

Helmut GrubmÃ¼ller

List of Publications by Year in descending order

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154
papers

16,822
citations

26630

56
h-index

17105

122
g-index

176
all docs

176
docs citations

176
times ranked

18600
citing authors

#	ARTICLE	IF	CITATIONS
1	Folding of VemP into translation-arresting secondary structure is driven by the ribosome exit tunnel. <i>Nucleic Acids Research</i> , 2022, 50, 2258-2269.	14.5	8
2	GROMACS in the Cloud: A Global Supercomputer to Speed Up Alchemical Drug Design. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1691-1711.	5.4	37
3	Effects of cryo-EM cooling on structural ensembles. <i>Nature Communications</i> , 2022, 13, 1709.	12.8	33
4	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> , 2022, 119, e2115516119.	7.1	7
5	Estimating ruggedness of free-energy landscapes of small globular proteins from principal component analysis of molecular dynamics trajectories. <i>Physical Review E</i> , 2022, 105, 044404.	2.1	6
6	Intersubunit Coupling Enables Fast CO ₂ -Fixation by Reductive Carboxylases. <i>ACS Central Science</i> , 2022, 8, 1091-1101.	11.3	10
7	A CUDA fast multipole method with highly efficient M2L far field evaluation. <i>International Journal of High Performance Computing Applications</i> , 2021, 35, 97-117.	3.7	3
8	ATP-Magnesium Coordination: Protein Structure-Based Force Field Evaluation and Corrections. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1922-1930.	5.3	19
9	Choice of fluorophore affects dynamic DNA nanostructures. <i>Nucleic Acids Research</i> , 2021, 49, 4186-4195.	14.5	20
10	Per Mut: Spatially Resolved Hydration Entropies from Atomistic Simulations. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2090-2098.	5.3	13
11	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> , 2021, 143, 6981-6989.	13.7	33
12	Tight docking of membranes before fusion represents a metastable state with unique properties. <i>Nature Communications</i> , 2021, 12, 3606.	12.8	20
13	GROMACS implementation of free energy calculations with non-pairwise Variationally derived Intermediates. <i>Computer Physics Communications</i> , 2021, 264, 107931.	7.5	7
14	Structural and mechanistic basis for translation inhibition by macrolide and ketolide antibiotics. <i>Nature Communications</i> , 2021, 12, 4466.	12.8	43
15	Spatially resolved free-energy contributions of Native fold and molten-globule-like Crambin. <i>Biophysical Journal</i> , 2021, 120, 3470-3482.	0.5	10
16	Time-Lagged Independent Component Analysis of Random Walks and Protein Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5766-5776.	5.3	27
17	Implementation of a Bayesian secondary structure estimation method for the SESCA circular dichroism analysis package. <i>Computer Physics Communications</i> , 2021, 266, 108022.	7.5	6
18	How proteins open fusion pores: insights from molecular simulations. <i>European Biophysics Journal</i> , 2021, 50, 279-293.	2.2	17

