

David van der Spoel

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.

149
papers

50,583
citations

53
h-index

166
g-index

166
ext. papers

57,086
ext. citations

6
avg. IF

7.64
L-index

#	Paper	IF	Citations
149	NMR refinement and peptide folding using the GROMACS software. <i>Journal of Biomolecular NMR</i> , 2021 , 75, 143-149	3	0
148	Accurate absolute free energies for ligand-protein binding based on non-equilibrium approaches. <i>Communications Chemistry</i> , 2021 , 4,	6.3	7
147	Systematic design of biomolecular force fields. <i>Current Opinion in Structural Biology</i> , 2021 , 67, 18-24	8.1	10
146	Microscopic origins of conductivity in molten salts unraveled by computer simulations. <i>Communications Chemistry</i> , 2021 , 4,	6.3	5
145	The structure of CO and CH at the interface of a poly(urethane urea) oligomer model from the microscopic point of view. <i>Journal of Chemical Physics</i> , 2021 , 155, 044704	3.9	0
144	An Intuitively Understandable Quality Measure for Theoretical Vibrational Spectra. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 5471-5475	6.4	7
143	Theoretical Infrared Spectra: Quantitative Similarity Measures and Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 3307-3315	6.4	14
142	Propagation of uncertainty in physicochemical data to force field predictions. <i>Physical Review Research</i> , 2020 , 2,	3.9	2
141	Making Soup: Preparing and Validating Models of the Bacterial Cytoplasm for Molecular Simulation. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 322-331	6.1	6
140	Toward a Computational Ecotoxicity Assay. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 3792-3803	6.2	2
139	A potential for molecular simulation of compounds with linear moieties. <i>Journal of Chemical Physics</i> , 2020 , 153, 084503	3.9	2
138	Systematically improved melting point prediction: a detailed physical simulation model is required. <i>Chemical Communications</i> , 2019 , 55, 12044-12047	5.8	7
137	Molten alkali halides - temperature dependence of structure, dynamics and thermodynamics. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 18516-18524	3.6	16
136	Prediction of Partition Coefficients of Environmental Toxins Using Computational Chemistry Methods. <i>ACS Omega</i> , 2019 , 4, 13772-13781	3.9	15
135	Role of Host-Guest Charge Transfer in Cyclodextrin Complexation: A Computational Study. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 17745-17756	3.8	1
134	Direct Link between Structure, Dynamics, and Thermodynamics in Molten Salts. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 25596-25602	3.8	10
133	Rotational and Translational Diffusion of Proteins as a Function of Concentration. <i>ACS Omega</i> , 2019 , 4, 20654-20664	3.9	7

