Helmut Grubmller

List of Publications by Citations

162 papers	12,063 citations	52 h-index	109 g-index
176 ext. papers	14,688 ext. citations	7.2 avg, IF	6.58 L-index

#	Paper	IF	Citations
162	CHARMM36m: an improved force field for folded and intrinsically disordered proteins. *Nature Methods*, **2017**, 14, 71-73	21.6	1819
161	Molecular anatomy of a trafficking organelle. *Cell*, **2006**, 127, 831-46	56.2	1670
160	Recognition dynamics up to microseconds revealed from an RDC-derived ubiquitin ensemble in solution. *Science*, **2008**, 320, 1471-5	33.3	872
159	Predicting slow structural transitions in macromolecular systems: Conformational flooding. *Physical Review E*, **1995**, 52, 2893-2906	2.4	502
158	Structural Ensembles of Intrinsically Disordered Proteins Depend Strongly on Force Field: A Comparison to Experiment. *Journal of Chemical Theory and Computation*, **2015**, 11, 5513-24	6.4	281
157	Generalized correlation for biomolecular dynamics. *Proteins: Structure, Function and Bioinformatics*, **2006**, 62, 1053-61	4.2	278
156	The dynamics and energetics of water permeation and proton exclusion in aquaporins. *Current Opinion in Structural Biology*, **2005**, 15, 176-83	8.1	242
155	The mechanism of proton exclusion in the aquaporin-1 water channel. *Journal of Molecular Biology*, **2003**, 333, 279-93	6.5	233
154	Kinetics, statistics, and energetics of lipid membrane electroporation studied by molecular dynamics simulations. *Biophysical Journal*, **2008**, 95, 1837-50	2.9	230
153	Structure and function of water channels. *Current Opinion in Structural Biology*, **2002**, 12, 509-15	8.1	227
152	Structure and mechanism of the reversible photoswitch of a fluorescent protein. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 13070-4	11.5	222
151	Mechanically induced titin kinase activation studied by force-probe molecular dynamics simulations. *Biophysical Journal*, **2005**, 88, 790-804	2.9	181
150	Membrane fusion. *Current Opinion in Cell Biology*, **2002**, 14, 488-95	9	167
149	Multistep binding of divalent cations to phospholipid bilayers: a molecular dynamics study. *Angewandte Chemie - International Edition*, **2004**, 43, 1021-4	16.4	164
148	Dynamic force spectroscopy of molecular adhesion bonds. *Physical Review Letters*, **2000**, 84, 6126-9	7.4	145
147	The 2018 biomembrane curvature and remodeling roadmap. *Journal Physics D: Applied Physics*, **2018**, 51,	3	133
146	Best bang for your buck: GPU nodes for GROMACS biomolecular simulations. *Journal of Computational Chemistry*, **2015**, 36, 1990-2008	3.5	130

145	Constant pH Molecular Dynamics in Explicit Solvent with λ-Dynamics. *Journal of Chemical Theory and Computation*, **2011**, 7, 1962-1978	6.4	130
144	More bang for your buck: Improved use of GPU nodes for GROMACS 2018. *Journal of Computational Chemistry*, **2019**, 40, 2418-2431	3.5	122
143	Essential dynamics of reversible peptide folding: memory-free conformational dynamics governed by internal hydrogen bonds. *Journal of Molecular Biology*, **2001**, 309, 299-313	6.5	119
142	Energy barriers and driving forces in tRNA translocation through the ribosome. *Nature Structural and Molecular Biology*, **2013**, 20, 1390-6	17.6	117
141	A refined structure of human aquaporin-1. *FEBS Letters*, **2001**, 504, 206-11	3.8	110
140	How SNARE molecules mediate membrane fusion: recent insights from molecular simulations. *Current Opinion in Structural Biology*, **2012**, 22, 187-96	8.1	109
139	Caught in the act: visualization of SNARE-mediated fusion events in molecular detail. *ChemBioChem* , **2011**, 12, 1049-55	3.8	109
138	Full correlation analysis of conformational protein dynamics. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 1294-312	4.2	108
137	Mechanical properties of the icosahedral shell of southern bean mosaic virus: a molecular dynamics study. *Biophysical Journal*, **2009**, 96, 1350-63	2.9	102
136	Speeding up parallel GROMACS on high-latency networks. *Journal of Computational Chemistry*, **2007**, 28, 2075-84	3.5	98
135	Structural heterogeneity and quantitative FRET efficiency distributions of polyprolines through a hybrid atomistic simulation and Monte Carlo approach. *PLoS ONE*, **2011**, 6, e19791	3.7	95
134	Hydrophobic mismatch sorts SNARE proteins into distinct membrane domains. *Nature Communications*, **2015**, 6, 5984	17.4	89
133	Chromophore protonation state controls photoswitching of the fluoroprotein asFP595. *PLoS Computational Biology*, **2008**, 4, e1000034	5	89
132	Photoswitching of the fluorescent protein asFP595: mechanism, proton pathways, and absorption spectra. *Angewandte Chemie - International Edition*, **2007**, 46, 530-6	16.4	89
131	Collective Langevin dynamics of conformational motions in proteins. *Journal of Chemical Physics*, **2006**, 124, 214903	3.9	89
130	Water permeation through gramicidin A: desformylation and the double helix: a molecular dynamics study. *Biophysical Journal*, **2002**, 82, 2934-42	2.9	80
129	Dynamics and energetics of permeation through aquaporins. What do we learn from molecular dynamics simulations?. *Handbook of Experimental Pharmacology*, **2009**, 57-76	3.2	76
128	Structural Basis for Polyproline-Mediated Ribosome Stalling and Rescue by the Translation Elongation Factor EF-P. *Molecular Cell*, **2017**, 68, 515-527.e6	17.6	73

