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	VMD: Visual molecular dynamics. Journal of Molecular Graphics, 1996, 14, 33-38.	1.1	46,937
2	Scalable molecular dynamics with NAMD. Journal of Computational Chemistry, 2005, 26, 1781-1802.	3.3	15,208
3	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	3.0	1,548
4	The crystal structure of the light-harvesting complex II (B800â€“850) from Rhodospirillum molischianum. Structure, 1996, 4, 581-597.	3.3	1,056
5	A Model for Photoreceptor-Based Magnetoreception in Birds. Biophysical Journal, 2000, 78, 707-718.	0.5	955
6	Flexible Fitting of Atomic Structures into Electron Microscopy Maps Using Molecular Dynamics. Structure, 2008, 16, 673-683.	3.3	833
7	Free energy calculation from steered molecular dynamics simulations using Jarzynskiâ€™s equality. Journal of Chemical Physics, 2003, 119, 3559-3566.	3.0	712
8	Mature HIV-1 capsid structure by cryo-electron microscopy and all-atom molecular dynamics. Nature, 2013, 497, 643-646.	27.8	712
9	Imaging Î±-Hemolysin with Molecular Dynamics: Ionic Conductance, Osmotic Permeability, and the Electrostatic Potential Map. Biophysical Journal, 2005, 88, 3745-3761.	0.5	620
10	Accelerating molecular modeling applications with graphics processors. Journal of Computational Chemistry, 2007, 28, 2618-2640.	3.3	619
11	Molecular Dynamics Simulations of the Complete Satellite Tobacco Mosaic Virus. Structure, 2006, 14, 437-449.	3.3	390
12	Photosynthetic apparatus of purple bacteria. Quarterly Reviews of Biophysics, 2002, 35, 1-62.	5.7	353
13	Molecular dynamics simulations of large macromolecular complexes. Current Opinion in Structural Biology, 2015, 31, 64-74.	5.7	347
14	GPU-accelerated molecular modeling coming of age. Journal of Molecular Graphics and Modelling, 2010, 29, 116-125.	2.4	336
15	Challenges in protein-folding simulations. Nature Physics, 2010, 6, 751-758.	16.7	310
16	Molecular dynamics flexible fitting: A practical guide to combine cryo-electron microscopy and X-ray crystallography. Methods, 2009, 49, 174-180.	3.8	305
17	Discovery Through the Computational Microscope. Structure, 2009, 17, 1295-1306.	3.3	302
18	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

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19	Cryo-EM structure of the ribosomeâ€“SecYE complex in the membrane environment. Nature Structural and Molecular Biology, 2011, 18, 614-621.	8.2	264
20	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
21	Imaging the Migration Pathways for O2, CO, NO, and Xe Inside Myoglobin. Biophysical Journal, 2006, 91, 1844-1857.	0.5	258
22	Steered molecular dynamics simulations of force-induced protein domain unfolding. Proteins: Structure, Function and Bioinformatics, 1999, 35, 453-463.	2.6	246
23	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
24	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
25	Structural mechanism of voltage-dependent gating in an isolated voltage-sensing domain. Nature Structural and Molecular Biology, 2014, 21, 244-252.	8.2	228
26	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
27	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
28	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
29	Energy transfer between carotenoids and bacteriochlorophylls in light-harvesting complex II of purple bacteria. Physical Review E, 1999, 59, 3293-3311.	2.1	161
30	Efficient light harvesting through carotenoids. Photosynthesis Research, 2000, 66, 125-144.	2.9	157
31	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
32	QwikMDâ€‰â€”â€‰Integrative Molecular Dynamics Toolkit for Novices and Experts. Scientific Reports, 2016, 6, 26536.	3.3	153
33	NAMD goes quantum: an integrative suite for hybrid simulations. Nature Methods, 2018, 15, 351-354.	19.0	149
34	FÃ¶rster Energy Transfer Theory as Reflected in the Structures of Photosynthetic Lightâ€Harvesting Systems. ChemPhysChem, 2011, 12, 518-531.	2.1	142
35	Constant-pH Molecular Dynamics Simulations for Large Biomolecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5933-5944.	5.3	139
36	Parallel Generalized Born Implicit Solvent Calculations with NAMD. Journal of Chemical Theory and Computation, 2011, 7, 3635-3642.	5.3	137

