David van der Spoel

List of Publications by Year
in descending order

160 papers	62,424 citations	26567 56 h-index	7718 150 g-index
166 all docs	166 docs citations	166 times ranked	48037 citing authors

#	Article	IF	Citations
1	GROMACS 4:â€‰ Algorithms for Highly Efficient, Load-Balanced, and Scalable Molecular Simulation. Journal of Chemical Theory and Computation, 2008, 4, 435-447.	2.3	13,875
2	GROMACS: Fast, flexible, and free. Journal of Computational Chemistry, 2005, 26, 1701-1718.	1.5	13,676
3	GROMACS: A message-passing parallel molecular dynamics implementation. Computer Physics Communications, 1995, 91, 43-56.	3.0	8,250
4	GROMACS 3.0: a package for molecular simulation and trajectory analysis. Journal of Molecular Modeling, 2001, 7, 306-317.	0.8	6,085
5	GROMACS 4.5: a high-throughput and highly parallel open source molecular simulation toolkit. Bioinformatics, 2013, 29, 845-854.	1.8	6,072
6	Potential for biomolecular imaging with femtosecond X-ray pulses. Nature, 2000, 406, 752-757.	13.7	1,773
7	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
8	Femtosecond diffractive imaging with a soft-X-ray free-electron laser. Nature Physics, 2006, 2, 839-843.	6.5	910
9	Water Determines the Structure and Dynamics of Proteins. Chemical Reviews, 2016, 116, 7673-7697.	23.0	645
10	Force Field Benchmark of Organic Liquids: Density, Enthalpy of Vaporization, Heat Capacities, Surface Tension, Isothermal Compressibility, Volumetric Expansion Coefficient, and Dielectric Constant. Journal of Chemical Theory and Computation, 2012, 8, 61-74.	2.3	609
11	A systematic study of water models for molecular simulation: Derivation of water models optimized for use with a reaction field. Journal of Chemical Physics, 1998, 108, 10220-10230.	1.2	581
12	A temperature predictor for parallel tempering simulations. Physical Chemistry Chemical Physics, 2008, 10, 2073.	1.3	437
13	Thermodynamics of Hydrogen Bonding in Hydrophilic and Hydrophobic Media. Journal of Physical Chemistry B, 2006, 110, 4393-4398.	1.2	404
14	Efficient docking of peptides to proteins without prior knowledge of the binding site. Protein Science, 2009, 11, 1729-1737.	3.1	370
15	Atomic-Scale Visualization of Inertial Dynamics. Science, 2005, 308, 392-395.	6.0	324
16	Molecular Dynamics Simulations of Dodecylphosphocholine Micelles at Three Different Aggregate Sizes:Â Micellar Structure and Chain Relaxation. Journal of Physical Chemistry B, 2000, 104, 6380-6388.	1.2	273
17	Dynamic properties of water/alcohol mixtures studied by computer simulation. Journal of Chemical Physics, 2003, 119, 7308-7317.	1.2	255
18	Blind docking of drug-sized compounds to proteins with up to a thousand residues. FEBS Letters, 2006, 580, 1447-1450.	1.3	253