127	Expansion of the fusion stalk and its implication for biological membrane fusion. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 11043-8	11.5	72
126	Quantitative structural analysis of importin-β flexibility: paradigm for solenoid protein structures. *Structure*, **2010**, 18, 1171-83	5.2	72
125	Urea impedes the hydrophobic collapse of partially unfolded proteins. *Biophysical Journal*, **2009**, 96, 3744-52	3.5	68
124	Accuracy and convergence of free energy differences calculated from nonequilibrium switching processes. *Journal of Computational Chemistry*, **2009**, 30, 447-56	3.5	66
123	A combined cryo-EM and molecular dynamics approach reveals the mechanism of ErmBL-mediated translation arrest. *Nature Communications*, **2016**, 7, 12026	17.4	66
122	Exploring protein dynamics space: the dynasome as the missing link between protein structure and function. *PLoS ONE*, **2012**, 7, e33931	3.7	65
121	The pathway to GTPase activation of elongation factor SelB on the ribosome. *Nature*, **2016**, 540, 80-85	50.4	63
120	Polar or apolar--the role of polarity for urea-induced protein denaturation. *PLoS Computational Biology*, **2008**, 4, e1000221	5	61
119	Mechanical coupling via the membrane fusion SNARE protein syntaxin 1A: a molecular dynamics study. *Biophysical Journal*, **2003**, 84, 1527-47	2.9	60
118	Molecular basis of the light-driven switching of the photochromic fluorescent protein Padron. *Journal of Biological Chemistry*, **2010**, 285, 14603-9	5.4	58
117	Kinase-activity-independent functions of atypical protein kinase C in Drosophila. *Journal of Cell Science*, **2009**, 122, 3759-71	5.3	58
116	Maximum likelihood trajectories from single molecule fluorescence resonance energy transfer experiments. *Journal of Chemical Physics*, **2003**, 119, 9920-9924	3.9	57
115	Predicting unimolecular chemical reactions: Chemical flooding. *Journal of Chemical Physics*, **2002**, 116, 897-905	3.9	56
114	Heterogeneous and rate-dependent streptavidin-biotin unbinding revealed by high-speed force spectroscopy and atomistic simulations. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 6594-6601	11.5	55
113	Estimating absolute configurational entropies of macromolecules: the minimally coupled subspace approach. *PLoS ONE*, **2010**, 5, e9179	3.7	53
112	An unusual hydrophobic core confers extreme flexibility to HEAT repeat proteins. *Biophysical Journal*, **2010**, 99, 1596-603	2.9	53
111	Flooding in GROMACS: accelerated barrier crossings in molecular dynamics. *Journal of Computational Chemistry*, **2006**, 27, 1693-702	3.5	53
110	Line-tension controlled mechanism for influenza fusion. *PLoS ONE*, **2012**, 7, e38302	3.7	51

