David van der Spoel

List of Publications by Year
in descending order

160 papers	62,424 citations	26630 56 h-index	7745 150 g-index
166 all docs	166 docs citations	166 times ranked	48037 citing authors

#	Article	IF	Citations
1	Quantitative predictions from molecular simulations using explicit or implicit interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1560.	14.6	14
2	Binding Networks Identify Targetable Protein Pockets for Mechanism-Based Drug Design. International Journal of Molecular Sciences, 2022, 23, 7313.	4.1	0
3	Systematic design of biomolecular force fields. Current Opinion in Structural Biology, 2021, 67, 18-24.	5.7	30
4	Microscopic origins of conductivity in molten salts unraveled by computer simulations. Communications Chemistry, 2021, 4, .	4.5	11
5	NMR refinement and peptide folding using the GROMACS software. Journal of Biomolecular NMR, 2021, 75, 143-149.	2.8	9
6	Classical molecular dynamics. Journal of Chemical Physics, 2021, 154, 100401.	3.0	28
7	Editorial overview: Theory and simulation and their new friends. Current Opinion in Structural Biology, 2021, 67, iii-v.	5.7	0
8	Accurate absolute free energies for ligandâ€“protein binding based on non-equilibrium approaches. Communications Chemistry, 2021, 4, .	4.5	49
9	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.	3.0	3
10	Making Soup: Preparing and Validating Models of the Bacterial Cytoplasm for Molecular Simulation. Journal of Chemical Information and Modeling, 2020, 60, 322-331.	5.4	17
11	Toward a Computational Ecotoxicity Assay. Journal of Chemical Information and Modeling, 2020, 60, 3792-3803.	5.4	5
12	A potential for molecular simulation of compounds with linear moieties. Journal of Chemical Physics, 2020, 153, 084503.	3.0	5
13	An Intuitively Understandable Quality Measure for Theoretical Vibrational Spectra. Journal of Physical Chemistry Letters, 2020, 11, 5471-5475.	4.6	13
14	Theoretical Infrared Spectra: Quantitative Similarity Measures and Force Fields. Journal of Chemical Theory and Computation, 2020, 16, 3307-3315.	5.3	31
15	Propagation of uncertainty in physicochemical data to force field predictions. Physical Review Research, 2020, 2, .	3.6	4
16	Molten alkali halides â€“ temperature dependence of structure, dynamics and thermodynamics. Physical Chemistry Chemical Physics, 2019, 21, 18516-18524.	2.8	19
17	Prediction of Partition Coefficients of Environmental Toxins Using Computational Chemistry Methods. ACS Omega, 2019, 4, 13772-13781.	3.5	24
18	Role of Hostâ€“Guest Charge Transfer in Cyclodextrin Complexation: A Computational Study. Journal of Physical Chemistry C, 2019, 123, 17745-17756.	3.1	5