132	Transient isomers in the photodissociation of bromiodomethane. <i>Journal of Chemical Physics</i> , 2018 , 148, 134307	3.9	5
131	The Alexandria library, a quantum-chemical database of molecular properties for force field development. <i>Scientific Data</i> , 2018 , 5, 180062	8.2	34
130	Force Field Benchmark of Amino Acids: I. Hydration and Diffusion in Different Water Models. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 1037-1052	6.1	56
129	Influence of Na ⁺ and Mg ²⁺ ions on RNA structures studied with molecular dynamics simulations. <i>Nucleic Acids Research</i> , 2018 , 46, 4872-4882	20.1	40
128	Impact of Dispersion Coefficient on Simulations of Proteins and Organic Liquids. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 8018-8027	3.4	12
127	Polarizable Drude Model with s-Type Gaussian or Slater Charge Density for General Molecular Mechanics Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 5553-5566	6.4	20
126	Phase-Transferable Force Field for Alkali Halides. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 5933-5948	6.4	24
125	Small Molecule Thermochemistry: A Tool for Empirical Force Field Development. <i>Journal of Physical Chemistry A</i> , 2018 , 122, 8982-8988	2.8	14
124	Statistical efficiency of methods for computing free energy of hydration. <i>Journal of Chemical Physics</i> , 2018 , 149, 144111	3.9	14
123	Comparison of Implicit and Explicit Solvent Models for the Calculation of Solvation Free Energy in Organic Solvents. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 1034-1043	6.4	96
122	Free-Energy Calculations of Ionic Hydration Consistent with the Experimental Hydration Free Energy of the Proton. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 2705-2712	6.4	30
121	Systematic exploration of multiple drug binding sites. <i>Journal of Cheminformatics</i> , 2017 , 9, 65	8.6	9
120	Mechanistic Insights into Autoinhibition of the Oncogenic Chromatin Remodeler ALC1. <i>Molecular Cell</i> , 2017 , 68, 847-859.e7	17.6	32
119	Membrane vesiculation induced by proteins of the dengue virus envelope studied by molecular dynamics simulations. <i>Journal of Physics Condensed Matter</i> , 2017 , 29, 504002	1.8	11
118	Evaluation of Generalized Born Models for Large Scale Affinity Prediction of Cyclodextrin Host-Guest Complexes. <i>Journal of Chemical Information and Modeling</i> , 2016 , 56, 2080-2092	6.1	18
117	Atomistic Simulation of Protein Encapsulation in Metal-Organic Frameworks. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 477-84	3.4	25
116	Exploration of Interfacial Hydration Networks of Target-Ligand Complexes. <i>Journal of Chemical Information and Modeling</i> , 2016 , 56, 148-58	6.1	17
115	Large-scale calculations of gas phase thermochemistry: Enthalpy of formation, standard entropy, and heat capacity. <i>Journal of Chemical Physics</i> , 2016 , 145, 114305	3.9	42

114	Water Determines the Structure and Dynamics of Proteins. <i>Chemical Reviews</i> , 2016 , 116, 7673-97	68.1	437
113	Binding of Pollutants to Biomolecules: A Simulation Study. <i>Chemical Research in Toxicology</i> , 2016 , 29, 1679-1688	4	5
112	Force Field Benchmark of Organic Liquids. 2. Gibbs Energy of Solvation. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 1192-201	6.1	57
111	Relationship between electronic properties and drug activity of seven quinoxaline compounds: A DFT study. <i>Journal of Molecular Structure</i> , 2015 , 1091, 196-202	3.4	17
110	Mobility-based prediction of hydration structures of protein surfaces. <i>Bioinformatics</i> , 2015 , 31, 1959-65	7.2	17
109	Generalized Born and Explicit Solvent Models for Free Energy Calculations in Organic Solvents: Cyclodextrin Dimerization. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5103-13	6.4	25
108	Impact of sludge deposition on biodiversity. <i>Ecotoxicology</i> , 2015 , 24, 1799-814	2.9	17
107	Implementation of extended Lagrangian dynamics in GROMACS for polarizable simulations using the classical Drude oscillator model. <i>Journal of Computational Chemistry</i> , 2015 , 36, 1473-9	3.5	60
106	Deconvoluting Protein (Un)folding Structural Ensembles Using X-Ray Scattering, Nuclear Magnetic Resonance Spectroscopy and Molecular Dynamics Simulation. <i>PLoS ONE</i> , 2015 , 10, e0125662	3.7	7
105	Properties of Organic Liquids when Simulated with Long-Range Lennard-Jones Interactions. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 2938-44	6.4	86
104	Deciphering solution scattering data with experimentally guided molecular dynamics simulations. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 780-7	6.4	40
103	Cooperative Binding of Cyclodextrin Dimers to Isoflavone Analogues Elucidated by Free Energy Calculations. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 7163-7173	3.8	26
102	MemBuilder: a web-based graphical interface to build heterogeneously mixed membrane bilayers for the GROMACS biomolecular simulation program. <i>Bioinformatics</i> , 2014 , 30, 439-41	7.2	44
101	CO ₂ and O ₂ distribution in Rubisco suggests the small subunit functions as a CO ₂ reservoir. <i>Journal of the American Chemical Society</i> , 2014 , 136, 3165-71	16.4	39
100	Thermodynamics of hydronium and hydroxide surface solvation. <i>Chemical Science</i> , 2014 , 5, 1745	9.4	42
99	Chemical properties, environmental fate, and degradation of seven classes of pollutants. <i>Chemical Research in Toxicology</i> , 2014 , 27, 713-37	4	78
98	Thiamin function, metabolism, uptake, and transport. <i>Biochemistry</i> , 2014 , 53, 821-35	3.2	171
97	An efficient and extensible format, library, and API for binary trajectory data from molecular simulations. <i>Journal of Computational Chemistry</i> , 2014 , 35, 260-9	3.5	9