109	Engineering fatty acid synthases for directed polyketide production. *Nature Chemical Biology*, **2017**, 13, 363-365	11.7	50
108	Structural basis for cooperativity of CRM1 export complex formation. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 960-5	11.5	50
107	do_x3dna: a tool to analyze structural fluctuations of dsDNA or dsRNA from molecular dynamics simulations. *Bioinformatics*, **2015**, 31, 2583-5	7.2	49
106	Anomalous surface diffusion of protons on lipid membranes. *Biophysical Journal*, **2014**, 107, 76-87	2.9	46
105	Elastic properties of photoswitchable azobenzene polymers from molecular dynamics simulations. *Angewandte Chemie - International Edition*, **2007**, 46, 2232-7	16.4	46
104	Determining equilibrium constants for dimerization reactions from molecular dynamics simulations. *Journal of Computational Chemistry*, **2011**, 32, 1919-28	3.5	45
103	The structure of the aquaporin-1 water channel: a comparison between cryo-electron microscopy and X-ray crystallography. *Journal of Molecular Biology*, **2003**, 325, 485-93	6.5	45
102	Importin-beta: structural and dynamic determinants of a molecular spring. *Structure*, **2008**, 16, 906-15	5.2	44
101	Torsional elasticity and energetics of F1-ATPase. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 7408-13	11.5	41
100	Proteins in the gas phase. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 408-425	7.9	40
99	Quantitative assessment of protein interaction with methyl-lysine analogues by hybrid computational and experimental approaches. *ACS Chemical Biology*, **2012**, 7, 150-4	4.9	38
98	Conformational dynamics of the F1-ATPase beta-subunit: a molecular dynamics study. *Biophysical Journal*, **2003**, 85, 1482-91	2.9	38
97	Automated cryo-EM structure refinement using correlation-driven molecular dynamics. *ELife*, **2019**, 8,	8.9	38
96	Estimation of absolute solvent and solvation shell entropies via permutation reduction. *Journal of Chemical Physics*, **2007**, 126, 014102	3.9	37
95	Keep It Flexible: Driving Macromolecular Rotary Motions in Atomistic Simulations with GROMACS. *Journal of Chemical Theory and Computation*, **2011**, 7, 1381-1393	6.4	33
94	Linear-scaling soft-core scheme for alchemical free energy calculations. *Journal of Computational Chemistry*, **2012**, 33, 25-33	3.5	32
93	Primary steps of pH-dependent insulin aggregation kinetics are governed by conformational flexibility. *ChemBioChem*, **2009**, 10, 1816-22	3.8	31
92	Multiple time step algorithms for molecular dynamics simulations of proteins: How good are they?. *Journal of Computational Chemistry*, **1998**, 19, 1534-1552	3.5	31

91	PspF-binding domain PspA1-144 and the PspA·F complex: New insights into the coiled-coil-dependent regulation of AAA+ proteins. *Molecular Microbiology*, **2015**, 98, 743-59	4.1	30
90	The fold of human aquaporin 1. *Journal of Molecular Biology*, **2000**, 300, 987-94	6.5	30
89	AMBER-DYES: Characterization of Charge Fluctuations and Force Field Parameterization of Fluorescent Dyes for Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2014**, 10, 5505-12	6.4	29
88	Fluctuations of primary ubiquitin folding intermediates in a force clamp. *Journal of Structural Biology*, **2007**, 157, 557-69	3.4	27
87	Lipid binding defects and perturbed synaptogenic activity of a Collybistin R290H mutant that causes epilepsy and intellectual disability. *Journal of Biological Chemistry*, **2015**, 290, 8256-70	5.4	26
86	g_contacts: Fast contact search in bio-molecular ensemble data. *Computer Physics Communications*, **2013**, 184, 2856-2859	4.2	26
85	A highly strained nuclear conformation of the exportin Cse1p revealed by molecular dynamics simulations. *Structure*, **2006**, 14, 1469-78	5.2	26
84	Microtubule assembly governed by tubulin allosteric gain in flexibility and lattice induced fit. *ELife*, **2018**, 7,	8.9	26
83	Photoswitching of the Fluorescent Protein asFP595: Mechanism, Proton Pathways, and Absorption Spectra. *Angewandte Chemie*, **2007**, 119, 536-542	3.6	25
82	Structure determination from single molecule X-ray scattering with three photons per image. *Nature Communications*, **2018**, 9, 2375	17.4	25
81	Molecular dynamics simulations of protein G challenge NMR-derived correlated backbone motions. *Angewandte Chemie - International Edition*, **2005**, 44, 3394-9	16.4	24
80	Dynamic contact network between ribosomal subunits enables rapid large-scale rotation during spontaneous translocation. *Nucleic Acids Research*, **2015**, 43, 6747-60	20.1	23
79	Primary changes of the mechanical properties of Southern Bean Mosaic Virus upon calcium removal. *Biophysical Journal*, **2010**, 98, 687-95	2.9	23
78	Charge-Neutral Constant pH Molecular Dynamics Simulations Using a Parsimonious Proton Buffer. *Journal of Chemical Theory and Computation*, **2016**, 12, 1040-51	6.4	22
77	SESCA: Predicting Circular Dichroism Spectra from Protein Molecular Structures. *Journal of Chemical Theory and Computation*, **2019**, 15, 5087-5102	6.4	22
76	A "force buffer" protecting immunoglobulin titin. *Angewandte Chemie - International Edition*, **2010**, 49, 3528-31	16.4	22
75	Cationic and Anionic Impact on the Electronic Structure of Liquid Water. *Journal of Physical Chemistry Letters*, **2017**, 8, 3759-3764	6.4	21
74	A GPU-Accelerated Fast Multipole Method for GROMACS: Performance and Accuracy. *Journal of Chemical Theory and Computation*, **2020**, 16, 6938-6949	6.4	21

