Bert L De Groot

List of Publications by Year
in descending order

186 papers	20,876 citations	18887 64 h-index	14012 133 g-index
211 all docs	211 docs citations	211 times ranked	23713 citing authors

#	Article	IF	Citations
1	<scp>Preâ€exascale HPC</scp> approaches for molecular dynamics simulations. Covidâ€19 research: A use case. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	6.2	6
2	Direct Detection of Bound Ammonium Ions in the Selectivity Filter of Ion Channels by Solid-State NMR. Journal of the American Chemical Society, 2022, 144, 4147-4157.	6.6	7
3	Pre-Exascale Computing of Proteinâ€“Ligand Binding Free Energies with Open Source Software for Drug Design. Journal of Chemical Information and Modeling, 2022, 62, 1172-1177.	2.5	22
4	GROMACS in the Cloud: A Global Supercomputer to Speed Up Alchemical Drug Design. Journal of Chemical Information and Modeling, 2022, 62, 1691-1711.	2.5	37
5	Repositioning Food and Drug Administration-Approved Drugs for Inhibiting Biliverdin IXÎ² Reductase B as a Novel Thrombocytopenia Therapeutic Target. Journal of Medicinal Chemistry, 2022, 65, 2548-2557.	2.9	1
6	A litmus test for classifying recognition mechanisms of transiently binding proteins. Nature Communications, 2022, 13, .	5.8	13
7	Non-equilibrium approach for binding free energies in cyclodextrins in SAMPL7: force fields and software. Journal of Computer-Aided Molecular Design, 2021, 35, 49-61.	1.3	23
8	Visualization of the mechanosensitive ion channel MscS under membrane tension. Nature, 2021, 590, 509-514.	13.7	77
9	ATPâ€“Magnesium Coordination: Protein Structure-Based Force Field Evaluation and Corrections. Journal of Chemical Theory and Computation, 2021, 17, 1922-1930.	2.3	19
10	Lipid-Protein Interactions Modulate the Conformational Equilibrium of a Potassium Channel. Biophysical Journal, 2021, 120, 157a.	0.2	0
11	Structure, gating and interactions of the voltage-dependent anion channel. European Biophysics Journal, 2021, 50, 159-172.	1.2	28
12	One Plus One Makes Three: Triangular Coupling of Correlated Amino Acid Mutations. Journal of Physical Chemistry Letters, 2021, 12, 3195-3201.	2.1	4
13	Structural plasticity of the selectivity filter in a nonselective ion channel. IUCrJ, 2021, 8, 421-430.	1.0	13
14	Challenges Encountered Applying Equilibrium and Nonequilibrium Binding Free Energy Calculations. Journal of Physical Chemistry B, 2021, 125, 4241-4261.	1.2	33
15	Accurate absolute free energies for ligandâ€“protein binding based on non-equilibrium approaches. Communications Chemistry, 2021, 4, .	2.0	49
16	The Persistent Question of Potassium Channel Permeation Mechanisms. Journal of Molecular Biology, 2021, 433, 167002.	2.0	55
17	Alchemical absolute proteinâ€“ligand binding free energies for drug design. Chemical Science, 2021, 12, 13958-13971.	3.7	48
18	Lipidâ€“protein forces predict conformational changes in a mechanosensitive channel. European Biophysics Journal, 2021, 50, 181-186.	1.2	3

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19	Comment on â€œDeficiencies in Molecular Dynamics Simulation-Based Prediction of Protein-DNA Binding Free Energy Landscapesâ€. Journal of Physical Chemistry B, 2020, 124, 1115-1123.	1.2	4
20	Large scale relative protein ligand binding affinities using non-equilibrium alchemy. Chemical Science, 2020, 11, 1140-1152.	3.7	147
21	Enhancing NMR derived ensembles with kinetics on multiple timescales. Journal of Biomolecular NMR, 2020, 74, 27-43.	1.6	12
22	Structural Basis for Glycerol Efflux and Selectivity of Human Aquaporin 7. Structure, 2020, 28, 215-222.e3.	1.6	43
23	Structural basis for antibiotic action of the B1 antivitamin 2â€²-methoxy-thiamine. Nature Chemical Biology, 2020, 16, 1237-1245.	3.9	13
24	A Î²-barrel for oil transport through lipid membranes: Dynamic NMR structures of AlkL. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 21014-21021.	3.3	52