96	Order Parameters and Algorithmic Approaches for Detection and Demarcation of Interfaces in Hydrate-Fluid and Ice-Fluid Systems. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 5606-15	6.4	0
95	Local partition coefficients govern solute permeability of cholesterol-containing membranes. <i>Biophysical Journal</i> , 2013 , 105, 2760-70	2.9	53
94	Quantification of Solvent Contribution to the Stability of Noncovalent Complexes. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 4542-51	6.4	33
93	Unexpected Effects of Cholesterol on Membrane Permeability. <i>Biophysical Journal</i> , 2013 , 104, 192a-193a	2.9	0
92	Sheet structures and dimer models of the two major tyrocidines, antimicrobial peptides from <i>Bacillus aneurinolyticus</i> . <i>Biochemistry</i> , 2013 , 52, 7798-806	3.2	21
91	Anopheles gambiae, Anoga-HrTH hormone, free and bound structure--a nuclear magnetic resonance experiment. <i>Peptides</i> , 2013 , 41, 94-100	3.8	13
90	GROMACS 4.5: a high-throughput and highly parallel open source molecular simulation toolkit. <i>Bioinformatics</i> , 2013 , 29, 845-54	7.2	4786
89	Insights on the solubility of CO ₂ in 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide from the microscopic point of view. <i>Environmental Science & Technology</i> , 2013 , 47, 7421-9	10.3	55
88	Fullerenes toxicity and electronic properties. <i>Environmental Chemistry Letters</i> , 2013 , 11, 105-118	13.3	38
87	Transcription-factor binding and sliding on DNA studied using micro- and macroscopic models. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013 , 110, 19796-801	11.5	67
86	GROMACS molecule & liquid database. <i>Bioinformatics</i> , 2012 , 28, 752-3	7.2	140
85	Screening for the Location of RNA using the Chloride Ion Distribution in Simulations of Virus Capsids. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 2474-83	6.4	19
84	Organic molecules on the surface of water droplets--an energetic perspective. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 9537-45	3.6	43
83	Free energy of separation of structure II clathrate hydrate in water and a light oil. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 5933-40	3.4	5
82	Insight into the structural deformations of beta-cyclodextrin caused by alcohol cosolvents and guest molecules. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 3880-9	3.4	31
81	Molecular recognition in different environments: Cyclodextrin dimer formation in organic solvents. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 12684-93	3.4	46
80	Force Field Benchmark of Organic Liquids: Density, Enthalpy of Vaporization, Heat Capacities, Surface Tension, Isothermal Compressibility, Volumetric Expansion Coefficient, and Dielectric Constant. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 61-74	6.4	476
79	Large influence of cholesterol on solute partitioning into lipid membranes. <i>Journal of the American Chemical Society</i> , 2012 , 134, 5351-61	16.4	124