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19	Direct Link between Structure, Dynamics, and Thermodynamics in Molten Salts. Journal of Physical Chemistry C, 2019, 123, 25596-25602.	3.1	14
20	Systematically improved melting point prediction: a detailed physical simulation model is required. Chemical Communications, 2019, 55, 12044-12047.	4.1	17
21	Ten simple rules on how to create open access and reproducible molecular simulations of biological systems. PLoS Computational Biology, 2019, 15, e1006649.	3.2	25
22	Rotational and Translational Diffusion of Proteins as a Function of Concentration. ACS Omega, 2019, 4, 20654-20664.	3.5	17
23	Transient isomers in the photodissociation of bromoiodomethane. Journal of Chemical Physics, 2018, 148, 134307.	3.0	6
24	The Alexandria library, a quantum-chemical database of molecular properties for force field development. Scientific Data, 2018, 5, 180062.	5.3	45
25	Force Field Benchmark of Amino Acids: I. Hydration and Diffusion in Different Water Models. Journal of Chemical Information and Modeling, 2018, 58, 1037-1052.	5.4	70
26	Influence of Na+ and Mg2+ ions on RNA structures studied with molecular dynamics simulations. Nucleic Acids Research, 2018, 46, 4872-4882.	14.5	76
27	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.	5.3	27
28	Phase-Transferable Force Field for Alkali Halides. Journal of Chemical Theory and Computation, 2018, 14, 5933-5948.	5.3	35
29	Small Molecule Thermochemistry: A Tool for Empirical Force Field Development. Journal of Physical Chemistry A, 2018, 122, 8982-8988.	2.5	25
30	Statistical efficiency of methods for computing free energy of hydration. Journal of Chemical Physics, 2018, 149, 144111.	3.0	16
31	Impact of Dispersion Coefficient on Simulations of Proteins and Organic Liquids. Journal of Physical Chemistry B, 2018, 122, 8018-8027.	2.6	16
32	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.	5.3	180
33	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.	4.6	40
34	Mechanistic Insights into Autoinhibition of the Oncogenic Chromatin Remodeler ALC1. Molecular Cell, 2017, 68, 847-859.e7.	9.7	53
35	Membrane vesiculation induced by proteins of the dengue virus envelope studied by molecular dynamics simulations. Journal of Physics Condensed Matter, 2017, 29, 504002.	1.8	14
36	Systematic exploration of multiple drug binding sites. Journal of Cheminformatics, 2017, 9, 65.	6.1	20

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37	Large-scale calculations of gas phase thermochemistry: Enthalpy of formation, standard entropy, and heat capacity. Journal of Chemical Physics, 2016, 145, .	3.0	60
38	Water Determines the Structure and Dynamics of Proteins. Chemical Reviews, 2016, 116, 7673-7697.	47.7	645
39	Binding of Pollutants to Biomolecules: A Simulation Study. Chemical Research in Toxicology, 2016, 29, 1679-1688.	3.3	7
40	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.	5.4	32
41	Atomistic Simulation of Protein Encapsulation in Metalâ€“Organic Frameworks. Journal of Physical Chemistry B, 2016, 120, 477-484.	2.6	35
42	Exploration of Interfacial Hydration Networks of Targetâ€“Ligand Complexes. Journal of Chemical Information and Modeling, 2016, 56, 148-158.	5.4	30
43	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.	3.3	79
44	Deconvoluting Protein (Un)folding Structural Ensembles Using X-Ray Scattering, Nuclear Magnetic Resonance Spectroscopy and Molecular Dynamics Simulation. PLoS ONE, 2015, 10, e0125662.	2.5	10
45	Properties of Organic Liquids when Simulated with Long-Range Lennard-Jones Interactions. Journal of Chemical Theory and Computation, 2015, 11, 2938-2944.	5.3	116
46	Deciphering Solution Scattering Data with Experimentally Guided Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2015, 11, 780-787.	5.3	45
47	Force Field Benchmark of Organic Liquids. 2. Gibbs Energy of Solvation. Journal of Chemical Information and Modeling, 2015, 55, 1192-1201.	5.4	77
48	Relationship between electronic properties and drug activity of seven quinoxaline compounds: A DFT study. Journal of Molecular Structure, 2015, 1091, 196-202.	3.6	23
49	Mobility-based prediction of hydration structures of protein surfaces. Bioinformatics, 2015, 31, 1959-1965.	4.1	30
50	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.	5.3	31
51	Impact of sludge deposition on biodiversity. Ecotoxicology, 2015, 24, 1799-1814.	2.4	24
52	An efficient and extensible format, library, and API for binary trajectory data from molecular simulations. Journal of Computational Chemistry, 2014, 35, 260-269.	3.3	14
53	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.	5.3	1
54	Cooperative Binding of Cyclodextrin Dimers to Isoflavone Analogues Elucidated by Free Energy Calculations. Journal of Physical Chemistry C, 2014, 118, 7163-7173.	3.1	35