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19	Thiamin Function, Metabolism, Uptake, and Transport. Biochemistry, 2014, 53, 821-835.	1.2	242
20	Clocking Femtosecond X Rays. Physical Review Letters, 2005, 94, 114801.	2.9	230
21	The Origin of Layer Structure Artifacts in Simulations of Liquid Water. Journal of Chemical Theory and Computation, 2006, 2, 1-11.	2.3	195
22	Scrutinizing Molecular Mechanics Force Fields on the Submicrosecond Timescale with NMR Data. Biophysical Journal, 2010, 99, 647-655.	0.2	192
23	Atomistic simulation of ion solvation in water explains surface preference of halides. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 6838-6842.	3.3	192
24	Comparison of Implicit and Explicit Solvent Models for the Calculation of Solvation Free Energy in Organic Solvents. Journal of Chemical Theory and Computation, 2017, 13, 1034-1043.	2.3	180
25	Reproducible Polypeptide Folding and Structure Prediction using Molecular Dynamics Simulations. Journal of Molecular Biology, 2005, 354, 173-183.	2.0	165
26	Molecular Dynamics Simulations of Water with Novel Shell-Model Potentials. Journal of Physical Chemistry B, 2001, 105, 2618-2626.	1.2	162
27	GROMACS molecule & liquid database. Bioinformatics, 2012, 28, 752-753.	1.8	161
28	Large Influence of Cholesterol on Solute Partitioning into Lipid Membranes. Journal of the American Chemical Society, 2012, 134, 5351-5361.	6.6	145
29	Protein Structures under Electrospray Conditions. Biochemistry, 2007, 46, 933-945.	1.2	120
30	Properties of Organic Liquids when Simulated with Long-Range Lennard-Jones Interactions. Journal of Chemical Theory and Computation, 2015, 11, 2938-2944.	2.3	116
31	Molecular dynamics simulations of Leu-enkephalin in water and DMSO. Biophysical Journal, 1997, 72, 2032-2041.	0.2	108
32	Speeding up parallel GROMACS on high-latency networks. Journal of Computational Chemistry, 2007, 28, 2075-2084.	1.5	107
33	Chemical Properties, Environmental Fate, and Degradation of Seven Classes of Pollutants. Chemical Research in Toxicology, 2014, 27, 713-737.	1.7	91
34	Protein Folding Kinetics and Thermodynamics from Atomistic Simulations. Physical Review Letters, 2006, 96, 238102.	2.9	85
35	Molecular dynamics simulations of peptides from BPTI: A closer look at amideâ€”aromatic interactions. Journal of Biomolecular NMR, 1996, 8, 229-238.	1.6	84
36	Transcription-factor binding and sliding on DNA studied using micro- and macroscopic models. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 19796-19801.	3.3	79

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37	Implementation of extended <scp>L</scp>agrangian dynamics in <scp>GROMACS</scp> for polarizable simulations using the classical <scp>D</scp>rude oscillator model. Journal of Computational Chemistry, 2015, 36, 1473-1479.	1.5	79
38	Proteins, Lipids, and Water in the Gas Phase. Macromolecular Bioscience, 2011, 11, 50-59.	2.1	77
39	Force Field Benchmark of Organic Liquids. 2. Gibbs Energy of Solvation. Journal of Chemical Information and Modeling, 2015, 55, 1192-1201.	2.5	77
40	Influence of Na+ and Mg2+ ions on RNA structures studied with molecular dynamics simulations. Nucleic Acids Research, 2018, 46, 4872-4882.	6.5	76
41	Deformation of Helix C in the Low Temperature L-intermediate of Bacteriorhodopsin. Journal of Biological Chemistry, 2004, 279, 2147-2158.	1.6	72
42	Bending of the calmodulin central helix: A theoretical study. Protein Science, 1996, 5, 2044-2053.	3.1	71
43	Virus Capsid Dissolution Studied by Microsecond Molecular Dynamics Simulations. PLoS Computational Biology, 2012, 8, e1002502.	1.5	70
44	Force Field Benchmark of Amino Acids: I. Hydration and Diffusion in Different Water Models. Journal of Chemical Information and Modeling, 2018, 58, 1037-1052.	2.5	70
45	Model for the dynamics of a water cluster in an x-ray free electron laser beam. Physical Review E, 2004, 70, 051904.	0.8	69
46	Local Partition Coefficients Govern Solute Permeability of Cholesterol-Containing Membranes. Biophysical Journal, 2013, 105, 2760-2770.	0.2	67
47	Insights on the Solubility of CO₂ in 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide from the Microscopic Point of View. Environmental Science & Technology, 2013, 47, 7421-7429.	4.6	65
48	Fluorescence Probe of Trp-Cage Protein Conformation in Solution and in Gas Phase. Journal of the American Chemical Society, 2007, 129, 6726-6735.	6.6	64
49	Evaporation from water clusters containing singly charged ions. Physical Chemistry Chemical Physics, 2007, 9, 5105.	1.3	64
50	Brute-Force Molecular Dynamics Simulations of Villin Headpiece:Â Comparison with NMR Parameters. Journal of Physical Chemistry B, 2003, 107, 11178-11187.	1.2	62
51	On the Feasibility of Nanocrystal Imaging Using Intense and Ultrashort X-ray Pulses. ACS Nano, 2011, 5, 139-146.	7.3	61
52	Time-Resolved WAXS Reveals Accelerated Conformational Changes in Iodoretinal-Substituted Proteorhodopsin. Biophysical Journal, 2011, 101, 1345-1353.	0.2	60
53	Large-scale calculations of gas phase thermochemistry: Enthalpy of formation, standard entropy, and heat capacity. Journal of Chemical Physics, 2016, 145, .	1.2	60
54	Prediction of NCÎ± bond cleavage frequencies in electron capture dissociation of Trp-cage dications by force-field molecular dynamics simulations. International Journal of Mass Spectrometry, 2006, 248, 124-135.	0.7	59