25	Non-active site mutants of HIV-1 protease influence resistance and sensitisation towards protease inhibitors. Retrovirology, 2020, 17, 13.	0.9	12
26	Simulating Streaming Potentials in Potassium Channels. Biophysical Journal, 2020, 118, 168a.	0.2	0
27	Force Field Error Diagnosis and Structure-Driven Correction for the ATP-Magnesium Complex. Biophysical Journal, 2020, 118, 143a.	0.2	0
28	The SAMPL6 SAMPLing challenge: assessing the reliability and efficiency of binding free energy calculations. Journal of Computer-Aided Molecular Design, 2020, 34, 601-633.	1.3	86
29	The structure of a potassium-selective ion channel reveals a hydrophobic gate regulating ion permeation. IUCrJ, 2020, 7, 835-843.	1.0	8
30	On the importance of statistics in molecular simulations for thermodynamics, kinetics and simulation box size. ELife, 2020, 9, .	2.8	34
31	The conduction pathway of potassium channels is water free under physiological conditions. Science Advances, 2019, 5, eaaw6756.	4.7	48
32	Predicting Kinase Inhibitor Resistance: Physics-Based and Data-Driven Approaches. ACS Central Science, 2019, 5, 1468-1474.	5.3	40
33	More bang for your buck: Improved use of GPU nodes for GROMACS 2018. Journal of Computational Chemistry, 2019, 40, 2418-2431.	1.5	286
34	Performance evaluation of molecular docking and free energy calculations protocols using the D3R Grand Challenge 4 dataset. Journal of Computer-Aided Molecular Design, 2019, 33, 1031-1043.	1.3	12
35	Lipid Bilayer Composition Influences the Activity ofÂthe Antimicrobial Peptide Dermcidin Channel. Biophysical Journal, 2019, 116, 1658-1666.	0.2	20
36	Identification of kinetic order parameters for non-equilibrium dynamics. Journal of Chemical Physics, 2019, 150, 164120.	1.2	31

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37	Thermodynamic Coupling - Free Energy Calculations of Correlated Amino Acid Mutations. Biophysical Journal, 2019, 116, 463a.	0.2	0
38	Pyruvate carboxylase deficiency type A and type C: Characterization of five novel pathogenic variants inPCand analysis of the genotypeâ€“phenotype correlation. Human Mutation, 2019, 40, 816-827.	1.1	16
39	A molecular mechanism for transthyretin amyloidogenesis. Nature Communications, 2019, 10, 925.	5.8	92
40	A pharmacological master key mechanism that unlocks the selectivity filter gate in K ⁺ channels. Science, 2019, 363, 875-880.	6.0	91
41	Molecular mechanism of a potassium channel gating through activation gate-selectivity filter coupling. Nature Communications, 2019, 10, 5366.	5.8	83
42	GROmaïs: A GROMACS-Based Toolset to Analyze Density Maps Derived from Molecular Dynamics Simulations. Biophysical Journal, 2019, 116, 4-11.	0.2	73
43	Conotoxin ÎºM-RIIIJ, a tool targeting asymmetric heteromeric K _v 1 channels. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 1059-1064.	3.3	17
44	Mechanistic Insights into Microsecond Time-Scale Motion of Solid Proteins Using Complementary ¹⁵N and ¹H Relaxation Dispersion Techniques. Journal of the American Chemical Society, 2019, 141, 858-869.	6.6	49
45	Interpretation of Interfacial Protein Spectra with Enhanced Molecular Simulation Ensembles. Journal of Chemical Theory and Computation, 2019, 15, 698-707.	2.3	4
46	Accurate Calculation of Free Energy Changes upon Amino Acid Mutation. Methods in Molecular Biology, 2019, 1851, 19-47.	0.4	32
47	Comment on 'Valid molecular dynamics simulations of human hemoglobin require a surprisingly large box size'. ELife, 2019, 8, .	2.8	35
48	Utilizing dipole-dipole cross-correlated relaxation for the measurement of angles between pairs of opposing CÎ±HÎ±-CÎ±HÎ± bonds in anti-parallel Î²-sheets. Methods, 2018, 138-139, 85-92.	1.9	8
49	In silico assessment of the conduction mechanism of the Ryanodine Receptor 1 reveals previously unknown exit pathways. Scientific Reports, 2018, 8, 6886.	1.6	13