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19	Small-sample limit of the Bennett acceptance ratio method and the variationally derived intermediates. <i>Physical Review E</i> , 2021, 104, 054133.	2.1	2
20	Atomistic Simulations of the Human Proteasome Inhibited by a Covalent Ligand. , 2021, , 47-57.		0
21	tRNA Dissociation from EF-Tu after GTP Hydrolysis: Primary Steps and Antibiotic Inhibition. <i>Biophysical Journal</i> , 2020, 118, 151-161.	0.5	19
22	Computing Spatially Resolved Rotational Hydration Entropies from Atomistic Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 108-118.	5.3	15
23	A GPU-Accelerated Fast Multipole Method for GROMACS: Performance and Accuracy. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6938-6949.	5.3	68
24	Sequential Water and Headgroup Merger: Membrane Poration Paths and Energetics from MD Simulations. <i>Biophysical Journal</i> , 2020, 119, 2418-2430.	0.5	8
25	How accurate is circular dichroism-based model validation?. <i>European Biophysics Journal</i> , 2020, 49, 497-510.	2.2	10
26	Microtubule instability driven by longitudinal and lateral strain propagation. <i>PLoS Computational Biology</i> , 2020, 16, e1008132.	3.2	15
27	Variationally derived intermediates for correlated free-energy estimates between intermediate states. <i>Physical Review E</i> , 2020, 102, 043312.	2.1	3
28	Determining Free-Energy Differences Through Variationally Derived Intermediates. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3504-3512.	5.3	15
29	Probing the Accuracy of Explicit Solvent Constant pH Molecular Dynamics Simulations for Peptides. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2561-2569.	5.3	13
30	GROMEX: A Scalable and Versatile Fast Multipole Method for Biomolecular Simulation. <i>Lecture Notes in Computational Science and Engineering</i> , 2020, , 517-543.	0.3	2
31	Microtubule instability driven by longitudinal and lateral strain propagation. , 2020, 16, e1008132.		0
32	Microtubule instability driven by longitudinal and lateral strain propagation. , 2020, 16, e1008132.		0
33	Microtubule instability driven by longitudinal and lateral strain propagation. , 2020, 16, e1008132.		0
34	Microtubule instability driven by longitudinal and lateral strain propagation. , 2020, 16, e1008132.		0
35	Microtubule instability driven by longitudinal and lateral strain propagation. , 2020, 16, e1008132.		0
36	Microtubule instability driven by longitudinal and lateral strain propagation. , 2020, 16, e1008132.		0

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37	SESCA: Predicting Circular Dichroism Spectra from Protein Molecular Structures. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5087-5102.	5.3	54
38	More bang for your buck: Improved use of GPU nodes for GROMACS 2018. <i>Journal of Computational Chemistry</i> , 2019, 40, 2418-2431.	3.3	286
39	Thermodynamic control of ~ 1 programmed ribosomal frameshifting. <i>Nature Communications</i> , 2019, 10, 4598.	12.8	34
40	Sharing Data from Molecular Simulations. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4093-4099.	5.4	26
41	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> , 2019, 116, 6594-6601.	7.1	95
42	Active role of elongation factor G in maintaining the mRNA reading frame during translation. <i>Science Advances</i> , 2019, 5, eaax8030.	10.3	38
43	Automated cryo-EM structure refinement using correlation-driven molecular dynamics. <i>ELife</i> , 2019, 8, .	6.0	83
44	Molecular simulations of the ribosome and associated translation factors. <i>Current Opinion in Structural Biology</i> , 2018, 49, 27-35.	5.7	33
45	Structure determination from single molecule X-ray scattering with three photons per image. <i>Nature Communications</i> , 2018, 9, 2375.	12.8	34
46	The 2018 biomembrane curvature and remodeling roadmap. <i>Journal Physics D: Applied Physics</i> , 2018, 51, 343001.	2.8	212
47	Transient Secondary and Tertiary Structure Formation Kinetics in the Intrinsically Disordered State of ϵ -Synuclein from Atomistic Simulations. <i>ChemPhysChem</i> , 2018, 19, 2507-2511.	2.1	17
48	Microtubule assembly governed by tubulin allosteric gain in flexibility and lattice induced fit. <i>ELife</i> , 2018, 7, .	6.0	42
49	Engineering fatty acid synthases for directed polyketide production. <i>Nature Chemical Biology</i> , 2017, 13, 363-365.	8.0	63
50	Mechanochemical Energy Transduction during the Main Rotary Step in the Synthesis Cycle of F_1F_0 -ATPase. <i>Journal of the American Chemical Society</i> , 2017, 139, 4025-4034.	13.7	23
51	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> , 2017, 13, 147-160.	5.3	27
52	Structural Basis for Polyproline-Mediated Ribosome Stalling and Rescue by the Translation Elongation Factor EF-P. <i>Molecular Cell</i> , 2017, 68, 515-527.e6.	9.7	118
53	CHARMM36m: an improved force field for folded and intrinsically disordered proteins. <i>Nature Methods</i> , 2017, 14, 71-73.	19.0	3,959
54	Cationic and Anionic Impact on the Electronic Structure of Liquid Water. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3759-3764.	4.6	26