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55	Temperature and structural changes of water clusters in vacuum due to evaporation. Journal of Chemical Physics, 2006, 125, 154508.	1.2	59
56	Toward prediction of functional protein pockets using blind docking and pocket search algorithms. Protein Science, 2011, 20, 880-893.	3.1	59
57	CO₂ and O₂ Distribution in Rubisco Suggests the Small Subunit Functions as a CO₂ Reservoir. Journal of the American Chemical Society, 2014, 136, 3165-3171.	6.6	59
58	Structural stability of electrosprayed proteins: temperature and hydration effects. Physical Chemistry Chemical Physics, 2009, 11, 8069.	1.3	57
59	Observation of Structural Anisotropy and the Onset of Liquidlike Motion During the Nonthermal Melting of InSb. Physical Review Letters, 2005, 95, 125701.	2.9	56
60	Molecular Recognition in Different Environments: Î²-Cyclodextrin Dimer Formation in Organic Solvents. Journal of Physical Chemistry B, 2012, 116, 12684-12693.	1.2	56
61	Thermodynamics of hydronium and hydroxide surface solvation. Chemical Science, 2014, 5, 1745.	3.7	56
62	Potential impact of an X-ray free electron laser on structural biology. Radiation Physics and Chemistry, 2004, 71, 905-916.	1.4	55
63	Auger electron cascades in water and ice. Chemical Physics, 2004, 299, 277-283.	0.9	55
64	MemBuilder: a web-based graphical interface to build heterogeneously mixed membrane bilayers for the GROMACS biomolecular simulation program. Bioinformatics, 2014, 30, 439-441.	1.8	54
65	Auger-electron cascades in diamond and amorphous carbon. Physical Review B, 2001, 64, .	1.1	53
66	Mechanistic Insights into Autoinhibition of the Oncogenic Chromatin Remodeler ALC1. Molecular Cell, 2017, 68, 847-859.e7.	4.5	53
67	Organic molecules on the surface of water droplets â€“ an energetic perspective. Physical Chemistry Chemical Physics, 2012, 14, 9537.	1.3	52
68	Accurate absolute free energies for ligandâ€“protein binding based on non-equilibrium approaches. Communications Chemistry, 2021, 4, .	2.0	49
69	A Direct Comparison of Protein Structure in the Gas and Solution Phase:â€‰ The Trp-cage. Journal of Physical Chemistry B, 2007, 111, 13147-13150.	1.2	46
70	Picosecond Melting of Ice by an Infrared Laser Pulse: A Simulation Study. Angewandte Chemie - International Edition, 2008, 47, 1417-1420.	7.2	46
71	Hawk: the image reconstruction package for coherent X-ray diffractive imaging. Journal of Applied Crystallography, 2010, 43, 1535-1539.	1.9	46
72	Deciphering Solution Scattering Data with Experimentally Guided Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2015, 11, 780-787.	2.3	45