50	Mechanism of Mechanosensitive Gating of the TREK-2 Potassium Channel. Biophysical Journal, 2018, 114, 1336-1343.	0.2	38
51	A single NaK channel conformation is not enough for non-selective ion conduction. Nature Communications, 2018, 9, 717.	5.8	52
52	Accurate Estimation of Ligand Binding Affinity Changes upon Protein Mutation. ACS Central Science, 2018, 4, 1708-1718.	5.3	82
53	Quantifying Asymmetry of Multimeric Proteins. Journal of Physical Chemistry A, 2018, 122, 7924-7930.	1.1	1
54	ATP as a Fuel Molecule: Evolutionary Selection of Magnesium-ATP Interaction Mode Facilitates Lossless Chemomechanical Coupling for ATPases. Biophysical Journal, 2018, 114, 680a.	0.2	1

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55	Consistent Prediction of Mutation Effect on Drug Binding in HIV-1 Protease Using Alchemical Calculations. Journal of Chemical Theory and Computation, 2018, 14, 3397-3408.	2.3	24
56	Direct knock-on of desolvated ions governs strict ion selectivity in K+ channels. Nature Chemistry, 2018, 10, 813-820.	6.6	170
57	pmx Webserver: A User Friendly Interface for Alchemistry. Journal of Chemical Information and Modeling, 2017, 57, 109-114.	2.5	50
58	Gating Charge Calculations by Computational Electrophysiology Simulations. Biophysical Journal, 2017, 112, 1396-1405.	0.2	11
59	Role of Pore-Lining Residues in Defining the Rate of Water Conduction by Aquaporin-0. Biophysical Journal, 2017, 112, 953-965.	0.2	14
60	Resolving the Atomistic Modes of Anle138b Inhibitory Action on Peptide Oligomer Formation. ACS Chemical Neuroscience, 2017, 8, 2791-2808.	1.7	26
61	Alchemical Free Energy Calculations for Nucleotide Mutations in Proteinâ€“DNA Complexes. Journal of Chemical Theory and Computation, 2017, 13, 6275-6289.	2.3	42
62	Temperature dependence of protein-water interactions in a gated yeast aquaporin. Scientific Reports, 2017, 7, 4016.	1.6	9
63	CHARMM36m: an improved force field for folded and intrinsically disordered proteins. Nature Methods, 2017, 14, 71-73.	9.0	3,959
64	Localization and Ordering of Lipids Around Aquaporin-0: Protein and Lipid Mobility Effects. Frontiers in Physiology, 2017, 8, 124.	1.3	24
65	Recent advances in measuring the kinetics of biomolecules by NMR relaxation dispersion spectroscopy. Archives of Biochemistry and Biophysics, 2017, 628, 81-91.	1.4	30
66	Crystal Structure of an Ammonia-Permeable Aquaporin. PLoS Biology, 2016, 14, e1002411.	2.6	108
67	Insights into the function of ion channels by computational electrophysiology simulations. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1741-1752.	1.4	60
68	Aquaporin 4 as a NH3 Channel. Journal of Biological Chemistry, 2016, 291, 19184-19195.	1.6	27
69	Voltage Dependence of Conformational Dynamics and Subconducting States of VDAC-1. Biophysical Journal, 2016, 111, 1223-1234.	0.2	28
70	Insights into the molecular basis for substrate binding and specificity of the wild-type L-arginine/agmatine antiporter AdiC. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 10358-10363.	3.3	82
71	An Atomistic View of Amyloidogenic Self-assembly: Structure and Dynamics of Heterogeneous Conformational States in the Pre-nucleation Phase. Scientific Reports, 2016, 6, 33156.	1.6	25
72	Accurate and Rigorous Prediction of the Changes in Protein Free Energies in a Largeâ€Scale Mutation Scan. Angewandte Chemie - International Edition, 2016, 55, 7364-7368.	7.2	111

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73	Partial least squares for dependent data. Biometrika, 2016, 103, 351-362.	1.3	10
74	A Non-canonical Voltage-Sensing Mechanism Controls Gating in K2P K+ Channels. Cell, 2016, 164, 937-949.	13.5	169
75	Allosteric switch regulates proteinâ€“protein binding through collective motion. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 3269-3274.	3.3	57