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55	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> , 2016, 138, 16620-16631.	13.7	18
56	A combined cryo-EM and molecular dynamics approach reveals the mechanism of ErmBL-mediated translation arrest. <i>Nature Communications</i> , 2016, 7, 12026.	12.8	103
57	Phi29 Connector-DNA Interactions Govern DNA Crunching and Rotation, Supporting the Check-Valve Model. <i>Biophysical Journal</i> , 2016, 110, 455-469.	0.5	10
58	The pathway to GTPase activation of elongation factor SelB on the ribosome. <i>Nature</i> , 2016, 540, 80-85.	27.8	93
59	Exploiting Lipid Permutation Symmetry to Compute Membrane Remodeling Free Energies. <i>Physical Review Letters</i> , 2016, 117, 188102.	7.8	27
60	A Quantitative Model for cAMP Binding to the Binding Domain of MloK1. <i>Biophysical Journal</i> , 2016, 111, 1668-1678.	0.5	4
61	BASDet: Bayesian approach(es) for structure determination from single molecule X-ray diffraction images. <i>Computer Physics Communications</i> , 2016, 201, 159-166.	7.5	2
62	Charge-Neutral Constant pH Molecular Dynamics Simulations Using a Parsimonious Proton Buffer. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1040-1051.	5.3	44
63	NuSol – Numerical solver for the 3D stationary nuclear Schrödinger equation. <i>Computer Physics Communications</i> , 2016, 198, 169-178.	7.5	28
64	Best bang for your buck: GPU nodes for GROMACS biomolecular simulations. <i>Journal of Computational Chemistry</i> , 2015, 36, 1990-2008.	3.3	195
65	PspF binding domain of PspA ₁₄₄ and the PspA-F complex: New insights into the coiled-coil dependent regulation of AAA+ proteins. <i>Molecular Microbiology</i> , 2015, 98, 743-759.	2.5	33
66	TatBC-Independent TatA/Tat Substrate Interactions Contribute to Transport Efficiency. <i>PLoS ONE</i> , 2015, 10, e0119761.	2.5	20
67	Binding Affinities Controlled by Shifting Conformational Equilibria: Opportunities and Limitations. <i>Biophysical Journal</i> , 2015, 108, 2585-2590.	0.5	10
68	Lipid Binding Defects and Perturbed Synaptogenic Activity of a Collybistin R290H Mutant That Causes Epilepsy and Intellectual Disability. <i>Journal of Biological Chemistry</i> , 2015, 290, 8256-8270.	3.4	32
69	MD Simulations and FRET Reveal an Environment-Sensitive Conformational Plasticity of Importin- β^2 . <i>Biophysical Journal</i> , 2015, 109, 277-286.	0.5	23
70	do_x3dna: a tool to analyze structural fluctuations of dsDNA or dsRNA from molecular dynamics simulations. <i>Bioinformatics</i> , 2015, 31, 2583-2585.	4.1	59
71	Hydrophobic mismatch sorts SNARE proteins into distinct membrane domains. <i>Nature Communications</i> , 2015, 6, 5984.	12.8	130
72	Structural Ensembles of Intrinsically Disordered Proteins Depend Strongly on Force Field: A Comparison to Experiment. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5513-5524.	5.3	368

