

# Helmut Grubmüller

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Effects of cryo-EM cooling on structural ensembles.. <i>Nature Communications</i> , <b>2022</b> , 13, 1709	17.4	1
161	Bending-torsional elasticity and energetics of the plus-end microtubule tip.. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2022</b> , 119, e2115516119	11.5	0
160	Estimating ruggedness of free-energy landscapes of small globular proteins from principal component analysis of molecular dynamics trajectories.. <i>Physical Review E</i> , <b>2022</b> , 105, 044404	2.4	1
159	Atomistic Simulations of the Human Proteasome Inhibited by a Covalent Ligand <b>2021</b> , 47-57		
158	Small-sample limit of the Bennett acceptance ratio method and the variationally derived intermediates.. <i>Physical Review E</i> , <b>2021</b> , 104, 054133	2.4	0
157	How proteins open fusion pores: insights from molecular simulations. <i>European Biophysics Journal</i> , <b>2021</b> , 50, 279-293	1.9	4
156	Choice of fluorophore affects dynamic DNA nanostructures. <i>Nucleic Acids Research</i> , <b>2021</b> , 49, 4186-4195	20.1	4
155	Per Mut: Spatially Resolved Hydration Entropies from Atomistic Simulations. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 2090-2098	6.4	5
154	Spatiotemporal Resolution of Conformational Changes in Biomolecules by Combining Pulsed Electron-Electron Double Resonance Spectroscopy with Microsecond Freeze-Hyperquenching. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 6981-6989	16.4	12
153	Tight docking of membranes before fusion represents a metastable state with unique properties. <i>Nature Communications</i> , <b>2021</b> , 12, 3606	17.4	3
152	GROMACS implementation of free energy calculations with non-pairwise Variationally derived Intermediates. <i>Computer Physics Communications</i> , <b>2021</b> , 264, 107931	4.2	3
151	A CUDA fast multipole method with highly efficient M2L far field evaluation. <i>International Journal of High Performance Computing Applications</i> , <b>2021</b> , 35, 97-117	1.8	1
150	ATP-Magnesium Coordination: Protein Structure-Based Force Field Evaluation and Corrections. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 1922-1930	6.4	1
149	Structural and mechanistic basis for translation inhibition by macrolide and ketolide antibiotics. <i>Nature Communications</i> , <b>2021</b> , 12, 4466	17.4	6
148	Spatially resolved free-energy contributions of native fold and molten-globule-like Crambin. <i>Biophysical Journal</i> , <b>2021</b> , 120, 3470-3482	2.9	2
147	Time-Lagged Independent Component Analysis of Random Walks and Protein Dynamics. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 5766-5776	6.4	3
146	Implementation of a Bayesian secondary structure estimation method for the SESCA circular dichroism analysis package. <i>Computer Physics Communications</i> , <b>2021</b> , 266, 108022	4.2	0

145	Variationally derived intermediates for correlated free-energy estimates between intermediate states. <i>Physical Review E</i> , <b>2020</b> , 102, 043312	2.4	3
144	Determining Free-Energy Differences Through Variationally Derived Intermediates. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 3504-3512	6.4	10
143	Probing the Accuracy of Explicit Solvent Constant pH Molecular Dynamics Simulations for Peptides. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 2561-2569	6.4	3
142	GROMEX: A Scalable and Versatile Fast Multipole Method for Biomolecular Simulation. <i>Lecture Notes in Computational Science and Engineering</i> , <b>2020</b> , 517-543	0.3	2