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37	Light harvesting complex II B850 excitation dynamics. Journal of Chemical Physics, 2009, 131, 225101.	3.0	136
38	Physical properties of the HIV-1 capsid from all-atom molecular dynamics simulations. Nature Communications, 2017, 8, 15959.	12.8	136
39	Molecular dynamics-based refinement and validation for sub-5 Ã... cryo-electron microscopy maps. ELife, 2016, 5, .	6.0	136
40	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
41	Robustness and Optimality of Light Harvesting in Cyanobacterial Photosystem I. Journal of Physical Chemistry B, 2002, 106, 7948-7960.	2.6	134
42	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
43	Cyclophilin A stabilizes the HIV-1 capsid through a novel non-canonical binding site. Nature Communications, 2016, 7, 10714.	12.8	126
44	Implementation of accelerated molecular dynamics in NAMD. Computational Science & Discovery, 2011, 4, 015002.	1.5	124
45	Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism. Cell, 2019, 179, 1098-1111.e23.	28.9	122
46	Electronic Excitations in Aggregates of Bacteriochlorophylls. Journal of Physical Chemistry B, 1998, 102, 7640-7650.	2.6	119
47	Generalized scalable multiple copy algorithms for molecular dynamics simulations in NAMD. Computer Physics Communications, 2014, 185, 908-916.	7.5	115
48	A system for interactive molecular dynamics simulation. , 2001, , .		108
49	Investigating a back door mechanism of actin phosphate release by steered molecular dynamics. , 1999, 35, 262-273.		106
50	CryoEM and computer simulations reveal a novel kinase conformational switch in bacterial chemotaxis signaling. ELife, 2015, 4, .	6.0	106
51	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
52	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
53	Introduction to the diffusion Monte Carlo method. American Journal of Physics, 1996, 64, 633-644.	0.7	98
54	Elucidating the Mechanism behind Irreversible Deformation of Viral Capsids. Biophysical Journal, 2009, 97, 2061-2069.	0.5	94

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55	Ultrastable cellulosome-adhesion complex tightens under load. Nature Communications, 2014, 5, 5635.	12.8	92
56	All-atom molecular dynamics of the HBV capsid reveals insights into biological function and cryo-EM resolution limits. ELife, 2018, 7, .	6.0	92
57	Mechanisms of Selectivity in Channels and Enzymes Studied with Interactive Molecular Dynamics. Biophysical Journal, 2003, 85, 36-48.	0.5	88
58	The effect of correlated bath fluctuations on exciton transfer. Journal of Chemical Physics, 2011, 134, 095102.	3.0	88
59	Phylogenetic Analysis of Metabolic Pathways. Journal of Molecular Evolution, 2001, 52, 471-489.	1.8	83
60	Mapping Mechanical Force Propagation through Biomolecular Complexes. Nano Letters, 2015, 15, 7370-7376.	9.1	83
61	Advances in the molecular dynamics flexible fitting method for cryo-EM modeling. Methods, 2016, 100, 50-60.	3.8	82
62	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
63	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
64	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
65	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
66	All-Atom Molecular Dynamics of Virus Capsids as Drug Targets. Journal of Physical Chemistry Letters, 2016, 7, 1836-1844.	4.6	73
67	Reaction paths based on mean first-passage times. Journal of Chemical Physics, 2003, 119, 1313-1319.	3.0	72
68	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
69	A structural model of the active ribosome-bound membrane protein insertase YidC. ELife, 2014, 3, e03035.	6.0	69
70	Protein-Induced Membrane Curvature Investigated through Molecular Dynamics Flexible Fitting. Biophysical Journal, 2009, 97, 321-329.	0.5	68
71	Computational Methodologies for Real-Space Structural Refinement of Large Macromolecular Complexes. Annual Review of Biophysics, 2016, 45, 253-278.	10.0	67
72	Symmetry-Restrained Flexible Fitting for Symmetric EM Maps. Structure, 2011, 19, 1211-1218.	3.3	66