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73	Dynamic contact network between ribosomal subunits enables rapid large-scale rotation during spontaneous translocation. <i>Nucleic Acids Research</i> , 2015, 43, 6747-6760.	14.5	36
74	Bayesian orientation estimate and structure information from sparse single-molecule x-ray diffraction images. <i>Physical Review E</i> , 2014, 90, 022714.	2.1	12
75	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> , 2014, 10, 5505-5512.	5.3	44
76	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> , 2014, 111, 11043-11048.	7.1	99
77	Free Energy Landscape of Rim-Pore Expansion in Membrane Fusion. <i>Biophysical Journal</i> , 2014, 107, 2287-2295.	0.5	30
78	Anomalous Surface Diffusion of Protons on Lipid Membranes. <i>Biophysical Journal</i> , 2014, 107, 76-87.	0.5	55
79	Elastic Properties and Heterogeneous Stiffness of the Phi29 Motor Connector Channel. <i>Biophysical Journal</i> , 2014, 106, 1338-1348.	0.5	21
80	Force Distribution Analysis of Mechanochemically Reactive Dimethylcyclobutene. <i>ChemPhysChem</i> , 2013, 14, 2687-2697.	2.1	15
81	Energy barriers and driving forces in tRNA translocation through the ribosome. <i>Nature Structural and Molecular Biology</i> , 2013, 20, 1390-1396.	8.2	150
82	Structural Determinants and Mechanism of Mammalian CRM1 Allostery. <i>Structure</i> , 2013, 21, 1350-1360.	3.3	17
83	g_contacts: Fast contact search in bio-molecular ensemble data. <i>Computer Physics Communications</i> , 2013, 184, 2856-2859.	7.5	37
84	Proteins in the gas phase. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2013, 3, 408-425.	14.6	49
85	Structural basis for cooperativity of CRM1 export complex formation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 960-965.	7.1	64
86	Quantitative Assessment of Protein Interaction with Methyl-Lysine Analogues by Hybrid Computational and Experimental Approaches. <i>ACS Chemical Biology</i> , 2012, 7, 150-154.	3.4	42
87	Universal Relaxation Governs the Nonequilibrium Elasticity of Biomolecules. <i>Physical Review Letters</i> , 2012, 109, 118304.	7.8	12
88	Exploring Protein Dynamics Space: The Dynasome as the Missing Link between Protein Structure and Function. <i>PLoS ONE</i> , 2012, 7, e33931.	2.5	83
89	How SNARE molecules mediate membrane fusion: Recent insights from molecular simulations. <i>Current Opinion in Structural Biology</i> , 2012, 22, 187-196.	5.7	121
90	Linear scaling soft-core scheme for alchemical free energy calculations. <i>Journal of Computational Chemistry</i> , 2012, 33, 25-33.	3.3	37

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91	Line-Tension Controlled Mechanism for Influenza Fusion. PLoS ONE, 2012, 7, e38302.	2.5	63
92	Constant pH Molecular Dynamics in Explicit Solvent with $\hat{\mu}$ -Dynamics. Journal of Chemical Theory and Computation, 2011, 7, 1962-1978.	5.3	163
93	Estimating the Orientational Entropy of Water at Protein Interfaces. Biophysical Journal, 2011, 100, 613a.	0.5	4
94	Velocity-Dependent Mechanical Unfolding of Bacteriorhodopsin Is Governed by a Dynamic Interaction Network. Biophysical Journal, 2011, 100, 1109-1119.	0.5	17
95	Keep It Flexible: Driving Macromolecular Rotary Motions in Atomistic Simulations with GROMACS. Journal of Chemical Theory and Computation, 2011, 7, 1381-1393.	5.3	42
96	Determining equilibrium constants for dimerization reactions from molecular dynamics simulations. Journal of Computational Chemistry, 2011, 32, 1919-1928.	3.3	69
97	Caught in the Act: Visualization of SNARE-Mediated Fusion Events in Molecular Detail. ChemBioChem, 2011, 12, 1049-1055.	2.6	134
98	Towards computational specificity screening of DNA-binding proteins. Nucleic Acids Research, 2011, 39, 8281-8290.	14.5	20
99	Torsional elasticity and energetics of F ₁ -ATPase. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 7408-7413.	7.1	46
100	Structural Heterogeneity and Quantitative FRET Efficiency Distributions of Polyprolines through a Hybrid Atomistic Simulation and Monte Carlo Approach. PLoS ONE, 2011, 6, e19791.	2.5	108
101	Quantitative Structural Analysis of Importin- β Flexibility: Paradigm for Solenoid Protein Structures. Structure, 2010, 18, 1171-1183.	3.3	89
102	A α -Force Buffer-Protecting Immunoglobulin Titin. Angewandte Chemie - International Edition, 2010, 49, 3528-3531.	13.8	23
103	Estimating Absolute Configurational Entropies of Macromolecules: The Minimally Coupled Subspace Approach. PLoS ONE, 2010, 5, e9179.	2.5	57
104	Molecular Basis of the Light-driven Switching of the Photochromic Fluorescent Protein Padron. Journal of Biological Chemistry, 2010, 285, 14603-14609.	3.4	65
105	Primary Changes of the Mechanical Properties of Southern Bean Mosaic Virus upon Calcium Removal. Biophysical Journal, 2010, 98, 687-695.	0.5	25
106	An Unusual Hydrophobic Core Confers Extreme Flexibility to HEAT Repeat Proteins. Biophysical Journal, 2010, 99, 1596-1603.	0.5	66
107	Adaptive anisotropic kernels for nonparametric estimation of absolute configurational entropies in high-dimensional configuration spaces. Physical Review E, 2009, 80, 011913.	2.1	21
108	Kinase-activity-independent functions of atypical protein kinase C in Drosophila. Journal of Cell Science, 2009, 122, 3759-3771.	2.0	67