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55	MemBuilder: a web-based graphical interface to build heterogeneously mixed membrane bilayers for the GROMACS biomolecular simulation program. Bioinformatics, 2014, 30, 439-441.	4.1	54
56	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.	13.7	59
57	Thermodynamics of hydronium and hydroxide surface solvation. Chemical Science, 2014, 5, 1745.	7.4	56
58	Chemical Properties, Environmental Fate, and Degradation of Seven Classes of Pollutants. Chemical Research in Toxicology, 2014, 27, 713-737.	3.3	91
59	Thiamin Function, Metabolism, Uptake, and Transport. Biochemistry, 2014, 53, 821-835.	2.5	242
60	Local Partition Coefficients Govern Solute Permeability of Cholesterol-Containing Membranes. Biophysical Journal, 2013, 105, 2760-2770.	0.5	67
61	Quantification of Solvent Contribution to the Stability of Noncovalent Complexes. Journal of Chemical Theory and Computation, 2013, 9, 4542-4551.	5.3	37
62	Unexpected Effects of Cholesterol on Membrane Permeability. Biophysical Journal, 2013, 104, 192a-193a.	0.5	0
63	Î²-Sheet Structures and Dimer Models of the Two Major Tyrocidines, Antimicrobial Peptides from Bacillus aneurinolyticus. Biochemistry, 2013, 52, 7798-7806.	2.5	25
64	Anopheles gambiae, Anoga-HrTH hormone, free and bound structure â€“ A nuclear magnetic resonance experiment. Peptides, 2013, 41, 94-100.	2.4	17
65	GROMACS 4.5: a high-throughput and highly parallel open source molecular simulation toolkit. Bioinformatics, 2013, 29, 845-854.	4.1	6,072
66	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.	10.0	65
67	Fullerenes toxicity and electronic properties. Environmental Chemistry Letters, 2013, 11, 105-118.	16.2	44
68	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.	7.1	79
69	GROMACS molecule & liquid database. Bioinformatics, 2012, 28, 752-753.	4.1	161
70	Structural Determinants of Solute Diffusion through Membranes. Biophysical Journal, 2012, 102, 712a.	0.5	0
71	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.	5.3	24
72	Organic molecules on the surface of water droplets â€“ an energetic perspective. Physical Chemistry Chemical Physics, 2012, 14, 9537.	2.8	52

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73	Free Energy of Separation of Structure II Clathrate Hydrate in Water and a Light Oil. Journal of Physical Chemistry B, 2012, 116, 5933-5940.	2.6	5
74	Insight into the Structural Deformations of Beta-Cyclodextrin Caused by Alcohol Cosolvents and Guest Molecules. Journal of Physical Chemistry B, 2012, 116, 3880-3889.	2.6	37
75	Molecular Recognition in Different Environments: Î²-Cyclodextrin Dimer Formation in Organic Solvents. Journal of Physical Chemistry B, 2012, 116, 12684-12693.	2.6	56
76	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.	5.3	609
77	Large Influence of Cholesterol on Solute Partitioning into Lipid Membranes. Journal of the American Chemical Society, 2012, 134, 5351-5361.	13.7	145
78	Virus Capsid Dissolution Studied by Microsecond Molecular Dynamics Simulations. PLoS Computational Biology, 2012, 8, e1002502.	3.2	70
79	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.	2.8	3
80	On the Feasibility of Nanocrystal Imaging Using Intense and Ultrashort X-ray Pulses. ACS Nano, 2011, 5, 139-146.	14.6	61
81	Time-Resolved WAXS Reveals Accelerated Conformational Changes in Iodoretinal-Substituted Proteorhodopsin. Biophysical Journal, 2011, 101, 1345-1353.	0.5	60
82	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.	7.1	192
83	Subunit Interface Dynamics in Hexadecameric Rubisco. Journal of Molecular Biology, 2011, 411, 1083-1098.	4.2	33
84	Open conformation of adipokinetic hormone receptor from the malaria mosquito facilitates hormone binding. Peptides, 2011, 32, 553-559.	2.4	12
85	Explosions of Methane Clusters Driven by Intense X-Ray FEL Pulses. , 2011, , .		0
86	GROMACSâ€"the road ahead. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 710-715.	14.6	43
87	Trajectory NG: portable, compressed, general molecular dynamics trajectories. Journal of Molecular Modeling, 2011, 17, 2669-2685.	1.8	14
88	Probing 13C chemical shielding tensors in cryptolepine and two bromo-substituted analogs for antiplasmodial activity. Journal of Molecular Modeling, 2011, 17, 3289-3297.	1.8	3
89	Toward prediction of functional protein pockets using blind docking and pocket search algorithms. Protein Science, 2011, 20, 880-893.	7.6	59
90	Proteins, Lipids, and Water in the Gas Phase. Macromolecular Bioscience, 2011, 11, 50-59.	4.1	77