76	Best bang for your buck: GPU nodes for <scp>GROMACS</scp> biomolecular simulations. Journal of Computational Chemistry, 2015, 36, 1990-2008.	1.5	195
77	H95 Is a pH-Dependent Gate in Aquaporin 4. Structure, 2015, 23, 2309-2318.	1.6	47
78	Binding Affinities Controlled by Shifting Conformational Equilibria: Opportunities and Limitations. Biophysical Journal, 2015, 108, 2585-2590.	0.2	10
79	Mechanisms of Anion Conduction by Coupled Glutamate Transporters. Cell, 2015, 160, 542-553.	13.5	114
80	The membrane anchor of the transcriptional activator SREBP is characterized by intrinsic conformational flexibility. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 12390-12395.	3.3	14
81	Structural Ensembles of Intrinsically Disordered Proteins Depend Strongly on Force Field: A Comparison to Experiment. Journal of Chemical Theory and Computation, 2015, 11, 5513-5524.	2.3	368
82	Improved validation of IDP ensembles by one-bond CÎ±â€“HÎ± scalar couplings. Journal of Biomolecular NMR, 2015, 63, 299-307.	1.6	4
83	His 95 Acts as a pH Gate in Aquaporin-4. Biophysical Journal, 2015, 108, 316a.	0.2	0
84	pmx: Automated protein structure and topology generation for alchemical perturbations. Journal of Computational Chemistry, 2015, 36, 348-354.	1.5	199
85	Population Shuffling of Protein Conformations. Angewandte Chemie - International Edition, 2015, 54, 207-210.	7.2	57
86	Calculation of Binding Free Energies. Methods in Molecular Biology, 2015, 1215, 173-209.	0.4	95
87	Quantifying Artifacts in Ewald Simulations of Inhomogeneous Systems with a Net Charge. Journal of Chemical Theory and Computation, 2014, 10, 381-390.	2.3	176
88	Ion permeation in K ⁺ channels occurs by direct Coulomb knock-on. Science, 2014, 346, 352-355.	6.0	271
89	A Designed Conformational Shift To Control Protein Binding Specificity. Angewandte Chemie - International Edition, 2014, 53, 10367-10371.	7.2	45
90	Spontaneous Aggregation of the Insulin-Derived Steric Zipper Peptide VEALYL Results in Different Aggregation Forms with Common Features. Journal of Molecular Biology, 2014, 426, 362-376.	2.0	21

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91	The identification of novel, high affinity AQP9 inhibitors in an intracellular binding site. Molecular Membrane Biology, 2013, 30, 246-260.	2.0	33
92	Phosphorylation Drives a Dynamic Switch in Serine/Arginine-Rich Proteins. Structure, 2013, 21, 2162-2174.	1.6	101
93	Discovery of Novel Human Aquaporin-1 Blockers. ACS Chemical Biology, 2013, 8, 249-256.	1.6	58
94	Molecular Recognition through Concerted Ubiquitin Backbone and Side Chain Motion Determined from NMR and MD Simulations. Biophysical Journal, 2013, 104, 30a.	0.2	0
95	Channel Crystal Structure and Antimicrobial Mechanism of Dermcidin from Human Skin. Biophysical Journal, 2013, 104, 241a.	0.2	0
96	Optimal Superpositioning of Flexible Molecule Ensembles. Biophysical Journal, 2013, 104, 196-207.	0.2	25
97	Collective Dynamics Underlying Allosteric Transitions in Hemoglobin. PLoS Computational Biology, 2013, 9, e1003232.	1.5	27
98	Probing the Energy Landscape of Activation Gating of the Bacterial Potassium Channel KcsA. PLoS Computational Biology, 2013, 9, e1003058.	1.5	31
99	Crystal structure and functional mechanism of a human antimicrobial membrane channel. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 4586-4591.	3.3	104
100	Phosphorylation of rat aquaporinâ€4 at Ser¹¹¹ is not required for channel gating. Glia, 2013, 61, 1101-1112.	2.5	34
101	Molecular driving forces defining lipid positions around aquaporin-0. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 9887-9892.	3.3	60
102	Driving Forces and Structural Determinants of Steric Zipper Peptide Oligomer Formation Elucidated by Atomistic Simulations. Journal of Molecular Biology, 2012, 421, 390-416.	2.0	64