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109	Primary Steps of pH-Dependent Insulin Aggregation Kinetics are Governed by Conformational Flexibility. <i>ChemBioChem</i> , 2009, 10, 1816-1822.	2.6	39
110	Inside Cover: Primary Steps of pH-Dependent Insulin Aggregation Kinetics are Governed by Conformational Flexibility (<i>ChemBioChem</i> 11/2009). <i>ChemBioChem</i> , 2009, 10, 1742-1742.	2.6	1
111	Accuracy and convergence of free energy differences calculated from nonequilibrium switching processes. <i>Journal of Computational Chemistry</i> , 2009, 30, 447-456.	3.3	81
112	Dynamics and Energetics of Permeation Through Aquaporins. What Do We Learn from Molecular Dynamics Simulations?. <i>Handbook of Experimental Pharmacology</i> , 2009, , 57-76.	1.8	92
113	Mechanical Properties of the Icosahedral Shell of Southern Bean Mosaic Virus: A Molecular Dynamics Study. <i>Biophysical Journal</i> , 2009, 96, 1350-1363.	0.5	117
114	Urea Impedes the Hydrophobic Collapse of Partially Unfolded Proteins. <i>Biophysical Journal</i> , 2009, 96, 3744-3752.	0.5	69
115	Molecular Determinants of Snurportin 1 Ligand Affinity and Structural Response upon Binding. <i>Biophysical Journal</i> , 2009, 97, 581-589.	0.5	7
116	Full correlation analysis of conformational protein dynamics. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 70, 1294-1312.	2.6	122
117	Importin- β : Structural and Dynamic Determinants of a Molecular Spring. <i>Structure</i> , 2008, 16, 906-915.	3.3	49
118	Kinetics, Statistics, and Energetics of Lipid Membrane Electroporation Studied by Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2008, 95, 1837-1850.	0.5	280
119	Recognition Dynamics Up to Microseconds Revealed from an RDC-Derived Ubiquitin Ensemble in Solution. <i>Science</i> , 2008, 320, 1471-1475.	12.6	963
120	Polar or Apolar? The Role of Polarity for Urea-Induced Protein Denaturation. <i>PLoS Computational Biology</i> , 2008, 4, e1000221.	3.2	65
121	Chromophore Protonation State Controls Photoswitching of the Fluoroprotein asFP595. <i>PLoS Computational Biology</i> , 2008, 4, e1000034.	3.2	98
122	Estimation of absolute solvent and solvation shell entropies via permutation reduction. <i>Journal of Chemical Physics</i> , 2007, 126, 014102.	3.0	43
123	Fluctuations of primary ubiquitin folding intermediates in a force clamp. <i>Journal of Structural Biology</i> , 2007, 157, 557-569.	2.8	28
124	Photoswitching of the Fluorescent Protein asFP595: Mechanism, Proton Pathways, and Absorption Spectra. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 530-536.	13.8	95
125	Elastic Properties of Photoswitchable Azobenzene Polymers from Molecular Dynamics Simulations. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 2232-2237.	13.8	46
126	Speeding up parallel GROMACS on high-latency networks. <i>Journal of Computational Chemistry</i> , 2007, 28, 2075-2084.	3.3	107