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73	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
74	Molecular dynamics study of phospholipase A2on a membrane surface. , 1996, 25, 12-27.		65
75	Separation of photo-induced radical pair in cryptochrome to a functionally critical distance. Scientific Reports, 2014, 4, 3845.	3.3	65
76	Mechanism for the Regulated Control of Bacterial Transcription Termination by a Universal Adaptor Protein. Molecular Cell, 2018, 71, 911-922.e4.	9.7	65
77	Overall energy conversion efficiency of a photosynthetic vesicle. ELife, 2016, 5, .	6.0	63
78	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
79	Photosynthetic Vesicle Architecture and Constraints on Efficient EnergyÂHarvesting. Biophysical Journal, 2010, 99, 67-75.	0.5	60
80	Molecular Dynamics Studies of Bacteriorhodopsin's Photocycles. Israel Journal of Chemistry, 1995, 35, 447-464.	2.3	58
81	Calculation of Lipid-Bilayer Permeabilities Using an Average Force. Journal of Chemical Theory and Computation, 2014, 10, 554-564.	5.3	57
82	Crystal Structure and Conformational Change Mechanism of a Bacterial Nramp-Family Divalent Metal Transporter. Structure, 2016, 24, 2102-2114.	3.3	56
83	Lateral Segregation of Photosystem I in Cyanobacterial Thylakoids. Plant Cell, 2017, 29, 1119-1136.	6.6	54
84	Dynamic profiling of double-stranded RNA binding proteins. Nucleic Acids Research, 2015, 43, 7566-7576.	14.5	53
85	Excitation energy trapping by the reaction center ofRhodobacter Sphaeroides. International Journal of Quantum Chemistry, 2000, 77, 139-151.	2.0	52
86	Molecular insights into the membrane-associated phosphatidylinositol 4-kinase IIÎ±. Nature Communications, 2014, 5, 3552.	12.8	52
87	Stereochemical errors and their implications for molecular dynamics simulations. BMC Bioinformatics, 2011, 12, 190.	2.6	50
88	xMDFF: molecular dynamics flexible fitting of low-resolution X-ray structures. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 2344-2355.	2.5	50
89	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
90	Structural model and excitonic properties of the dimeric RCâ€“LH1â€“PufX complex from Rhodobacter sphaeroides. Chemical Physics, 2009, 357, 188-197.	1.9	48

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91	Light Harvesting by Lamellar Chromatophores in Rhodospirillum photometricum. Biophysical Journal, 2014, 106, 2503-2510.	0.5	48
92	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
93	Intrinsic Stepwise Translocation of Stretched ssDNA in Graphene Nanopores. Nano Letters, 2015, 15, 8322-8330.	9.1	47
94	CryoEM structure of MxB reveals a novel oligomerization interface critical for HIV restriction. Science Advances, 2017, 3, e1701264.	10.3	47
95	Excited state dynamics in photosynthetic reaction center and light harvesting complex 1. Journal of Chemical Physics, 2012, 137, 065101.	3.0	46
96	Multilevel Summation Method for Electrostatic Force Evaluation. Journal of Chemical Theory and Computation, 2015, 11, 766-779.	5.3	46
97	Expansion method for stationary states of quantum billiards. American Journal of Physics, 1999, 67, 133-141.	0.7	44
98	Applications of the molecular dynamics flexible fitting method. Journal of Structural Biology, 2011, 173, 420-427.	2.8	44
99	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
100	Predicting the structure of the light-harvesting complex II ofrhodospirillum molischianum. Protein Science, 1995, 4, 1670-1682.	7.6	43
101	Excitons and excitation transfer in the photosynthetic unit of purple bacteria. Journal of Luminescence, 1998, 76-77, 310-321.	3.1	43
102	Modeling transport through synthetic nanopores. IEEE Nanotechnology Magazine, 2009, 3, 20-28.	1.3	43
103	Diffusive Models of Membrane Permeation with Explicit Orientational Freedom. Journal of Chemical Theory and Computation, 2014, 10, 2710-2718.	5.3	43
104	Assembly of Nsp1 Nucleoporins Provides Insight into Nuclear Pore Complex Gating. PLoS Computational Biology, 2014, 10, e1003488.	3.2	42
105	Synaptotagminâ€™s Role in Neurotransmitter Release Likely Involves Ca 2+ -induced Conformational Transition. Biophysical Journal, 2014, 107, 1156-1166.	0.5	42
106	GPU-accelerated analysis and visualization of large structures solved by molecular dynamics flexible fitting. Faraday Discussions, 2014, 169, 265-283.	3.2	37
107	Atomic detail visualization of photosynthetic membranes with GPU-accelerated ray tracing. Parallel Computing, 2016, 55, 17-27.	2.1	37
108	Atomic Modeling of an Immature Retroviral Lattice Using Molecular Dynamics and Mutagenesis. Structure, 2015, 23, 1414-1425.	3.3	35