103	New Soft-Core Potential Function for Molecular Dynamics Based Alchemical Free Energy Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2373-2382.	2.3	92
104	Partial Least-Squares Functional Mode Analysis: Application to the Membrane Proteins AQP1, Aqy1, and CLC-ec1. Biophysical Journal, 2012, 103, 786-796.	0.2	57
105	Design of Peptide-Membrane Interactions to Modulate Single-File Water Transport through Modified Gramicidin Channels. Biophysical Journal, 2012, 103, 1698-1705.	0.2	8
106	Î²-Barrel Mobility Underlies Closure of the Voltage-Dependent Anion Channel. Structure, 2012, 20, 1540-1549.	1.6	104
107	A Molecular Switch Driving Inactivation in the Cardiac K+ Channel hERG. PLoS ONE, 2012, 7, e41023.	1.1	19
108	Molecular Dynamics in Principal Component Space. Journal of Physical Chemistry B, 2012, 116, 8350-8354.	1.2	21

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109	Identification of Selective Inhibitors of the Potassium Channel Kv1.1â€“1.2₍₃₎ by Highâ€Throughput Virtual Screening and Automated Patch Clamp. ChemMedChem, 2012, 7, 1775-1783.	1.6	20
110	Comment on â€œMolecular Selectivity in Aquaporin Channels Studied by the 3D-RISM Theoryâ€. Journal of Physical Chemistry B, 2011, 115, 8364-8366.	1.2	5
111	Computational Electrophysiology: The Molecular Dynamics of Ion Channel Permeation and Selectivity in Atomistic Detail. Biophysical Journal, 2011, 101, 809-817.	0.2	214
112	Computational Electrophysiology on Vdac-1 reveals Mechanism of Anion Flux. Biophysical Journal, 2011, 100, 267a.	0.2	0
113	Mapping the Conformational Dynamics and Pathways of Spontaneous Steric Zipper Peptide Oligomerization. PLoS ONE, 2011, 6, e19129.	1.1	45
114	Towards computional specificity screening of DNA-binding proteins. Nucleic Acids Research, 2011, 39, 8281-8290.	6.5	20
115	Aquaporin-9 Protein Is the Primary Route of Hepatocyte Glycerol Uptake for Glycerol Gluconeogenesis in Mice. Journal of Biological Chemistry, 2011, 286, 44319-44325.	1.6	101
116	Binding of glutamate to the umami receptor. Biophysical Chemistry, 2010, 152, 139-144.	1.5	55
117	Toward a Consensus Model of the hERG Potassium Channel. ChemMedChem, 2010, 5, 455-467.	1.6	66
118	The antiâ€protozoal drug pentamidine blocks K_{IR}2.xâ€mediated inward rectifier current by entering the cytoplasmic pore region of the channel. British Journal of Pharmacology, 2010, 159, 1532-1541.	2.7	42
119	Functional dynamics in the voltage-dependent anion channel. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 22546-22551.	3.3	97
120	Conformational Transitions upon Ligand Binding: Holo-Structure Prediction from Apo Conformations. PLoS Computational Biology, 2010, 6, e1000634.	1.5	117
121	Spontaneous Quaternary and Tertiary T-R Transitions of Human Hemoglobin in Molecular Dynamics Simulation. PLoS Computational Biology, 2010, 6, e1000774.	1.5	57
122	Augmentation of Single Channel Water Permeability by Modification of Membrane Anchoring. Biophysical Journal, 2010, 98, 279a-280a.	0.2	0
123	Protein Thermostability Calculations Using Alchemical Free Energy Simulations. Biophysical Journal, 2010, 98, 2309-2316.	0.2	176
124	Scrutinizing Molecular Mechanics Force Fields on the Submicrosecond Timescale with NMR Data. Biophysical Journal, 2010, 99, 647-655.	0.2	192
125	Voltage-Regulated Water Flux through Aquaporin Channels In Silico. Biophysical Journal, 2010, 99, L97-L99.	0.2	69
126	Potentials of Mean Force and Permeabilities for Carbon Dioxide, Ammonia, and Water Flux across a Rhesus Protein Channel and Lipid Membranes. Journal of the American Chemical Society, 2010, 132, 13251-13263.	6.6	88

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127	g_whamâ€"A Free Weighted Histogram Analysis Implementation Including Robust Error and Autocorrelation Estimates. Journal of Chemical Theory and Computation, 2010, 6, 3713-3720.	2.3	1,284
