal of hand surgery Asian-Pacific volume, The, 2018, , 433-443.	0.4	0
10	Structural characterization of mRNA-tRNA translocation intermediates. journal of hand surgery Asian-Pacific volume, The, 2018, , 450-455.	0.4	0
11	Quantitative Characterization of Domain Motions in Molecular Machines. journal of hand surgery Asian-Pacific volume, The, 2018, , 532-541.	0.4	0
12	Computational de novo design of antibodies binding to a peptide with high affinity. Biotechnology and Bioengineering, 2017, 114, 1331-1342.	3.3	25
13	Quantitative Characterization of Domain Motions in Molecular Machines. Journal of Physical Chemistry B, 2017, 121, 3747-3756.	2.6	10
14	Permeability of a Fluid Lipid Bilayer to Short-Chain Alcohols from First Principles. Journal of Chemical Theory and Computation, 2017, 13, 2523-2532.	5.3	33
15	Lateral Segregation of Photosystem I in Cyanobacterial Thylakoids. Plant Cell, 2017, 29, 1119-1136.	6.6	54
16	Chemomechanical Coupling in Hexameric Proteinâ€“Protein Interfaces Harnesses Energy within V-Type ATPases. Journal of the American Chemical Society, 2017, 139, 293-310.	13.7	44
17	CHARMM-GUI MDFF/xMDFF Utilizer for Molecular Dynamics Flexible Fitting Simulations in Various Environments. Journal of Physical Chemistry B, 2017, 121, 3718-3723.	2.6	24
18	CryoEM structure of MxB reveals a novel oligomerization interface critical for HIV restriction. Science Advances, 2017, 3, e1701264.	10.3	47

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19	Physical properties of the HIV-1 capsid from all-atom molecular dynamics simulations. Nature Communications, 2017, 8, 15959.	12.8	136
20	Constant-pH Molecular Dynamics Simulations for Large Biomolecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5933-5944.	5.3	139
21	Overall energy conversion efficiency of a photosynthetic vesicle. ELife, 2016, 5, .	6.0	63
22	The Water Permeability and Pore Entrance Structure of Aquaporin-4 Depend on Lipid Bilayer Thickness. Biophysical Journal, 2016, 111, 90-99.	0.5	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.	12.8	126
25	Electrically Tunable Quenching of DNA Fluctuations in Biased Solid-State Nanopores. ACS Nano, 2016, 10, 4482-4488.	14.6	22
26	Contributions of Charged Residues in Structurally Dynamic Capsid Surface Loops to Rous Sarcoma Virus Assembly. Journal of Virology, 2016, 90, 5700-5714.	3.4	12
27	Disulfide Bridges: Bringing Together Frustrated Structure in a Bioactive Peptide. Biophysical Journal, 2016, 110, 1744-1752.	0.5	27
28	All-Atom Molecular Dynamics of Virus Capsids as Drug Targets. Journal of Physical Chemistry Letters, 2016, 7, 1836-1844.	4.6	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.	5.3	80
30	Computational Methodologies for Real-Space Structural Refinement of Large Macromolecular Complexes. Annual Review of Biophysics, 2016, 45, 253-278.	10.0	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.	13.7	48
33	Mechanism of the Primary Charge Transfer Reaction in the Cytochrome bc₁ Complex. Journal of Physical Chemistry B, 2016, 120, 11369-11380.	2.6	30
34	Binding Site Recognition and Docking Dynamics of a Single Electron Transport Protein: Cytochrome c₂. Journal of the American Chemical Society, 2016, 138, 12077-12089.	13.7	15
35	Conserved methionine dictates substrate preference in Nramp-family divalent metal transporters. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 10310-10315.	7.1	72
36	Crystal Structure and Conformational Change Mechanism of a Bacterial Nramp-Family Divalent Metal Transporter. Structure, 2016, 24, 2102-2114.	3.3	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.	1.3	23
39	QwikMDâ€‰â€”â€‰Integrative Molecular Dynamics Toolkit for Novices and Experts. Scientific Reports, 2016, 6, 26536.	3.3	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.	2.5	25
41	Structure of the human 26S proteasome at a resolution of 3.9 Ã.... Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 7816-7821.	7.1	174
42	Advances in the molecular dynamics flexible fitting method for cryo-EM modeling. Methods, 2016, 100, 50-60.	3.8	82
43	Atomic detail visualization of photosynthetic membranes with GPU-accelerated ray tracing. Parallel Computing, 2016, 55, 17-27.	2.1	37
44	Molecular dynamics-based refinement and validation for sub-5 Ã... cryo-electron microscopy maps. ELife, 2016, 5, .	6.0	136