141	tRNA Dissociation from EF-Tu after GTP Hydrolysis: Primary Steps and Antibiotic Inhibition. <i>Biophysical Journal</i> , <b>2020</b> , 118, 151-161	2.9	5
140	Computing Spatially Resolved Rotational Hydration Entropies from Atomistic Simulations. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 108-118	6.4	8
139	A GPU-Accelerated Fast Multipole Method for GROMACS: Performance and Accuracy. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 6938-6949	6.4	21
138	Sequential Water and Headgroup Merger: Membrane Poration Paths and Energetics from MD Simulations. <i>Biophysical Journal</i> , <b>2020</b> , 119, 2418-2430	2.9	4
137	How accurate is circular dichroism-based model validation?. <i>European Biophysics Journal</i> , <b>2020</b> , 49, 497-510		4
136	Microtubule instability driven by longitudinal and lateral strain propagation. <i>PLoS Computational Biology</i> , <b>2020</b> , 16, e1008132	5	6
135	Microtubule instability driven by longitudinal and lateral strain propagation <b>2020</b> , 16, e1008132		
134	Microtubule instability driven by longitudinal and lateral strain propagation <b>2020</b> , 16, e1008132		
133	Microtubule instability driven by longitudinal and lateral strain propagation <b>2020</b> , 16, e1008132		
132	Microtubule instability driven by longitudinal and lateral strain propagation <b>2020</b> , 16, e1008132		
131	Microtubule instability driven by longitudinal and lateral strain propagation <b>2020</b> , 16, e1008132		
130	Microtubule instability driven by longitudinal and lateral strain propagation <b>2020</b> , 16, e1008132		
129	Sharing Data from Molecular Simulations. <i>Journal of Chemical Information and Modeling</i> , <b>2019</b> , 59, 4093-4099		11
128	Heterogeneous and rate-dependent streptavidin-biotin unbinding revealed by high-speed force spectroscopy and atomistic simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2019</b> , 116, 6594-6601	11.5	55

127	SESCA: Predicting Circular Dichroism Spectra from Protein Molecular Structures. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 5087-5102	6.4	22
126	More bang for your buck: Improved use of GPU nodes for GROMACS 2018. <i>Journal of Computational Chemistry</i> , <b>2019</b> , 40, 2418-2431	3.5	122
125	Thermodynamic control of -1 programmed ribosomal frameshifting. <i>Nature Communications</i> , <b>2019</b> , 10, 4598	17.4	16
124	Automated cryo-EM structure refinement using correlation-driven molecular dynamics. <i>ELife</i> , <b>2019</b> , 8,	8.9	38
123	Active role of elongation factor G in maintaining the mRNA reading frame during translation. <i>Science Advances</i> , <b>2019</b> , 5, eaax8030	14.3	18
122	The 2018 biomembrane curvature and remodeling roadmap. <i>Journal Physics D: Applied Physics</i> , <b>2018</b> , 51,	3	133
121	Transient Secondary and Tertiary Structure Formation Kinetics in the Intrinsically Disordered State of $\beta$ Synuclein from Atomistic Simulations. <i>ChemPhysChem</i> , <b>2018</b> , 19, 2507-2511	3.2	11
120	Microtubule assembly governed by tubulin allosteric gain in flexibility and lattice induced fit. <i>ELife</i> , <b>2018</b> , 7,	8.9	26
119	Molecular simulations of the ribosome and associated translation factors. <i>Current Opinion in Structural Biology</i> , <b>2018</b> , 49, 27-35	8.1	19
118	Structure determination from single molecule X-ray scattering with three photons per image. <i>Nature Communications</i> , <b>2018</b> , 9, 2375	17.4	25
117	Engineering fatty acid synthases for directed polyketide production. <i>Nature Chemical Biology</i> , <b>2017</b> , 13, 363-365	11.7	50
116	Mechanochemical Energy Transduction during the Main Rotary Step in the Synthesis Cycle of F-ATPase. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 4025-4034	16.4	13