73	NuSol Numerical solver for the 3D stationary nuclear Schr inger equation. *Computer Physics Communications*, **2016**, 198, 169-178	4.2	20
72	Free energy landscape of rim-pore expansion in membrane fusion. *Biophysical Journal*, **2014**, 107, 2287-95	2.9	20
71	Elastic properties and heterogeneous stiffness of the phi29 motor connector channel. *Biophysical Journal*, **2014**, 106, 1338-48	2.9	19
70	Adaptive anisotropic kernels for nonparametric estimation of absolute configurational entropies in high-dimensional configuration spaces. *Physical Review E*, **2009**, 80, 011913	2.4	19
69	Molecular simulations of the ribosome and associated translation factors. *Current Opinion in Structural Biology*, **2018**, 49, 27-35	8.1	19
68	Active role of elongation factor G in maintaining the mRNA reading frame during translation. *Science Advances*, **2019**, 5, eaax8030	14.3	18
67	Velocity-dependent mechanical unfolding of bacteriorhodopsin is governed by a dynamic interaction network. *Biophysical Journal*, **2011**, 100, 1109-19	2.9	17
66	Towards computational specificity screening of DNA-binding proteins. *Nucleic Acids Research*, **2011**, 39, 8281-90	20.1	17
65	Thermodynamic control of -1 programmed ribosomal frameshifting. *Nature Communications*, **2019**, 10, 4598	17.4	16
64	Structural determinants and mechanism of mammalian CRM1 allostery. *Structure*, **2013**, 21, 1350-60	5.2	16
63	MD simulations and FRET reveal an environment-sensitive conformational plasticity of importin- *Biophysical Journal*, **2015**, 109, 277-86	2.9	15
62	TatBC-independent TatA/Tat substrate interactions contribute to transport efficiency. *PLoS ONE*, **2015**, 10, e0119761	3.7	15
61	The Low Barrier Hydrogen Bond in the Photoactive Yellow Protein: A Vacuum Artifact Absent in the Crystal and Solution. *Journal of the American Chemical Society*, **2016**, 138, 16620-16631	16.4	15
60	Force distribution analysis of mechanochemically reactive dimethylcyclobutene. *ChemPhysChem*, **2013**, 14, 2687-97	3.2	14
59	Elastic Properties of Photoswitchable Azobenzene Polymers from Molecular Dynamics Simulations. *Angewandte Chemie*, **2007**, 119, 2282-2287	3.6	14
58	Mechanochemical Energy Transduction during the Main Rotary Step in the Synthesis Cycle of F-ATPase. *Journal of the American Chemical Society*, **2017**, 139, 4025-4034	16.4	13
57	Exploiting Lipid Permutation Symmetry to Compute Membrane Remodeling Free Energies. *Physical Review Letters*, **2016**, 117, 188102	7.4	13
56	Accurate Three States Model for Amino Acids with Two Chemically Coupled Titrating Sites in Explicit Solvent Atomistic Constant pH Simulations and pK(a) Calculations. *Journal of Chemical Theory and Computation*, **2017**, 13, 147-160	6.4	12