45	Structural Refinement of Proteins by Restrained Molecular Dynamics Simulations with Non-interacting Molecular Fragments. PLoS Computational Biology, 2015, 11, e1004368.	3.2	26
46	CryoEM and computer simulations reveal a novel kinase conformational switch in bacterial chemotaxis signaling. ELife, 2015, 4, .	6.0	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.	7.1	76
48	Atomic Modeling of an Immature Retroviral Lattice Using Molecular Dynamics and Mutagenesis. Structure, 2015, 23, 1414-1425.	3.3	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.	13.7	29
50	Molecular dynamics simulations of large macromolecular complexes. Current Opinion in Structural Biology, 2015, 31, 64-74.	5.7	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.	7.1	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.	3.1	75
53	Dynamic profiling of double-stranded RNA binding proteins. Nucleic Acids Research, 2015, 43, 7566-7576.	14.5	53
54	Mapping Mechanical Force Propagation through Biomolecular Complexes. Nano Letters, 2015, 15, 7370-7376.	9.1	83

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55	Intrinsic Stepwise Translocation of Stretched ssDNA in Graphene Nanopores. Nano Letters, 2015, 15, 8322-8330.	9.1	47
56	Multilevel Summation Method for Electrostatic Force Evaluation. Journal of Chemical Theory and Computation, 2015, 11, 766-779.	5.3	46
57	Structure, function, and quantum dynamics of pigmentâ€“protein complexes. , 2014, , 123-143.		3
58	Ultrastable cellulosome-adhesion complex tightens under load. Nature Communications, 2014, 5, 5635.	12.8	92
59	Molecular insights into the membrane-associated phosphatidylinositol 4-kinase IIÎ±. Nature Communications, 2014, 5, 3552.	12.8	52
60	Assembly of Nsp1 Nucleoporins Provides Insight into Nuclear Pore Complex Gating. PLoS Computational Biology, 2014, 10, e1003488.	3.2	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. Journal of Chemical Theory and Computation, 2014, 10, 5276-5285.	5.3	66
63	Integration of energy and electron transfer processes in the photosynthetic membrane of Rhodobacter sphaeroides. Biochimica Et Biophysica Acta - Bioenergetics, 2014, 1837, 1769-1780.	1.0	99
64	Structural mechanism of voltage-dependent gating in an isolated voltage-sensing domain. Nature Structural and Molecular Biology, 2014, 21, 244-252.	8.2	228
65	A Highly Tilted Membrane Configuration for the Prefusion State of Synaptobrevin. Biophysical Journal, 2014, 107, 2112-2121.	0.5	34
66	GPU-accelerated analysis and visualization of large structures solved by molecular dynamics flexible fitting. Faraday Discussions, 2014, 169, 265-283.	3.2	37
67	xMDFF: molecular dynamics flexible fitting of low-resolution X-ray structures. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 2344-2355.	2.5	50
68	Calculation of Lipid-Bilayer Permeabilities Using an Average Force. Journal of Chemical Theory and Computation, 2014, 10, 554-564.	5.3	57
69	Synaptotagminâ€™s Role in Neurotransmitter Release Likely Involves Ca 2+ -induced Conformational Transition. Biophysical Journal, 2014, 107, 1156-1166.	0.5	42
70	Generalized scalable multiple copy algorithms for molecular dynamics simulations in NAMD. Computer Physics Communications, 2014, 185, 908-916.	7.5	115
71	Macrolide antibiotics allosterically predispose the ribosome for translation arrest. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 9804-9809.	7.1	99
72	Diffusive Models of Membrane Permeation with Explicit Orientational Freedom. Journal of Chemical Theory and Computation, 2014, 10, 2710-2718.	5.3	43

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73	Light Harvesting by Lamellar Chromatophores in Rhodospirillum photometricum. Biophysical Journal, 2014, 106, 2503-2510.	0.5	48
74	Separation of photo-induced radical pair in cryptochrome to a functionally critical distance. Scientific Reports, 2014, 4, 3845.	3.3	65
75	A structural model of the active ribosome-bound membrane protein insertase YidC. ELife, 2014, 3, e03035.	6.0	69
76	Mature HIV-1 capsid structure by cryo-electron microscopy and all-atom molecular dynamics. Nature, 2013, 497, 643-646.	27.8	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. Journal of Chemical Physics, 2012, 137, 065101.	3.0	46