115	Accurate Three States Model for Amino Acids with Two Chemically Coupled Titrating Sites in Explicit Solvent Atomistic Constant pH Simulations and pK(a) Calculations. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 147-160	6.4	12
114	Structural Basis for Polyproline-Mediated Ribosome Stalling and Rescue by the Translation Elongation Factor EF-P. <i>Molecular Cell</i> , <b>2017</b> , 68, 515-527.e6	17.6	73
113	CHARMM36m: an improved force field for folded and intrinsically disordered proteins. <i>Nature Methods</i> , <b>2017</b> , 14, 71-73	21.6	1819
112	Cationic and Anionic Impact on the Electronic Structure of Liquid Water. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 3759-3764	6.4	21
111	NuSol $\square$ Numerical solver for the 3D stationary nuclear Schrödinger equation. <i>Computer Physics Communications</i> , <b>2016</b> , 198, 169-178	4.2	20
110	The pathway to GTPase activation of elongation factor SelB on the ribosome. <i>Nature</i> , <b>2016</b> , 540, 80-85	50.4	63

109	Exploiting Lipid Permutation Symmetry to Compute Membrane Remodeling Free Energies. <i>Physical Review Letters</i> , <b>2016</b> , 117, 188102	7.4	13
108	A Quantitative Model for cAMP Binding to the Binding Domain of MloK1. <i>Biophysical Journal</i> , <b>2016</b> , 111, 1668-1678	2.9	4
107	BASDet: Bayesian approach(es) for structure determination from single molecule X-ray diffraction images. <i>Computer Physics Communications</i> , <b>2016</b> , 201, 159-166	4.2	1
106	Charge-Neutral Constant pH Molecular Dynamics Simulations Using a Parsimonious Proton Buffer. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 1040-51	6.4	22
105	The Low Barrier Hydrogen Bond in the Photoactive Yellow Protein: A Vacuum Artifact Absent in the Crystal and Solution. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 16620-16631	16.4	15
104	A combined cryo-EM and molecular dynamics approach reveals the mechanism of ErmBL-mediated translation arrest. <i>Nature Communications</i> , <b>2016</b> , 7, 12026	17.4	66
103	Phi29 Connector-DNA Interactions Govern DNA Crunching and Rotation, Supporting the Check-Valve Model. <i>Biophysical Journal</i> , <b>2016</b> , 110, 455-469	2.9	8
102	Lipid binding defects and perturbed synaptogenic activity of a Collybistin R290H mutant that causes epilepsy and intellectual disability. <i>Journal of Biological Chemistry</i> , <b>2015</b> , 290, 8256-70	5.4	26
101	MD simulations and FRET reveal an environment-sensitive conformational plasticity of importin- $\beta$ . <i>Biophysical Journal</i> , <b>2015</b> , 109, 277-86	2.9	15
100	do_x3dna: a tool to analyze structural fluctuations of dsDNA or dsRNA from molecular dynamics simulations. <i>Bioinformatics</i> , <b>2015</b> , 31, 2583-5	7.2	49
99	Hydrophobic mismatch sorts SNARE proteins into distinct membrane domains. <i>Nature Communications</i> , <b>2015</b> , 6, 5984	17.4	89
98	Structural Ensembles of Intrinsically Disordered Proteins Depend Strongly on Force Field: A Comparison to Experiment. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 5513-24	6.4	281
97	Dynamic contact network between ribosomal subunits enables rapid large-scale rotation during spontaneous translocation. <i>Nucleic Acids Research</i> , <b>2015</b> , 43, 6747-60	20.1	23
96	Best bang for your buck: GPU nodes for GROMACS biomolecular simulations. <i>Journal of Computational Chemistry</i> , <b>2015</b> , 36, 1990-2008	3.5	130
95	PspF-binding domain PspA1-144 and the PspAIF complex: New insights into the coiled-coil-dependent regulation of AAA+ proteins. <i>Molecular Microbiology</i> , <b>2015</b> , 98, 743-59	4.1	30