78	Virus capsid dissolution studied by microsecond molecular dynamics simulations. <i>PLoS Computational Biology</i> , 2012 , 8, e1002502	5	53
77	Carbonyl charge solvation patterns may relate to fragmentation classes in collision-activated dissociation. <i>Journal of the American Society for Mass Spectrometry</i> , 2012 , 23, 1319-25	3.5	3
76	Time-resolved WAXS reveals accelerated conformational changes in iodoretinal-substituted proteorhodopsin. <i>Biophysical Journal</i> , 2011 , 101, 1345-53	2.9	54
75	Atomistic simulation of ion solvation in water explains surface preference of halides. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011 , 108, 6838-6842	11.5	171
74	Subunit interface dynamics in hexadecameric rubisco. <i>Journal of Molecular Biology</i> , 2011 , 411, 1083-98	6.5	29
73	Open conformation of adipokinetic hormone receptor from the malaria mosquito facilitates hormone binding. <i>Peptides</i> , 2011 , 32, 553-9	3.8	10
72	GROMACS: the road ahead. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011 , 1, 710-715	7.9	38
71	Trajectory NG: portable, compressed, general molecular dynamics trajectories. <i>Journal of Molecular Modeling</i> , 2011 , 17, 2669-85	2	12
70	Probing π chemical shielding tensors in cryptolepine and two bromo-substituted analogs for antiplasmodial activity. <i>Journal of Molecular Modeling</i> , 2011 , 17, 3289-97	2	3
69	Toward prediction of functional protein pockets using blind docking and pocket search algorithms. <i>Protein Science</i> , 2011 , 20, 880-93	6.3	50
68	Proteins, lipids, and water in the gas phase. <i>Macromolecular Bioscience</i> , 2011 , 11, 50-9	5.5	65
67	On the feasibility of nanocrystal imaging using intense and ultrashort X-ray pulses. <i>ACS Nano</i> , 2011 , 5, 139-46	16.7	59
66	Scrutinizing molecular mechanics force fields on the submicrosecond timescale with NMR data. <i>Biophysical Journal</i> , 2010 , 99, 647-55	2.9	175
65	g_wham: Free Weighted Histogram Analysis Implementation Including Robust Error and Autocorrelation Estimates. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 3713-3720	6.4	930
64	Hawk: the image reconstruction package for coherent X-ray diffractive imaging. <i>Journal of Applied Crystallography</i> , 2010 , 43, 1535-1539	3.8	41
63	Structural variability and the incoherent addition of scattered intensities in single-particle diffraction. <i>Physical Review E</i> , 2009 , 80, 031905	2.4	20
62	A density functional study of ^{15}N chemical shielding tensors in quinolines. <i>Chemical Physics Letters</i> , 2009 , 476, 196-200	2.5	7
61	Solution conformations of an insect neuropeptide: crustacean cardioactive peptide (CCAP). <i>Peptides</i> , 2009 , 30, 557-64	3.8	15

60	Structural stability of electrosprayed proteins: temperature and hydration effects. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 8069-78	3.6	43
59	Molecular dynamics simulations of a membrane protein-micelle complex in vacuo. <i>Journal of the American Chemical Society</i> , 2009 , 131, 16606-7	16.4	31
58	Encapsulation of myoglobin in a cetyl trimethylammonium bromide micelle in vacuo: a simulation study. <i>Biochemistry</i> , 2009 , 48, 1006-15	3.2	32
57	A proposed time-resolved X-ray scattering approach to track local and global conformational changes in membrane transport proteins. <i>Structure</i> , 2008 , 16, 21-8	5.2	18
56	Structural studies of melting on the picosecond time scale. <i>Physical Chemistry Chemical Physics</i> , 2008 , 10, 6344-9	3.6	11
55	A temperature predictor for parallel tempering simulations. <i>Physical Chemistry Chemical Physics</i> , 2008 , 10, 2073-7	3.6	352
54	A theoretical study of repeating sequence in HRP II: a combination of molecular dynamics simulations and ¹⁷ O quadrupole coupling tensors. <i>Biophysical Chemistry</i> , 2008 , 137, 76-80	3.5	1
53	Picosecond melting of ice by an infrared laser pulse: a simulation study. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 1417-20	16.4	27
52	Role of spin state on the geometry and nuclear quadrupole resonance parameters in hemin complex. <i>Biophysical Chemistry</i> , 2008 , 134, 200-6	3.5	3
51	GROMACS 4: Algorithms for Highly Efficient, Load-Balanced, and Scalable Molecular Simulation. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 435-47	6.4	11706
50	Fluorescence probe of Trp-cage protein conformation in solution and in gas phase. <i>Journal of the American Chemical Society</i> , 2007 , 129, 6726-35	16.4	59
49	Evaporation from water clusters containing singly charged ions. <i>Physical Chemistry Chemical Physics</i> , 2007 , 9, 5105-11	3.6	55
48	A direct comparison of protein structure in the gas and solution phase: the Trp-cage. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 13147-50	3.4	42
47	Protein structures under electrospray conditions. <i>Biochemistry</i> , 2007 , 46, 933-45	3.2	109
46	Speeding up parallel GROMACS on high-latency networks. <i>Journal of Computational Chemistry</i> , 2007 , 28, 2075-84	3.5	98
45	Protein Folding Properties from Molecular Dynamics Simulations. <i>Lecture Notes in Computer Science</i> , 2007 , 109-115	0.9	2
44	Temperature and structural changes of water clusters in vacuum due to evaporation. <i>Journal of Chemical Physics</i> , 2006 , 125, 154508	3.9	55
43	Thermodynamics of hydrogen bonding in hydrophilic and hydrophobic media. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 4393-8	3.4	323