79	GPU/CPU Algorithm for Generalized Born/Solvent-Accessible Surface Area Implicit Solvent Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2521-2530.	5.3	49
80	Open Quantum Dynamics Calculations with the Hierarchy Equations of Motion on Parallel Computers. Journal of Chemical Theory and Computation, 2012, 8, 2808-2816.	5.3	157
81	Parallel Generalized Born Implicit Solvent Calculations with NAMD. Journal of Chemical Theory and Computation, 2011, 7, 3635-3642.	5.3	137
82	Implementation of accelerated molecular dynamics in NAMD. Computational Science & Discovery, 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. Journal of Chemical Physics, 2011, 134, 095102.	3.0	88
85	Applications of the molecular dynamics flexible fitting method. Journal of Structural Biology, 2011, 173, 420-427.	2.8	44
86	High-Performance Scalable Molecular Dynamics Simulations of a Polarizable Force Field Based on Classical Drude Oscillators in NAMD. Journal of Physical Chemistry Letters, 2011, 2, 87-92.	4.6	233
87	Cryo-EM structure of the ribosomeâ€“SecYE complex in the membrane environment. Nature Structural and Molecular Biology, 2011, 18, 614-621.	8.2	264
88	Symmetry-Restrained Flexible Fitting for Symmetric EM Maps. Structure, 2011, 19, 1211-1218.	3.3	66
89	Stereochemical errors and their implications for molecular dynamics simulations. BMC Bioinformatics, 2011, 12, 190.	2.6	50
90	FÃ¶rster Energy Transfer Theory as Reflected in the Structures of Photosynthetic Lightâ€Harvesting Systems. ChemPhysChem, 2011, 12, 518-531.	2.1	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.	2.4	336
93	Selfâ€Assembly of Photosynthetic Membranes. ChemPhysChem, 2010, 11, 1154-1159.	2.1	23
94	Challenges in protein-folding simulations. Nature Physics, 2010, 6, 751-758.	16.7	310
95	Energy transfer dynamics in an RCâ€“LH1â€“PufX tubular photosynthetic membrane. New Journal of Physics, 2010, 12, 085005.	2.9	23
96	Photosynthetic Vesicle Architecture and Constraints on Efficient EnergyÂHarvesting. Biophysical Journal, 2010, 99, 67-75.	0.5	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.	7.1	219
98	Discovery Through the Computational Microscope. Structure, 2009, 17, 1295-1306.	3.3	302
99	Modeling transport through synthetic nanopores. IEEE Nanotechnology Magazine, 2009, 3, 20-28.	1.3	43
100	Structural model and excitonic properties of the dimeric RCâ€“LH1â€“PufX complex from Rhodobacter sphaeroides. Chemical Physics, 2009, 357, 188-197.	1.9	48
101	Molecular dynamics flexible fitting: A practical guide to combine cryo-electron microscopy and X-ray crystallography. Methods, 2009, 49, 174-180.	3.8	305
102	Protein-Induced Membrane Curvature Investigated through Molecular Dynamics Flexible Fitting. Biophysical Journal, 2009, 97, 321-329.	0.5	68
103	Elucidating the Mechanism behind Irreversible Deformation of Viral Capsids. Biophysical Journal, 2009, 97, 2061-2069.	0.5	94
104	Membrane Curvature Induced by Aggregates of LH2s and Monomeric LH1s. Biophysical Journal, 2009, 97, 2978-2984.	0.5	28
105	Light harvesting complex II B850 excitation dynamics. Journal of Chemical Physics, 2009, 131, 225101.	3.0	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.	3.3	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.	7.1	166

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109	Modeling Induction Phenomena in Intermolecular Interactions with an Ab Initio Force Field. Journal of Chemical Theory and Computation, 2007, 3, 1914-1926.	5.3	34
110	Accelerating molecular modeling applications with graphics processors. Journal of Computational Chemistry, 2007, 28, 2618-2640.	3.3	619
111	Imaging the Migration Pathways for O2, CO, NO, and Xe Inside Myoglobin. Biophysical Journal, 2006, 91, 1844-1857.	0.5	258
112	Molecular Dynamics Simulations of the Complete Satellite Tobacco Mosaic Virus. Structure, 2006, 14, 437-449.	3.3	390
113	Scalable molecular dynamics with NAMD. Journal of Computational Chemistry, 2005, 26, 1781-1802.	3.3	15,208
114	Structural dynamics of the lac repressor-DNA complex revealed by a multiscale simulation. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6783-6788.	7.1	135
115	Imaging Î±-Hemolysin with Molecular Dynamics: Ionic Conductance, Osmotic Permeability, and the Electrostatic Potential Map. Biophysical Journal, 2005, 88, 3745-3761.	0.5	620