94	TatBC-independent TatA/Tat substrate interactions contribute to transport efficiency. <i>PLoS ONE</i> , <b>2015</b> , 10, e0119761	3.7	15
93	Binding affinities controlled by shifting conformational equilibria: opportunities and limitations. <i>Biophysical Journal</i> , <b>2015</b> , 108, 2585-2590	2.9	9
92	Free energy landscape of rim-pore expansion in membrane fusion. <i>Biophysical Journal</i> , <b>2014</b> , 107, 2287-259	2.0	20

91	Anomalous surface diffusion of protons on lipid membranes. <i>Biophysical Journal</i> , <b>2014</b> , 107, 76-87	2.9	46
90	Elastic properties and heterogeneous stiffness of the phi29 motor connector channel. <i>Biophysical Journal</i> , <b>2014</b> , 106, 1338-48	2.9	19
89	Bayesian orientation estimate and structure information from sparse single-molecule x-ray diffraction images. <i>Physical Review E</i> , <b>2014</b> , 90, 022714	2.4	12
88	AMBER-DYES: Characterization of Charge Fluctuations and Force Field Parameterization of Fluorescent Dyes for Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 5505-12	6.4	29
87	Expansion of the fusion stalk and its implication for biological membrane fusion. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2014</b> , 111, 11043-8	11.5	72
86	Force distribution analysis of mechanochemically reactive dimethylcyclobutene. <i>ChemPhysChem</i> , <b>2013</b> , 14, 2687-97	3.2	14
85	Energy barriers and driving forces in tRNA translocation through the ribosome. <i>Nature Structural and Molecular Biology</i> , <b>2013</b> , 20, 1390-6	17.6	117
84	Structural determinants and mechanism of mammalian CRM1 allostery. <i>Structure</i> , <b>2013</b> , 21, 1350-60	5.2	16
83	g_contacts: Fast contact search in bio-molecular ensemble data. <i>Computer Physics Communications</i> , <b>2013</b> , 184, 2856-2859	4.2	26
82	Proteins in the gas phase. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2013</b> , 3, 408-425	4.5	40
81	Structural basis for cooperativity of CRM1 export complex formation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2013</b> , 110, 960-5	11.5	50
80	How SNARE molecules mediate membrane fusion: recent insights from molecular simulations. <i>Current Opinion in Structural Biology</i> , <b>2012</b> , 22, 187-96	8.1	109
79	Linear-scaling soft-core scheme for alchemical free energy calculations. <i>Journal of Computational Chemistry</i> , <b>2012</b> , 33, 25-33	3.5	32
78	Quantitative assessment of protein interaction with methyl-lysine analogues by hybrid computational and experimental approaches. <i>ACS Chemical Biology</i> , <b>2012</b> , 7, 150-4	4.9	38
77	Universal relaxation governs the nonequilibrium elasticity of biomolecules. <i>Physical Review Letters</i> , <b>2012</b> , 109, 118304	7.4	11
76	Exploring protein dynamics space: the dynasome as the missing link between protein structure and function. <i>PLoS ONE</i> , <b>2012</b> , 7, e33931	3.7	65
75	Line-tension controlled mechanism for influenza fusion. <i>PLoS ONE</i> , <b>2012</b> , 7, e38302	3.7	51
74	Estimating the Orientational Entropy of Water at Protein Interfaces. <i>Biophysical Journal</i> , <b>2011</b> , 100, 6132-9	2.9	3

73	Velocity-dependent mechanical unfolding of bacteriorhodopsin is governed by a dynamic interaction network. <i>Biophysical Journal</i> , <b>2011</b> , 100, 1109-19	2.9	17
72	Keep It Flexible: Driving Macromolecular Rotary Motions in Atomistic Simulations with GROMACS. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 1381-1393	6.4	33