42	The Origin of Layer Structure Artifacts in Simulations of Liquid Water. <i>Journal of Chemical Theory and Computation</i> , 2006 , 2, 1-11	6.4	164
41	Lifting a wet glass from a table: a microscopic picture. <i>Langmuir</i> , 2006 , 22, 5666-72	4	13
40	Blind docking of drug-sized compounds to proteins with up to a thousand residues. <i>FEBS Letters</i> , 2006 , 580, 1447-50	3.8	215
39	Femtosecond diffractive imaging with a soft-X-ray free-electron laser. <i>Nature Physics</i> , 2006 , 2, 839-843	16.2	778
38	Probing solution- and gas-phase structures of Trp-cage cations by chiral substitution and spectroscopic techniques. <i>International Journal of Mass Spectrometry</i> , 2006 , 253, 263-273	1.9	29
37	Prediction of NC α bond cleavage frequencies in electron capture dissociation of Trp-cage dications by force-field molecular dynamics simulations. <i>International Journal of Mass Spectrometry</i> , 2006 , 248, 124-135	1.9	58
36	Protein folding kinetics and thermodynamics from atomistic simulations. <i>Physical Review Letters</i> , 2006 , 96, 238102	7.4	80
35	Improved GROMACS Scaling on Ethernet Switched Clusters. <i>Lecture Notes in Computer Science</i> , 2006 , 404-405	0.9	2
34	Atomic-scale visualization of inertial dynamics. <i>Science</i> , 2005 , 308, 392-5	33.3	286
33	Reproducible polypeptide folding and structure prediction using molecular dynamics simulations. <i>Journal of Molecular Biology</i> , 2005 , 354, 173-83	6.5	150
32	GROMACS: fast, flexible, and free. <i>Journal of Computational Chemistry</i> , 2005 , 26, 1701-18	3.5	10273
31	Interactive visualization of electron density slices. <i>Journal of Applied Crystallography</i> , 2005 , 38, 563-565	3.8	3
30	Observation of structural anisotropy and the onset of liquidlike motion during the nonthermal melting of InSb. <i>Physical Review Letters</i> , 2005 , 95, 125701	7.4	49
29	Clocking femtosecond X rays. <i>Physical Review Letters</i> , 2005 , 94, 114801	7.4	196
28	Model for the dynamics of a water cluster in an x-ray free electron laser beam. <i>Physical Review E</i> , 2004 , 70, 051904	2.4	65
27	Deformation of helix C in the low temperature L-intermediate of bacteriorhodopsin. <i>Journal of Biological Chemistry</i> , 2004 , 279, 2147-58	5.4	66
26	Potential impact of an X-ray free electron laser on structural biology. <i>Radiation Physics and Chemistry</i> , 2004 , 71, 905-916	2.5	53
25	Auger electron cascades in water and ice. <i>Chemical Physics</i> , 2004 , 299, 277-283	2.3	49