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73	The Alexandria library, a quantum-chemical database of molecular properties for force field development. Scientific Data, 2018, 5, 180062.	2.4	45
74	Fullerenes toxicity and electronic properties. Environmental Chemistry Letters, 2013, 11, 105-118.	8.3	44
75	GROMACSâ€"the road ahead. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 710-715.	6.2	43
76	Modeling of enzymeâ€"substrate complexes for the metalloproteases MMP-3, ADAM-9 and ADAM-10. Journal of Computer-Aided Molecular Design, 2003, 17, 551-565.	1.3	42
77	Free-Energy Calculations of Ionic Hydration Consistent with the Experimental Hydration Free Energy of the Proton. Journal of Physical Chemistry Letters, 2017, 8, 2705-2712.	2.1	40
78	Space-time evolution of electron cascades in diamond. Physical Review B, 2002, 66, .	1.1	38
79	Insight into the Structural Deformations of Beta-Cyclodextrin Caused by Alcohol Cosolvents and Guest Molecules. Journal of Physical Chemistry B, 2012, 116, 3880-3889.	1.2	37
80	Quantification of Solvent Contribution to the Stability of Noncovalent Complexes. Journal of Chemical Theory and Computation, 2013, 9, 4542-4551.	2.3	37
81	Encapsulation of Myoglobin in a Cetyl Trimethylammonium Bromide Micelle in Vacuo: A Simulation Study. Biochemistry, 2009, 48, 1006-1015.	1.2	36
82	Cooperative Binding of Cyclodextrin Dimers to Isoflavone Analogues Elucidated by Free Energy Calculations. Journal of Physical Chemistry C, 2014, 118, 7163-7173.	1.5	35
83	Atomistic Simulation of Protein Encapsulation in Metalâ€"Organic Frameworks. Journal of Physical Chemistry B, 2016, 120, 477-484.	1.2	35
84	Phase-Transferable Force Field for Alkali Halides. Journal of Chemical Theory and Computation, 2018, 14, 5933-5948.	2.3	35
85	Towards phase transferable potential functions: Methodology and application to nitrogen. Journal of Chemical Physics, 1995, 103, 2272-2285.	1.2	33
86	Subunit Interface Dynamics in Hexadecameric Rubisco. Journal of Molecular Biology, 2011, 411, 1083-1098.	2.0	33
87	Evaluation of Generalized Born Models for Large Scale Affinity Prediction of Cyclodextrin Hostâ€"Guest Complexes. Journal of Chemical Information and Modeling, 2016, 56, 2080-2092.	2.5	32
88	Probing solution- and gas-phase structures of Trp-cage cations by chiral substitution and spectroscopic techniques. International Journal of Mass Spectrometry, 2006, 253, 263-273.	0.7	31
89	Molecular Dynamics Simulations of a Membrane Proteinâ^'Micelle Complex in Vacuo. Journal of the American Chemical Society, 2009, 131, 16606-16607.	6.6	31
90	Generalized Born and Explicit Solvent Models for Free Energy Calculations in Organic Solvents: Cyclodextrin Dimerization. Journal of Chemical Theory and Computation, 2015, 11, 5103-5113.	2.3	31

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91	Theoretical Infrared Spectra: Quantitative Similarity Measures and Force Fields. Journal of Chemical Theory and Computation, 2020, 16, 3307-3315.	2.3	31
92	Mobility-based prediction of hydration structures of protein surfaces. Bioinformatics, 2015, 31, 1959-1965.	1.8	30
93	Exploration of Interfacial Hydration Networks of Targetâ€“Ligand Complexes. Journal of Chemical Information and Modeling, 2016, 56, 148-158.	2.5	30
94	Systematic design of biomolecular force fields. Current Opinion in Structural Biology, 2021, 67, 18-24.	2.6	30
95	Classical molecular dynamics. Journal of Chemical Physics, 2021, 154, 100401.	1.2	28
96	Polarizable Drude Model with s-Type Gaussian or Slater Charge Density for General Molecular Mechanics Force Fields. Journal of Chemical Theory and Computation, 2018, 14, 5553-5566.	2.3	27
97	Structural variability and the incoherent addition of scattered intensities in single-particle diffraction. Physical Review E, 2009, 80, 031905.	0.8	25
98	Î²-Sheet Structures and Dimer Models of the Two Major Tyrocidines, Antimicrobial Peptides from Bacillus aneurinolyticus. Biochemistry, 2013, 52, 7798-7806.	1.2	25
99	Small Molecule Thermochemistry: A Tool for Empirical Force Field Development. Journal of Physical Chemistry A, 2018, 122, 8982-8988.	1.1	25
100	Ten simple rules on how to create open access and reproducible molecular simulations of biological systems. PLoS Computational Biology, 2019, 15, e1006649.	1.5	25
101	Screening for the Location of RNA using the Chloride Ion Distribution in Simulations of Virus Capsids. Journal of Chemical Theory and Computation, 2012, 8, 2474-2483.	2.3	24
102	Impact of sludge deposition on biodiversity. Ecotoxicology, 2015, 24, 1799-1814.	1.1	24
103	Prediction of Partition Coefficients of Environmental Toxins Using Computational Chemistry Methods. ACS Omega, 2019, 4, 13772-13781.	1.6	24
104	Relationship between electronic properties and drug activity of seven quinoxaline compounds: A DFT study. Journal of Molecular Structure, 2015, 1091, 196-202.	1.8	23
105	A Proposed Time-Resolved X-Ray Scattering Approach to Track Local and Global Conformational Changes in Membrane Transport Proteins. Structure, 2008, 16, 21-28.	1.6	20
106	Systematic exploration of multiple drug binding sites. Journal of Cheminformatics, 2017, 9, 65.	2.8	20
107	Molten alkali halides â€“ temperature dependence of structure, dynamics and thermodynamics. Physical Chemistry Chemical Physics, 2019, 21, 18516-18524.	1.3	19
108	Molecular modeling of the RNA binding N-terminal part of cowpea chlorotic mottle virus coat protein in solution with phosphate ions. Biophysical Journal, 1996, 71, 2920-2932.	0.2	18