55	Bayesian orientation estimate and structure information from sparse single-molecule x-ray diffraction images. *Physical Review E*, **2014**, 90, 022714	2.4	12
54	Spatiotemporal Resolution of Conformational Changes in Biomolecules by Combining Pulsed Electron-Electron Double Resonance Spectroscopy with Microsecond Freeze-Hyperquenching. *Journal of the American Chemical Society*, **2021**, 143, 6981-6989	16.4	12
53	Sharing Data from Molecular Simulations. *Journal of Chemical Information and Modeling*, **2019**, 59, 4093-4099	4.1	11
52	Transient Secondary and Tertiary Structure Formation Kinetics in the Intrinsically Disordered State of α-Synuclein from Atomistic Simulations. *ChemPhysChem*, **2018**, 19, 2507-2511	3.2	11
51	Universal relaxation governs the nonequilibrium elasticity of biomolecules. *Physical Review Letters*, **2012**, 109, 118304	7.4	11
50	Determining Free-Energy Differences Through Variationally Derived Intermediates. *Journal of Chemical Theory and Computation*, **2020**, 16, 3504-3512	6.4	10
49	What happens if the room at the bottom runs out? A close look at small water pores. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 7421-2	11.5	10
48	Binding affinities controlled by shifting conformational equilibria: opportunities and limitations. *Biophysical Journal*, **2015**, 108, 2585-2590	2.9	9
47	Computing Spatially Resolved Rotational Hydration Entropies from Atomistic Simulations. *Journal of Chemical Theory and Computation*, **2020**, 16, 108-118	6.4	8
46	Phi29 Connector-DNA Interactions Govern DNA Crunching and Rotation, Supporting the Check-Valve Model. *Biophysical Journal*, **2016**, 110, 455-469	2.9	8
45	Molecular determinants of snurportin 1 ligand affinity and structural response upon binding. *Biophysical Journal*, **2009**, 97, 581-9	2.9	6
44	Microtubule instability driven by longitudinal and lateral strain propagation. *PLoS Computational Biology*, **2020**, 16, e1008132	5	6
43	Structural and mechanistic basis for translation inhibition by macrolide and ketolide antibiotics. *Nature Communications*, **2021**, 12, 4466	17.4	6
42	tRNA Dissociation from EF-Tu after GTP Hydrolysis: Primary Steps and Antibiotic Inhibition. *Biophysical Journal*, **2020**, 118, 151-161	2.9	5
41	Per|Mut: Spatially Resolved Hydration Entropies from Atomistic Simulations. *Journal of Chemical Theory and Computation*, **2021**, 17, 2090-2098	6.4	5
40	A Quantitative Model for cAMP Binding to the Binding Domain of MloK1. *Biophysical Journal*, **2016**, 111, 1668-1678	2.9	4
39	How proteins open fusion pores: insights from molecular simulations. *European Biophysics Journal*, **2021**, 50, 279-293	1.9	4
38	Sequential Water and Headgroup Merger: Membrane Poration Paths and Energetics from MD Simulations. *Biophysical Journal*, **2020**, 119, 2418-2430	2.9	4