24	Molecular dynamics simulations of peptides from the central domain of smooth muscle caldesmon. <i>Journal of Biomolecular Structure and Dynamics</i> , 2004 , 21, 555-66	3.6	9
23	Modeling of enzyme-substrate complexes for the metalloproteases MMP-3, ADAM-9 and ADAM-10. <i>Journal of Computer-Aided Molecular Design</i> , 2003 , 17, 551-65	4.2	37
22	Brute-Force Molecular Dynamics Simulations of Villin Headpiece: Comparison with NMR Parameters. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 11178-11187	3.4	58
21	Dynamic properties of water/alcohol mixtures studied by computer simulation. <i>Journal of Chemical Physics</i> , 2003 , 119, 7308-7317	3.9	238
20	Efficient docking of peptides to proteins without prior knowledge of the binding site. <i>Protein Science</i> , 2002 , 11, 1729-37	6.3	314
19	Space-time evolution of electron cascades in diamond. <i>Physical Review B</i> , 2002 , 66,	3.3	36
18	GROMACS 3.0: a package for molecular simulation and trajectory analysis. <i>Journal of Molecular Modeling</i> , 2001 , 7, 306-317	2	5502
17	Auger-electron cascades in diamond and amorphous carbon. <i>Physical Review B</i> , 2001 , 64,	3.3	44
16	Molecular Dynamics Simulations of Water with Novel Shell-Model Potentials. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 2618-2626	3.4	151
15	Potential for biomolecular imaging with femtosecond X-ray pulses. <i>Nature</i> , 2000 , 406, 752-7	50.4	1498
14	Molecular Dynamics Simulations of Dodecylphosphocholine Micelles at Three Different Aggregate Sizes: Micellar Structure and Chain Relaxation. <i>Journal of Physical Chemistry B</i> , 2000 , 104, 6380-6388	3.4	250
13	The solution conformations of amino acids from molecular dynamics simulations of Gly-X-Gly peptides: comparison with NMR parameters. <i>Biochemistry and Cell Biology</i> , 1998 , 76, 164-170	3.6	15
12	A systematic study of water models for molecular simulation: Derivation of water models optimized for use with a reaction field. <i>Journal of Chemical Physics</i> , 1998 , 108, 10220-10230	3.9	514
11	The solution conformations of amino acids from molecular dynamics simulations of Gly-X-Gly peptides: comparison with NMR parameters. <i>Biochemistry and Cell Biology</i> , 1998 , 76, 164-70	3.6	2
10	Molecular dynamics simulations of Leu-enkephalin in water and DMSO. <i>Biophysical Journal</i> , 1997 , 72, 2032-41	2.9	99
9	Molecular modeling of the RNA binding N-terminal part of cowpea chlorotic mottle virus coat protein in solution with phosphate ions. <i>Biophysical Journal</i> , 1996 , 71, 2920-32	2.9	18
8	Molecular dynamics simulations of N-terminal peptides from a nucleotide binding protein. <i>Proteins: Structure, Function and Bioinformatics</i> , 1996 , 24, 450-66	4.2	16
7	Molecular dynamics simulations of peptides from BPTI: a closer look at amide-aromatic interactions. <i>Journal of Biomolecular NMR</i> , 1996 , 8, 229-38	3	79

6	Phosphorylation-induced torsion-angle strain in the active center of HPr, detected by NMR and restrained molecular dynamics refinement. <i>Protein Science</i> , 1996 , 5, 442-6	6.3	6
5	Bending of the calmodulin central helix: a theoretical study. <i>Protein Science</i> , 1996 , 5, 2044-53	6.3	66
4	Towards phase transferable potential functions: Methodology and application to nitrogen. <i>Journal of Chemical Physics</i> , 1995 , 103, 2272-2285	3.9	29
3	GROMACS: A message-passing parallel molecular dynamics implementation. <i>Computer Physics Communications</i> , 1995 , 91, 43-56	4.2	6589
2	Molecular Modeling of Inhibitors at Qi and Qo Sites in Cytochrome bc1 Complex110-127		
1	Quantitative predictions from molecular simulations using explicit or implicit interactions. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> ,e1560	7.9	4