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109	Molecular dynamics simulations of N-terminal peptides from a nucleotide binding protein. , 1996, 24, 450-466.		17
110	Anopheles gambiae, Anoga-HrTH hormone, free and bound structure â€“ A nuclear magnetic resonance experiment. Peptides, 2013, 41, 94-100.	1.2	17
111	Systematically improved melting point prediction: a detailed physical simulation model is required. Chemical Communications, 2019, 55, 12044-12047.	2.2	17
112	Rotational and Translational Diffusion of Proteins as a Function of Concentration. ACS Omega, 2019, 4, 20654-20664.	1.6	17
113	Making Soup: Preparing and Validating Models of the Bacterial Cytoplasm for Molecular Simulation. Journal of Chemical Information and Modeling, 2020, 60, 322-331.	2.5	17
114	The solution conformations of amino acids from molecular dynamics simulations of Gly-X-Gly peptides: comparison with NMR parameters. Biochemistry and Cell Biology, 1998, 76, 164-170.	0.9	16
115	Solution conformations of an insect neuropeptide: Crustacean cardioactive peptide (CCAP). Peptides, 2009, 30, 557-564.	1.2	16
116	Statistical efficiency of methods for computing free energy of hydration. Journal of Chemical Physics, 2018, 149, 144111.	1.2	16
117	Impact of Dispersion Coefficient on Simulations of Proteins and Organic Liquids. Journal of Physical Chemistry B, 2018, 122, 8018-8027.	1.2	16
118	Lifting a Wet Glass from a Table:Â A Microscopic Picture. Langmuir, 2006, 22, 5666-5672.	1.6	14
119	Trajectory NG: portable, compressed, general molecular dynamics trajectories. Journal of Molecular Modeling, 2011, 17, 2669-2685.	0.8	14
120	An efficient and extensible format, library, and API for binary trajectory data from molecular simulations. Journal of Computational Chemistry, 2014, 35, 260-269.	1.5	14
121	Membrane vesiculation induced by proteins of the dengue virus envelope studied by molecular dynamics simulations. Journal of Physics Condensed Matter, 2017, 29, 504002.	0.7	14
122	Direct Link between Structure, Dynamics, and Thermodynamics in Molten Salts. Journal of Physical Chemistry C, 2019, 123, 25596-25602.	1.5	14
123	Quantitative predictions from molecular simulations using explicit or implicit interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1560.	6.2	14
124	An Intuitively Understandable Quality Measure for Theoretical Vibrational Spectra. Journal of Physical Chemistry Letters, 2020, 11, 5471-5475.	2.1	13
125	Structural studies of melting on the picosecond time scale. Physical Chemistry Chemical Physics, 2008, 10, 6344.	1.3	12
126	Open conformation of adipokinetic hormone receptor from the malaria mosquito facilitates hormone binding. Peptides, 2011, 32, 553-559.	1.2	12