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91	Macromol. Biosci. 1/2011. Macromolecular Bioscience, 2011, 11, .	4.1	0
92	Hawk: the image reconstruction package for coherent X-ray diffractive imaging. Journal of Applied Crystallography, 2010, 43, 1535-1539.	4.5	46
93	Scrutinizing Molecular Mechanics Force Fields on the Submicrosecond Timescale with NMR Data. Biophysical Journal, 2010, 99, 647-655.	0.5	192
94	g_whamâ€"A Free Weighted Histogram Analysis Implementation Including Robust Error and Autocorrelation Estimates. Journal of Chemical Theory and Computation, 2010, 6, 3713-3720.	5.3	1,284
95	Detection of Functional Modes in Protein Dynamics. Biophysical Journal, 2010, 98, 566a.	0.5	1
96	Structural variability and the incoherent addition of scattered intensities in single-particle diffraction. Physical Review E, 2009, 80, 031905.	2.1	25
97	A density functional study of 15N chemical shielding tensors in quinolines. Chemical Physics Letters, 2009, 476, 196-200.	2.6	7
98	Efficient docking of peptides to proteins without prior knowledge of the binding site. Protein Science, 2009, 11, 1729-1737.	7.6	370
99	Solution conformations of an insect neuropeptide: Crustacean cardioactive peptide (CCAP). Peptides, 2009, 30, 557-564.	2.4	16
100	Structural stability of electrosprayed proteins: temperature and hydration effects. Physical Chemistry Chemical Physics, 2009, 11, 8069.	2.8	57
101	Molecular Dynamics Simulations of a Membrane Proteinâ^'Micelle Complex in Vacuo. Journal of the American Chemical Society, 2009, 131, 16606-16607.	13.7	31
102	Encapsulation of Myoglobin in a Cetyl Trimethylammonium Bromide Micelle in Vacuo: A Simulation Study. Biochemistry, 2009, 48, 1006-1015.	2.5	36
103	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.	2.8	1
104	Picosecond Melting of Ice by an Infrared Laser Pulse: A Simulation Study. Angewandte Chemie - International Edition, 2008, 47, 1417-1420.	13.8	46
105	Role of spin state on the geometry and nuclear quadrupole resonance parameters in hemin complex. Biophysical Chemistry, 2008, 134, 200-206.	2.8	3
106	GROMACS 4:â€‰ Algorithms for Highly Efficient, Load-Balanced, and Scalable Molecular Simulation. Journal of Chemical Theory and Computation, 2008, 4, 435-447.	5.3	13,875
107	A Proposed Time-Resolved X-Ray Scattering Approach to Track Local and Global Conformational Changes in Membrane Transport Proteins. Structure, 2008, 16, 21-28.	3.3	20
108	Structural studies of melting on the picosecond time scale. Physical Chemistry Chemical Physics, 2008, 10, 6344.	2.8	12