37	How accurate is circular dichroism-based model validation?. *European Biophysics Journal*, **2020**, 49, 497-510	1.9	4
36	Choice of fluorophore affects dynamic DNA nanostructures. *Nucleic Acids Research*, **2021**, 49, 4186-4195	20.1	4
35	Variationally derived intermediates for correlated free-energy estimates between intermediate states. *Physical Review E*, **2020**, 102, 043312	2.4	3
34	Probing the Accuracy of Explicit Solvent Constant pH Molecular Dynamics Simulations for Peptides. *Journal of Chemical Theory and Computation*, **2020**, 16, 2561-2569	6.4	3
33	Estimating the Orientational Entropy of Water at Protein Interfaces. *Biophysical Journal*, **2011**, 100, 613a	2.9	3
32	Molekulare Nanomaschinen unter der Lupe: Proteindynamik-Simulationen. *Physik in Unserer Zeit*, **2006**, 37, 73-79	0.1	3
31	Kraftspektroskopie von einzelnen Biomolekülen: Biologische Makromoleküle besser begreifen – mit Einzelmolekül-Kraftmessungen und Computersimulationen. *Physik Journal*, **2001**, 57, 55-61		3
30	Tight docking of membranes before fusion represents a metastable state with unique properties. *Nature Communications*, **2021**, 12, 3606	17.4	3
29	GROMACS implementation of free energy calculations with non-pairwise Variationally derived Intermediates. *Computer Physics Communications*, **2021**, 264, 107931	4.2	3
28	Time-Lagged Independent Component Analysis of Random Walks and Protein Dynamics. *Journal of Chemical Theory and Computation*, **2021**, 17, 5766-5776	6.4	3
27	Schrittweise Bindung zweiwertiger Kationen an Phospholipid-Membranen: eine Molekúldynamikstudie. *Angewandte Chemie*, **2004**, 116, 1039-1042	3.6	2
26	GROMEX: A Scalable and Versatile Fast Multipole Method for Biomolecular Simulation. *Lecture Notes in Computational Science and Engineering*, **2020**, 517-543	0.3	2
25	Sequential water and headgroup merger: Membrane poration paths and energetics from MD simulations		2
24	Spatially resolved free-energy contributions of native fold and molten-globule-like Crambin. *Biophysical Journal*, **2021**, 120, 3470-3482	2.9	2
23	BASDet: Bayesian approach(es) for structure determination from single molecule X-ray diffraction images. *Computer Physics Communications*, **2016**, 201, 159-166	4.2	1
22	Inside Cover: Primary Steps of pH-Dependent Insulin Aggregation Kinetics are Governed by Conformational Flexibility (ChemBioChem 11/2009). *ChemBioChem*, **2009**, 10, 1742-1742	3.8	1
21	Microtubule instability driven by longitudinal and lateral strain propagation		1
20	Effects of cryo-EM cooling on structural ensembles		1

19	Choice of fluorophore affects dynamic DNA nanostructures		1
18	A CUDA fast multipole method with highly efficient M2L far field evaluation. *International Journal of High Performance Computing Applications*, **2021**, 35, 97-117	1.8	1
17	ATP-Magnesium Coordination: Protein Structure-Based Force Field Evaluation and Corrections. *Journal of Chemical Theory and Computation*, **2021**, 17, 1922-1930	6.4	1
16	Nanomechanics combined with HDX reveal allosteric drug binding sites of CFTR NBD1		1
15	Effects of cryo-EM cooling on structural ensembles.. *Nature Communications*, **2022**, 13, 1709	17.4	1
14	Estimating ruggedness of free-energy landscapes of small globular proteins from principal component analysis of molecular dynamics trajectories.. *Physical Review E*, **2022**, 105, 044404	2.4	1
13	Small-sample limit of the Bennett acceptance ratio method and the variationally derived intermediates.. *Physical Review E*, **2021**, 104, 054133	2.4	0
12	Implementation of a Bayesian secondary structure estimation method for the SESCA circular dichroism analysis package. *Computer Physics Communications*, **2021**, 266, 108022	4.2	0
11	Bending-torsional elasticity and energetics of the plus-end microtubule tip.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119, e2115516119	11.5	0
10	Ein Kraftpuffer schützt Titinimmunglobulin. *Angewandte Chemie*, **2010**, 122, 3607-3610	3.6	
9	Cover Picture: Multistep Binding of Divalent Cations to Phospholipid Bilayers: A Molecular Dynamics Study (Angew. Chem. Int. Ed. 8/2004). *Angewandte Chemie - International Edition*, **2004**, 43, 911-911	16.4	
8	Titelbild: Schrittweise Bindung zweiwertiger Kationen an Phospholipid-Membranen: eine Molekül dynamikstudie (Angew. Chem. 8/2004). *Angewandte Chemie*, **2004**, 116, 929-929	3.6	
7	Atomistic Simulations of the Human Proteasome Inhibited by a Covalent Ligand **2021**, 47-57		
6	Microtubule instability driven by longitudinal and lateral strain propagation **2020**, 16, e1008132		
5	Microtubule instability driven by longitudinal and lateral strain propagation **2020**, 16, e1008132		
4	Microtubule instability driven by longitudinal and lateral strain propagation **2020**, 16, e1008132		
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1 Microtubule instability driven by longitudinal and lateral strain propagation **2020**, 16, e1008132