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127	Microscopic origins of conductivity in molten salts unraveled by computer simulations. Communications Chemistry, 2021, 4, .	2.0	11
128	Deconvoluting Protein (Un)folding Structural Ensembles Using X-Ray Scattering, Nuclear Magnetic Resonance Spectroscopy and Molecular Dynamics Simulation. PLoS ONE, 2015, 10, e0125662.	1.1	10
129	Molecular Dynamics Simulations of Peptides from the Central Domain of Smooth Muscle Caldesmon. Journal of Biomolecular Structure and Dynamics, 2004, 21, 555-565.	2.0	9
130	NMR refinement and peptide folding using the GROMACS software. Journal of Biomolecular NMR, 2021, 75, 143-149.	1.6	9
131	A density functional study of 15N chemical shielding tensors in quinolines. Chemical Physics Letters, 2009, 476, 196-200.	1.2	7
132	Binding of Pollutants to Biomolecules: A Simulation Study. Chemical Research in Toxicology, 2016, 29, 1679-1688.	1.7	7
133	Phosphorylationâ€induced torsionâ€angle strain in the active center of HPr, detected by NMR and restrained molecular dynamics refinement. Protein Science, 1996, 5, 442-446.	3.1	6
134	Transient isomers in the photodissociation of bromoiodomethane. Journal of Chemical Physics, 2018, 148, 134307.	1.2	6
135	Free Energy of Separation of Structure II Clathrate Hydrate in Water and a Light Oil. Journal of Physical Chemistry B, 2012, 116, 5933-5940.	1.2	5
136	Role of Hostâ€“Guest Charge Transfer in Cyclodextrin Complexation: A Computational Study. Journal of Physical Chemistry C, 2019, 123, 17745-17756.	1.5	5
137	Toward a Computational Ecotoxicity Assay. Journal of Chemical Information and Modeling, 2020, 60, 3792-3803.	2.5	5
138	A potential for molecular simulation of compounds with linear moieties. Journal of Chemical Physics, 2020, 153, 084503.	1.2	5
139	Propagation of uncertainty in physicochemical data to force field predictions. Physical Review Research, 2020, 2, .	1.3	4
140	Interactive visualization of electron density slices. Journal of Applied Crystallography, 2005, 38, 563-565.	1.9	3
141	Role of spin state on the geometry and nuclear quadrupole resonance parameters in hemin complex. Biophysical Chemistry, 2008, 134, 200-206.	1.5	3
142	Probing 13C chemical shielding tensors in cryptolepine and two bromo-substituted analogs for antiplasmodial activity. Journal of Molecular Modeling, 2011, 17, 3289-3297.	0.8	3
143	Carbonyl Charge Solvation Patterns May Relate to Fragmentation Classes in Collision-Activated Dissociation. Journal of the American Society for Mass Spectrometry, 2012, 23, 1319-1325.	1.2	3
144	The structure of CO2 and CH4 at the interface of a poly(urethane urea) oligomer model from the microscopic point of view. Journal of Chemical Physics, 2021, 155, 044704.	1.2	3

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145	Protein Folding Properties from Molecular Dynamics Simulations. Lecture Notes in Computer Science, 2007, , 109-115.	1.0	3
146	Improved GROMACS Scaling on Ethernet Switched Clusters. Lecture Notes in Computer Science, 2006, , 404-405.	1.0	2
147	The solution conformations of amino acids from molecular dynamics simulations of Gly-X-Gly peptides: comparison with NMR parameters. Biochemistry and Cell Biology, 1998, 76, 164-70.	0.9	2
148	A theoretical study of repeating sequence in HRP II: A combination of molecular dynamics simulations and 17O quadrupole coupling tensors. Biophysical Chemistry, 2008, 137, 76-80.	1.5	1
149	Detection of Functional Modes in Protein Dynamics. Biophysical Journal, 2010, 98, 566a.	0.2	1
150	Order Parameters and Algorithmic Approaches for Detection and Demarcation of Interfaces in Hydrateâ€“Fluid and Iceâ€“Fluid Systems. Journal of Chemical Theory and Computation, 2014, 10, 5606-5615.	2.3	1
151	Energy Utilization, Catalysis and Evolution-Emergent Properties of Life. Current Chemical Biology, 2007, 1, 53-57.	0.2	1
152	Ultrafast structural studies on biological molecules by x-rays. , 1999, , .		0
153	<title>Radiation-induced electron cascade in diamond and amorphous carbon</title>. , 2001, , .		0
154	Molecular Modeling of Inhibitors at Qi and Qo Sites in Cytochromebc1 Complex. , 0, , 110-127.		0
155	Explosions of Methane Clusters Driven by Intense X-Ray FEL Pulses. , 2011, , .		0
156	Macromol. Biosci. 1/2011. Macromolecular Bioscience, 2011, 11, .	2.1	0
157	Structural Determinants of Solute Diffusion through Membranes. Biophysical Journal, 2012, 102, 712a.	0.2	0
158	Unexpected Effects of Cholesterol on Membrane Permeability. Biophysical Journal, 2013, 104, 192a-193a.	0.2	0
159	Editorial overview: Theory and simulation and their new friends. Current Opinion in Structural Biology, 2021, 67, iii-v.	2.6	0
160	Binding Networks Identify Targetable Protein Pockets for Mechanism-Based Drug Design. International Journal of Molecular Sciences, 2022, 23, 7313.	1.8	0