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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	A Highly Tilted Membrane Configuration for the Prefusion State of Synaptobrevin. Biophysical Journal, 2014, 107, 2112-2121.	0.5	34
111	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
112	Structure prediction of a complex between the chromosomal protein HMG-D and DNA. , 1998, 30, 113-135.		30
113	Mechanism of the Primary Charge Transfer Reaction in the Cytochrome bc₁ Complex. Journal of Physical Chemistry B, 2016, 120, 11369-11380.	2.6	30
114	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
115	In Situ Conformational Changes of the Escherichia coli Serine Chemoreceptor in Different Signaling States. MBio, 2019, 10, .	4.1	29
116	Membrane Curvature Induced by Aggregates of LH2s and Monomeric LH1s. Biophysical Journal, 2009, 97, 2978-2984.	0.5	28
117	Disulfide Bridges: Bringing Together Frustrated Structure in a Bioactive Peptide. Biophysical Journal, 2016, 110, 1744-1752.	0.5	27
118	Structural Refinement of Proteins by Restrained Molecular Dynamics Simulations with Non-interacting Molecular Fragments. PLoS Computational Biology, 2015, 11, e1004368.	3.2	26
119	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
120	Computational de novo design of antibodies binding to a peptide with high affinity. Biotechnology and Bioengineering, 2017, 114, 1331-1342.	3.3	25
121	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
122	Selfâ€Assembly of Photosynthetic Membranes. ChemPhysChem, 2010, 11, 1154-1159.	2.1	23
123	Energy transfer dynamics in an RCâ€“LH1â€“PufX tubular photosynthetic membrane. New Journal of Physics, 2010, 12, 085005.	2.9	23
124	Evaluation of Emerging Energy-Efficient Heterogeneous Computing Platforms for Biomolecular and Cellular Simulation Workloads. , 2016, 2016, 89-100.		23
125	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
126	Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering. , 2016, 2016, 1048-1057.		22

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127	Electrically Tunable Quenching of DNA Fluctuations in Biased Solid-State Nanopores. ACS Nano, 2016, 10, 4482-4488.	14.6	22
128	The Water Permeability and Pore Entrance Structure of Aquaporin-4 Depend on Lipid Bilayer Thickness. Biophysical Journal, 2016, 111, 90-99.	0.5	20
129	Early experiences scaling VMD molecular visualization and analysis jobs on blue waters. , 2013, , .		17
130	Theory of heterogeneous relaxation in compartmentalized tissues. Magnetic Resonance in Medicine, 1997, 37, 666-675.	3.0	15
131	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
132	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
133	Free-energy simulations reveal molecular mechanism for functional switch of a DNA helicase. ELife, 2018, 7, .	6.0	15
134	Velocity reassignment echoes in proteins. Journal of Chemical Physics, 1995, 103, 3124-3139.	3.0	12
135	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
136	Quantitative Characterization of Domain Motions in Molecular Machines. Journal of Physical Chemistry B, 2017, 121, 3747-3756.	2.6	10
137	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
138	Petascale Tcl with NAMD, VMD, and Swift/T. , 2014, , .		9
139	Steered molecular dynamics simulations of forceâ€induced protein domain unfolding. Proteins: Structure, Function and Bioinformatics, 1999, 35, 453-463.	2.6	8
140	High Performance Molecular Visualization: In-Situ and Parallel Rendering with EGL. , 2016, 2016, 1014-1023.		6
141	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
142	Physik der Photosynthese: Wie Bakterien die Quantenphysik ausnutzen, um effizient Photosynthese zu betreiben. Physik Journal, 2001, 57, 49-53.	0.1	4
143	The Light-Harvesting Apparatus in Purple Photosynthetic Bacteria: Introduction to a Quantum Biological Device. , 2011, , 19-48.		3
144	Structure, function, and quantum dynamics of pigmentâ€“protein complexes. , 2014, , 123-143.		3

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145	Viewing the Mechanisms of Translation through the Computational Microscope. , 2011, , 142-157.		3
146	Towards an Understanding of Membrane Channels. , 0, , 153-190.		3
147	NEURONAL OSCILLATIONS AND STOCHASTIC LIMIT CYCLES. International Journal of Neural Systems, 1996, 07, 399-402.	5.2	2
148	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
149	Steered molecular dynamics simulations of force-induced protein domain unfolding. , 1999, 35, 453.		1
150	Contributory presentations/posters. Journal of Biosciences, 1999, 24, 33-198.	1.1	0
151	Understanding Structure and Function of Membrane Proteins Using Free Energy Calculations. , 0, , 187-211.		0
152	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
153	Structural characterization of mRNA-tRNA translocation intermediates. journal of hand surgery Asian-Pacific volume, The, 2018, , 450-455.	0.4	0
154	Quantitative Characterization of Domain Motions in Molecular Machines. journal of hand surgery Asian-Pacific volume, The, 2018, , 532-541.	0.4	0