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127	Collective Langevin dynamics of conformational motions in proteins. <i>Journal of Chemical Physics</i> , 2006, 124, 214903.	3.0	114
128	Molecular Anatomy of a Trafficking Organelle. <i>Cell</i> , 2006, 127, 831-846.	28.9	1,985
129	A Highly Strained Nuclear Conformation of the Exportin Cse1p Revealed by Molecular Dynamics Simulations. <i>Structure</i> , 2006, 14, 1469-1478.	3.3	27
130	Flooding in GROMACS: Accelerated barrier crossings in molecular dynamics. <i>Journal of Computational Chemistry</i> , 2006, 27, 1693-1702.	3.3	63
131	The dynamics and energetics of water permeation and proton exclusion in aquaporins. <i>Current Opinion in Structural Biology</i> , 2005, 15, 176-183.	5.7	263
132	Molecular Dynamics Simulations of Protein G Challenge NMR-Derived Correlated Backbone Motions. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 3394-3399.	13.8	25
133	Generalized correlation for biomolecular dynamics. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 62, 1053-1061.	2.6	380
134	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> , 2005, 102, 13070-13074.	7.1	253
135	Mechanically Induced Titin Kinase Activation Studied by Force-Probe Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2005, 88, 790-804.	0.5	195
136	Multistep Binding of Divalent Cations to Phospholipid Bilayers: A Molecular Dynamics Study. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 1021-1024.	13.8	173
137	Cover Picture: Multistep Binding of Divalent Cations to Phospholipid Bilayers: A Molecular Dynamics Study (<i>Angew. Chem. Int. Ed.</i> 8/2004). <i>Angewandte Chemie - International Edition</i> , 2004, 43, 911-911.	13.8	0
138	The Structure of the Aquaporin-1 Water Channel: A Comparison between Cryo-electron Microscopy and X-ray Crystallography. <i>Journal of Molecular Biology</i> , 2003, 325, 485-493.	4.2	51
139	The Mechanism of Proton Exclusion in the Aquaporin-1 Water Channel. <i>Journal of Molecular Biology</i> , 2003, 333, 279-293.	4.2	257
140	Conformational Dynamics of the F1-ATPase $\hat{\gamma}$ -Subunit: A Molecular Dynamics Study. <i>Biophysical Journal</i> , 2003, 85, 1482-1491.	0.5	38
141	Mechanical Coupling via the Membrane Fusion SNARE Protein Syntaxin 1A: A Molecular Dynamics Study. <i>Biophysical Journal</i> , 2003, 84, 1527-1547.	0.5	66
142	Maximum likelihood trajectories from single molecule fluorescence resonance energy transfer experiments. <i>Journal of Chemical Physics</i> , 2003, 119, 9920-9924.	3.0	62
143	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> , 2003, 100, 7421-7422.	7.1	10
144	Predicting unimolecular chemical reactions: Chemical flooding. <i>Journal of Chemical Physics</i> , 2002, 116, 897-905.	3.0	63

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145	Water Permeation through Gramicidin A: Desformylation and the Double Helix: A Molecular Dynamics Study. <i>Biophysical Journal</i> , 2002, 82, 2934-2942.	0.5	89
146	Membrane fusion. <i>Current Opinion in Cell Biology</i> , 2002, 14, 488-495.	5.4	181
147	Structure and Function of Water Channels. <i>Current Opinion in Structural Biology</i> , 2002, 12, 509-515.	5.7	246
148	Essential dynamics of reversible peptide folding: memory-free conformational dynamics governed by internal hydrogen bonds. <i>Journal of Molecular Biology</i> , 2001, 309, 299-313.	4.2	126
149	A refined structure of human aquaporin-1. <i>FEBS Letters</i> , 2001, 504, 206-211.	2.8	120
150	Kraftspektroskopie von einzelnen Biomolekülen: Biologische Makromoleküle besser begreifen – mit Einzelmolekülkraftmessungen und Computersimulationen. <i>Physik Journal</i> , 2001, 57, 55-61.	0.1	4
151	Dynamic Force Spectroscopy of Molecular Adhesion Bonds. <i>Physical Review Letters</i> , 2000, 84, 6126-6129.	7.8	152
152	The Fold of Human Aquaporin 1. <i>Journal of Molecular Biology</i> , 2000, 300, 987-994.	4.2	34
153	Multiple time step algorithms for molecular dynamics simulations of proteins: How good are they?. <i>Journal of Computational Chemistry</i> , 1998, 19, 1534-1552.	3.3	33
154	Predicting slow structural transitions in macromolecular systems: Conformational flooding. <i>Physical Review E</i> , 1995, 52, 2893-2906.	2.1	573