71	Determining equilibrium constants for dimerization reactions from molecular dynamics simulations. <i>Journal of Computational Chemistry</i> , <b>2011</b> , 32, 1919-28	3.5	45
70	Caught in the act: visualization of SNARE-mediated fusion events in molecular detail. <i>ChemBioChem</i> , <b>2011</b> , 12, 1049-55	3.8	109
69	Constant pH Molecular Dynamics in Explicit Solvent with E Dynamics. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 1962-1978	6.4	130
68	Towards computational specificity screening of DNA-binding proteins. <i>Nucleic Acids Research</i> , <b>2011</b> , 39, 8281-90	20.1	17
67	Torsional elasticity and energetics of F1-ATPase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2011</b> , 108, 7408-13	11.5	41
66	Structural heterogeneity and quantitative FRET efficiency distributions of polyprolines through a hybrid atomistic simulation and Monte Carlo approach. <i>PLoS ONE</i> , <b>2011</b> , 6, e19791	3.7	95
65	Estimating absolute configurational entropies of macromolecules: the minimally coupled subspace approach. <i>PLoS ONE</i> , <b>2010</b> , 5, e9179	3.7	53
64	Molecular basis of the light-driven switching of the photochromic fluorescent protein Padron. <i>Journal of Biological Chemistry</i> , <b>2010</b> , 285, 14603-9	5.4	58
63	Primary changes of the mechanical properties of Southern Bean Mosaic Virus upon calcium removal. <i>Biophysical Journal</i> , <b>2010</b> , 98, 687-95	2.9	23
62	An unusual hydrophobic core confers extreme flexibility to HEAT repeat proteins. <i>Biophysical Journal</i> , <b>2010</b> , 99, 1596-603	2.9	53
61	Quantitative structural analysis of importin- $\beta$ flexibility: paradigm for solenoid protein structures. <i>Structure</i> , <b>2010</b> , 18, 1171-83	5.2	72
60	Ein Kraftpuffer schützt Titinimmunglobulin. <i>Angewandte Chemie</i> , <b>2010</b> , 122, 3607-3610	3.6	
59	A "force buffer" protecting immunoglobulin titin. <i>Angewandte Chemie - International Edition</i> , <b>2010</b> , 49, 3528-31	16.4	22
58	Adaptive anisotropic kernels for nonparametric estimation of absolute configurational entropies in high-dimensional configuration spaces. <i>Physical Review E</i> , <b>2009</b> , 80, 011913	2.4	19
57	Kinase-activity-independent functions of atypical protein kinase C in Drosophila. <i>Journal of Cell Science</i> , <b>2009</b> , 122, 3759-71	5.3	58
56	Primary steps of pH-dependent insulin aggregation kinetics are governed by conformational flexibility. <i>ChemBioChem</i> , <b>2009</b> , 10, 1816-22	3.8	31

55	Inside Cover: Primary Steps of pH-Dependent Insulin Aggregation Kinetics are Governed by Conformational Flexibility (ChemBioChem 11/2009). <i>ChemBioChem</i> , <b>2009</b> , 10, 1742-1742	3.8	1
54	Accuracy and convergence of free energy differences calculated from nonequilibrium switching processes. <i>Journal of Computational Chemistry</i> , <b>2009</b> , 30, 447-56	3.5	66
53	Dynamics and energetics of permeation through aquaporins. What do we learn from molecular dynamics simulations?. <i>Handbook of Experimental Pharmacology</i> , <b>2009</b> , 57-76	3.2	76
52	Mechanical properties of the icosahedral shell of southern bean mosaic virus: a molecular dynamics study. <i>Biophysical Journal</i> , <b>2009</b> , 96, 1350-63	2.9	102
51	Urea impedes the hydrophobic collapse of partially unfolded proteins. <i>Biophysical Journal</i> , <b>2009</b> , 96, 3744-52	4.5	68
50	Molecular determinants of snurportin 1 ligand affinity and structural response upon binding. <i>Biophysical Journal</i> , <b>2009</b> , 97, 581-9	2.9	6
49	Importin-beta: structural and dynamic determinants of a molecular spring. <i>Structure</i> , <b>2008</b> , 16, 906-15	5.2	44