128	Detection of Functional Modes in Protein Dynamics. Biophysical Journal, 2010, 98, 566a.	0.2	1
129	Dynamics and energetics of solute permeation through the Plasmodium falciparum aquaglyceroporin. Physical Chemistry Chemical Physics, 2010, 12, 10246.	1.3	34
130	Crystal Structure of a Yeast Aquaporin at 1.15 Ã... Reveals a Novel Gating Mechanism. PLoS Biology, 2009, 7, e1000130.	2.6	150
131	tCONCOORDâ€GUI: Visually supported conformational sampling of bioactive molecules. Journal of Computational Chemistry, 2009, 30, 1160-1166.	1.5	36
132	The Thermodynamic Influence of Trapped Water Molecules on a Proteinâ€"Ligand Interaction. Angewandte Chemie - International Edition, 2009, 48, 5207-5210.	7.2	36
133	Domain motions of hyaluronan lyase underlying processive hyaluronan translocation. Proteins: Structure, Function and Bioinformatics, 2009, 76, 30-46.	1.5	11
134	Predicting free energy changes using structural ensembles. Nature Methods, 2009, 6, 3-4.	9.0	228
135	Determinants of Water Permeability through Nanoscopic Hydrophilic Channels. Biophysical Journal, 2009, 96, 925-938.	0.2	34
136	Secondary Structure Propensities in Peptide Folding Simulations: A Systematic Comparison of Molecular Mechanics Interaction Schemes. Biophysical Journal, 2009, 97, 599-608.	0.2	109
137	Detection of Functional Modes in Protein Dynamics. PLoS Computational Biology, 2009, 5, e1000480.	1.5	126
138	Self-consistent residual dipolar coupling based model-free analysis for the robust determination of nanosecond to microsecond protein dynamics. Journal of Biomolecular NMR, 2008, 41, 139-155.	1.6	100
139	The Molecular Mechanism of Toxin-Induced Conformational Changes in a Potassium Channel: Relation to C-Type Inactivation. Structure, 2008, 16, 747-754.	1.6	52
140	The Atomistic Mechanism of Conformational Transition in Adenylate Kinase: A TEE-REX Molecular Dynamics Study. Structure, 2008, 16, 1175-1182.	1.6	55
141	Kinetics, Statistics, and Energetics of Lipid Membrane Electroporation Studied by Molecular Dynamics Simulations. Biophysical Journal, 2008, 95, 1837-1850.	0.2	280
142	Not Only Enthalpy: Large Entropy Contribution to Ion Permeation Barriers in Single-File Channels. Biophysical Journal, 2008, 95, 2275-2282.	0.2	13
143	Recognition Dynamics Up to Microseconds Revealed from an RDC-Derived Ubiquitin Ensemble in Solution. Science, 2008, 320, 1471-1475.	6.0	963
144	Residual dipolar couplings as a tool to study molecular recognition of ubiquitin. Biochemical Society Transactions, 2008, 36, 1433-1437.	1.6	36

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145	Vacuolar Protein Sorting: Two Different Functional States of the AAA-ATPase Vps4p. Journal of Molecular Biology, 2008, 377, 352-363.	2.0	41
146	Mechanism of selectivity in aquaporins and aquaglyceroporins. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 1198-1203.	3.3	378
147	Invariance of Single-File Water Mobility in Gramicidin-like Peptidic Pores as Function of Pore Length. Biophysical Journal, 2007, 92, 3930-3937.	0.2	31
148	Molecular Dynamics Simulations Using Temperature-Enhanced Essential Dynamics Replica Exchange. Biophysical Journal, 2007, 92, 4262-4270.	0.2	52
149	Short-Range Order and Collective Dynamics of DMPC Bilayers: A Comparison between Molecular Dynamics Simulations, X-Ray, and Neutron Scattering Experiments. Biophysical Journal, 2007, 93, 3156-3168.	0.2	77
150	Speeding up parallel GROMACS on high-latency networks. Journal of Computational Chemistry, 2007, 28, 2075-2084.	1.5	107
151	Atomic contacts in protein structures. A detailed analysis of atomic radii, packing, and overlaps. Proteins: Structure, Function and Bioinformatics, 2007, 68, 595-601.	1.5	29
152	Geometry-Based Sampling of Conformational Transitions in Proteins. Structure, 2007, 15, 1482-1492.	1.6	115