116	Free energy calculation from steered molecular dynamics simulations using Jarzynskiâ€™s equality. Journal of Chemical Physics, 2003, 119, 3559-3566.	3.0	712
117	Mechanisms of Selectivity in Channels and Enzymes Studied with Interactive Molecular Dynamics. Biophysical Journal, 2003, 85, 36-48.	0.5	88
118	Reaction paths based on mean first-passage times. Journal of Chemical Physics, 2003, 119, 1313-1319.	3.0	72
119	Robustness and Optimality of Light Harvesting in Cyanobacterial Photosystem I. Journal of Physical Chemistry B, 2002, 106, 7948-7960.	2.6	134
120	General random matrix approach to account for the effect of static disorder on the spectral properties of light harvesting systems. Physical Review E, 2002, 65, 031916.	2.1	62
121	Photosynthetic apparatus of purple bacteria. Quarterly Reviews of Biophysics, 2002, 35, 1-62.	5.7	353
122	Excitons in a photosynthetic light-harvesting system: A combined molecular dynamics, quantum chemistry, and polaron model study. Physical Review E, 2002, 65, 031919.	2.1	261
123	Kinetics of Excitation Migration and Trapping in the Photosynthetic Unit of Purple Bacteria. Journal of Physical Chemistry B, 2001, 105, 8259-8267.	2.6	128
124	Phylogenetic Analysis of Metabolic Pathways. Journal of Molecular Evolution, 2001, 52, 471-489.	1.8	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. Physik Journal, 2001, 57, 49-53.	0.1	4

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127	Excitation energy trapping by the reaction center ofRhodobacter Sphaeroides. International Journal of Quantum Chemistry, 2000, 77, 139-151.	2.0	52
128	Efficient light harvesting through carotenoids. Photosynthesis Research, 2000, 66, 125-144.	2.9	157
129	A Model for Photoreceptor-Based Magnetoreception in Birds. Biophysical Journal, 2000, 78, 707-718.	0.5	955
130	Contributory presentations/posters. Journal of Biosciences, 1999, 24, 33-198.	1.1	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. Proteins: Structure, Function and Bioinformatics, 1999, 35, 453-463.	2.6	246
133	Energy transfer between carotenoids and bacteriochlorophylls in light-harvesting complex II of purple bacteria. Physical Review E, 1999, 59, 3293-3311.	2.1	161
134	Expansion method for stationary states of quantum billiards. American Journal of Physics, 1999, 67, 133-141.	0.7	44
135	Investigating a back door mechanism of actin phosphate release by steered molecular dynamics. Proteins: Structure, Function and Bioinformatics, 1999, 35, 262-273.	2.6	1
136	Steered molecular dynamics simulations of force-induced protein domain unfolding. , 1999, 35, 453.		1
137	Steered molecular dynamics simulations of forceâ€induced protein domain unfolding. Proteins: Structure, Function and Bioinformatics, 1999, 35, 453-463.	2.6	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.	3.1	43
140	Electronic Excitations in Aggregates of Bacteriochlorophylls. Journal of Physical Chemistry B, 1998, 102, 7640-7650.	2.6	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.	2.6	282
142	Theory of heterogeneous relaxation in compartmentalized tissues. Magnetic Resonance in Medicine, 1997, 37, 666-675.	3.0	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.	2.6	230
144	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.	2.6	5

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145	NEURONAL OSCILLATIONS AND STOCHASTIC LIMIT CYCLES. International Journal of Neural Systems, 1996, 07, 399-402.	5.2	2
146	Introduction to the diffusion Monte Carlo method. American Journal of Physics, 1996, 64, 633-644.	0.7	98
147	The crystal structure of the light-harvesting complex II (B800â€“850) from Rhodospirillum molischianum. Structure, 1996, 4, 581-597.	3.3	1,056
148	Molecular dynamics study of phospholipase A2on a membrane surface. , 1996, 25, 12-27.		65
149	VMD: Visual molecular dynamics. Journal of Molecular Graphics, 1996, 14, 33-38.	1.1	46,937
150	Molecular Dynamics Studies of Bacteriorhodopsin's Photocycles. Israel Journal of Chemistry, 1995, 35, 447-464.	2.3	58
151	Predicting the structure of the light-harvesting complex II ofrhodospirillum molischianum. Protein Science, 1995, 4, 1670-1682.	7.6	43
152	Velocity reassignment echoes in proteins. Journal of Chemical Physics, 1995, 103, 3124-3139.	3.0	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