48	Kinetics, statistics, and energetics of lipid membrane electroporation studied by molecular dynamics simulations. <i>Biophysical Journal</i> , <b>2008</b> , 95, 1837-50	2.9	230
47	Recognition dynamics up to microseconds revealed from an RDC-derived ubiquitin ensemble in solution. <i>Science</i> , <b>2008</b> , 320, 1471-5	33.3	872
46	Polar or apolar--the role of polarity for urea-induced protein denaturation. <i>PLoS Computational Biology</i> , <b>2008</b> , 4, e1000221	5	61
45	Chromophore protonation state controls photoswitching of the fluoroprotein asFP595. <i>PLoS Computational Biology</i> , <b>2008</b> , 4, e1000034	5	89
44	Full correlation analysis of conformational protein dynamics. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2008</b> , 70, 1294-312	4.2	108
43	Photoswitching of the fluorescent protein asFP595: mechanism, proton pathways, and absorption spectra. <i>Angewandte Chemie - International Edition</i> , <b>2007</b> , 46, 530-6	16.4	89
42	Elastic properties of photoswitchable azobenzene polymers from molecular dynamics simulations. <i>Angewandte Chemie - International Edition</i> , <b>2007</b> , 46, 2232-7	16.4	46
41	Photoswitching of the Fluorescent Protein asFP595: Mechanism, Proton Pathways, and Absorption Spectra. <i>Angewandte Chemie</i> , <b>2007</b> , 119, 536-542	3.6	25
40	Elastic Properties of Photoswitchable Azobenzene Polymers from Molecular Dynamics Simulations. <i>Angewandte Chemie</i> , <b>2007</b> , 119, 2282-2287	3.6	14
39	Speeding up parallel GROMACS on high-latency networks. <i>Journal of Computational Chemistry</i> , <b>2007</b> , 28, 2075-84	3.5	98
38	Estimation of absolute solvent and solvation shell entropies via permutation reduction. <i>Journal of Chemical Physics</i> , <b>2007</b> , 126, 014102	3.9	37



37	Fluctuations of primary ubiquitin folding intermediates in a force clamp. <i>Journal of Structural Biology</i> , <b>2007</b> , 157, 557-69	3.4	27
36	A highly strained nuclear conformation of the exportin Cse1p revealed by molecular dynamics simulations. <i>Structure</i> , <b>2006</b> , 14, 1469-78	5.2	26
35	Flooding in GROMACS: accelerated barrier crossings in molecular dynamics. <i>Journal of Computational Chemistry</i> , <b>2006</b> , 27, 1693-702	3.5	53
34	Collective Langevin dynamics of conformational motions in proteins. <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 214903	3.9	89
33	Molecular anatomy of a trafficking organelle. <i>Cell</i> , <b>2006</b> , 127, 831-46	56.2	1670
32	Molekulare Nanomaschinen unter der Lupe: Proteindynamik-Simulationen. <i>Physik in Unserer Zeit</i> , <b>2006</b> , 37, 73-79	0.1	3
31	Generalized correlation for biomolecular dynamics. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2006</b> , 62, 1053-61	4.2	278
30	Mechanically induced titin kinase activation studied by force-probe molecular dynamics simulations. <i>Biophysical Journal</i> , <b>2005</b> , 88, 790-804	2.9	181
29	The dynamics and energetics of water permeation and proton exclusion in aquaporins. <i>Current Opinion in Structural Biology</i> , <b>2005</b> , 15, 176-83	8.1	242
28	Molecular dynamics simulations of protein G challenge NMR-derived correlated backbone motions. <i>Angewandte Chemie - International Edition</i> , <b>2005</b> , 44, 3394-9	16.4	24
27	Structure and mechanism of the reversible photoswitch of a fluorescent protein. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2005</b> , 102, 13070-4	11.5	222
26	Multistep binding of divalent cations to phospholipid bilayers: a molecular dynamics study. <i>Angewandte Chemie - International Edition</i> , <b>2004</b> , 43, 1021-4	16.4	164