153	Acyl chain order parameter profiles in phospholipid bilayers: computation from molecular dynamics simulations and comparison with 2H NMR experiments. European Biophysics Journal, 2007, 36, 919-931.	1.2	304
154	Does CO2 Permeate through Aquaporin-1?. Biophysical Journal, 2006, 91, 842-848.	0.2	131
155	Molecular Anatomy of a Trafficking Organelle. Cell, 2006, 127, 831-846.	13.5	1,985
156	Alternate Structural Conformations of Streptococcus pneumoniae Hyaluronan Lyase: Insights into Enzyme Flexibility and Underlying Molecular Mechanism of Action. Journal of Molecular Biology, 2006, 358, 1165-1178.	2.0	21
157	Sequential N- to C-terminal SNARE complex assembly drives priming and fusion of secretory vesicles. EMBO Journal, 2006, 25, 955-966.	3.5	251
158	Ligand-Release Pathways in the Pheromone-Binding Protein of Bombyx mori. Structure, 2006, 14, 1567-1576.	1.6	29
159	Quaternary Ammonium Compounds as Water Channel Blockers. Journal of Biological Chemistry, 2006, 281, 14207-14214.	1.6	120
160	Mobility of a One-Dimensional Confined File of Water Molecules as a Function of File Length. Physical Review Letters, 2006, 96, 148101.	2.9	46
161	The 4.5Ã... Structure of Human AQP2. Journal of Molecular Biology, 2005, 350, 278-289.	2.0	74
162	The 5Ã... Structure of Heterologously Expressed Plant Aquaporin SoPIP2;1. Journal of Molecular Biology, 2005, 350, 611-616.	2.0	68

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163	Probing Conformational Disorder in Neurotensin by Two-Dimensional Solid-State NMR and Comparison to Molecular Dynamics Simulations. Biophysical Journal, 2005, 89, 2113-2120.	0.2	52
164	The Structure of the Aquaporin-1 Water Channel: A Comparison between Cryo-electron Microscopy and X-ray Crystallography. Journal of Molecular Biology, 2003, 325, 485-493.	2.0	51
165	The Mechanism of Proton Exclusion in the Aquaporin-1 Water Channel. Journal of Molecular Biology, 2003, 333, 279-293.	2.0	257
166	Structure and Flexibility of Streptococcus agalactiaeHyaluronate Lyase Complex with Its Substrate. Journal of Biological Chemistry, 2002, 277, 36678-36688.	1.6	73
167	Mechanism of Hyaluronan Degradation byStreptococcus pneumoniae Hyaluronate Lyase. Journal of Biological Chemistry, 2002, 277, 28287-28297.	1.6	113
168	Progress in the analysis of membrane protein structure and function. FEBS Letters, 2002, 529, 65-72.	1.3	74
169	Water Permeation through Gramicidin A: Desformylation and the Double Helix: A Molecular Dynamics Study. Biophysical Journal, 2002, 82, 2934-2942.	0.2	89
170	Essential dynamics of reversible peptide folding: memory-free conformational dynamics governed by internal hydrogen bonds. Journal of Molecular Biology, 2001, 309, 299-313.	2.0	126
171	A refined structure of human aquaporin-1. FEBS Letters, 2001, 504, 206-211.	1.3	120
172	Water Permeation Across Biological Membranes: Mechanism and Dynamics of Aquaporin-1 and GlpF. Science, 2001, 294, 2353-2357.	6.0	431
173	Conformations of the rhodopsin third cytoplasmic loop grafted onto bacteriorhodopsin. Structure, 2000, 8, 643-653.	1.6	23
174	The Fold of Human Aquaporin 1. Journal of Molecular Biology, 2000, 300, 987-994.	2.0	34
175	Conformational changes in the chaperonin GroEL: new insights into the allosteric mechanism 1 1Edited by A. R. Fersht. Journal of Molecular Biology, 1999, 286, 1241-1249.	2.0	67
176	A kinetic model for the internal motions of proteins: diffusion between multiple harmonic wells. Proteins: Structure, Function and Bioinformatics, 1999, 35, 283-92.	1.5	17
177	Domain motions in bacteriophage T4 lysozyme: A comparison between molecular dynamics and crystallographic data. , 1998, 31, 116-127.		155
178	Protein dynamics derived from clusters of crystal structures. Biophysical Journal, 1997, 73, 2891-2896.	0.2	75
179	Prediction of protein conformational freedom from distance constraints. , 1997, 29, 240-251.		240
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