25	Cover Picture: Multistep Binding of Divalent Cations to Phospholipid Bilayers: A Molecular Dynamics Study (Angew. Chem. Int. Ed. 8/2004). <i>Angewandte Chemie - International Edition</i> , <b>2004</b> , 43, 911-911	16.4	
24	Schrittweise Bindung zweiwertiger Kationen an Phospholipid-Membranen: eine Molek�ldynamikstudie. <i>Angewandte Chemie</i> , <b>2004</b> , 116, 1039-1042	3.6	2
23	Titelbild: Schrittweise Bindung zweiwertiger Kationen an Phospholipid-Membranen: eine Molek�ldynamikstudie (Angew. Chem. 8/2004). <i>Angewandte Chemie</i> , <b>2004</b> , 116, 929-929	3.6	
22	What happens if the room at the bottom runs out? A close look at small water pores. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2003</b> , 100, 7421-2	11.5	10
21	The structure of the aquaporin-1 water channel: a comparison between cryo-electron microscopy and X-ray crystallography. <i>Journal of Molecular Biology</i> , <b>2003</b> , 325, 485-93	6.5	45
20	The mechanism of proton exclusion in the aquaporin-1 water channel. <i>Journal of Molecular Biology</i> , <b>2003</b> , 333, 279-93	6.5	233

19	Conformational dynamics of the F1-ATPase beta-subunit: a molecular dynamics study. <i>Biophysical Journal</i> , <b>2003</b> , 85, 1482-91	2.9	38
18	Mechanical coupling via the membrane fusion SNARE protein syntaxin 1A: a molecular dynamics study. <i>Biophysical Journal</i> , <b>2003</b> , 84, 1527-47	2.9	60
17	Maximum likelihood trajectories from single molecule fluorescence resonance energy transfer experiments. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 9920-9924	3.9	57
16	Membrane fusion. <i>Current Opinion in Cell Biology</i> , <b>2002</b> , 14, 488-95	9	167
15	Structure and function of water channels. <i>Current Opinion in Structural Biology</i> , <b>2002</b> , 12, 509-15	8.1	227
14	Predicting unimolecular chemical reactions: Chemical flooding. <i>Journal of Chemical Physics</i> , <b>2002</b> , 116, 897-905	3.9	56
13	Water permeation through gramicidin A: desformylation and the double helix: a molecular dynamics study. <i>Biophysical Journal</i> , <b>2002</b> , 82, 2934-42	2.9	80
12	Essential dynamics of reversible peptide folding: memory-free conformational dynamics governed by internal hydrogen bonds. <i>Journal of Molecular Biology</i> , <b>2001</b> , 309, 299-313	6.5	119
11	A refined structure of human aquaporin-1. <i>FEBS Letters</i> , <b>2001</b> , 504, 206-11	3.8	110
10	Kraftspektroskopie von einzelnen Biomolekülen: Biologische Makromoleküle besser begreifen □ mit Einzelmolekülkraftmessungen und Computersimulationen. <i>Physik Journal</i> , <b>2001</b> , 57, 55-61		3
9	Dynamic force spectroscopy of molecular adhesion bonds. <i>Physical Review Letters</i> , <b>2000</b> , 84, 6126-9	7.4	145
8	The fold of human aquaporin 1. <i>Journal of Molecular Biology</i> , <b>2000</b> , 300, 987-94	6.5	30
7	Multiple time step algorithms for molecular dynamics simulations of proteins: How good are they?. <i>Journal of Computational Chemistry</i> , <b>1998</b> , 19, 1534-1552	3.5	31
6	Predicting slow structural transitions in macromolecular systems: Conformational flooding. <i>Physical Review E</i> , <b>1995</b> , 52, 2893-2906	2.4	502
5	Microtubule instability driven by longitudinal and lateral strain propagation		1
4	Effects of cryo-EM cooling on structural ensembles		1
3	Sequential water and headgroup merger: Membrane poration paths and energetics from MD simulations		2
2	Choice of fluorophore affects dynamic DNA nanostructures		1

1 Nanomechanics combined with HDX reveal allosteric drug binding sites of CFTR NBD1

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