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109	A temperature predictor for parallel tempering simulations. Physical Chemistry Chemical Physics, 2008, 10, 2073.	2.8	437
110	Fluorescence Probe of Trp-Cage Protein Conformation in Solution and in Gas Phase. Journal of the American Chemical Society, 2007, 129, 6726-6735.	13.7	64
111	Evaporation from water clusters containing singly charged ions. Physical Chemistry Chemical Physics, 2007, 9, 5105.	2.8	64
112	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.	2.6	46
113	Protein Structures under Electrospray Conditions. Biochemistry, 2007, 46, 933-945.	2.5	120
114	Speeding up parallel GROMACS on high-latency networks. Journal of Computational Chemistry, 2007, 28, 2075-2084.	3.3	107
115	Protein Folding Properties from Molecular Dynamics Simulations. Lecture Notes in Computer Science, 2007, , 109-115.	1.3	3
116	Energy Utilization, Catalysis and Evolution-Emergent Properties of Life. Current Chemical Biology, 2007, 1, 53-57.	0.5	1
117	Thermodynamics of Hydrogen Bonding in Hydrophilic and Hydrophobic Media. Journal of Physical Chemistry B, 2006, 110, 4393-4398.	2.6	404
118	The Origin of Layer Structure Artifacts in Simulations of Liquid Water. Journal of Chemical Theory and Computation, 2006, 2, 1-11.	5.3	195
119	Lifting a Wet Glass from a Table:Â A Microscopic Picture. Langmuir, 2006, 22, 5666-5672.	3.5	14
120	Blind docking of drug-sized compounds to proteins with up to a thousand residues. FEBS Letters, 2006, 580, 1447-1450.	2.8	253
121	Femtosecond diffractive imaging with a soft-X-ray free-electron laser. Nature Physics, 2006, 2, 839-843.	16.7	910
122	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.	1.5	31
123	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.	1.5	59
124	Protein Folding Kinetics and Thermodynamics from Atomistic Simulations. Physical Review Letters, 2006, 96, 238102.	7.8	85
125	Temperature and structural changes of water clusters in vacuum due to evaporation. Journal of Chemical Physics, 2006, 125, 154508.	3.0	59
126	Improved GROMACS Scaling on Ethernet Switched Clusters. Lecture Notes in Computer Science, 2006, , 404-405.	1.3	2

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127	GROMACS: Fast, flexible, and free. Journal of Computational Chemistry, 2005, 26, 1701-1718.	3.3	13,676
128	Interactive visualization of electron density slices. Journal of Applied Crystallography, 2005, 38, 563-565.	4.5	3
129	Observation of Structural Anisotropy and the Onset of Liquidlike Motion During the Nonthermal Melting of InSb. Physical Review Letters, 2005, 95, 125701.	7.8	56
130	Clocking Femtosecond X Rays. Physical Review Letters, 2005, 94, 114801.	7.8	230
131	Atomic-Scale Visualization of Inertial Dynamics. Science, 2005, 308, 392-395.	12.6	324
132	Reproducible Polypeptide Folding and Structure Prediction using Molecular Dynamics Simulations. Journal of Molecular Biology, 2005, 354, 173-183.	4.2	165
133	Model for the dynamics of a water cluster in an x-ray free electron laser beam. Physical Review E, 2004, 70, 051904.	2.1	69
134	Deformation of Helix C in the Low Temperature L-intermediate of Bacteriorhodopsin. Journal of Biological Chemistry, 2004, 279, 2147-2158.	3.4	72
135	Potential impact of an X-ray free electron laser on structural biology. Radiation Physics and Chemistry, 2004, 71, 905-916.	2.8	55
136	Auger electron cascades in water and ice. Chemical Physics, 2004, 299, 277-283.	1.9	55
137	Molecular Dynamics Simulations of Peptides from the Central Domain of Smooth Muscle Caldesmon. Journal of Biomolecular Structure and Dynamics, 2004, 21, 555-565.	3.5	9
138	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.	2.9	42
139	Brute-Force Molecular Dynamics Simulations of Villin Headpiece:Â Comparison with NMR Parameters. Journal of Physical Chemistry B, 2003, 107, 11178-11187.	2.6	62
140	Dynamic properties of water/alcohol mixtures studied by computer simulation. Journal of Chemical Physics, 2003, 119, 7308-7317.	3.0	255
141	Space-time evolution of electron cascades in diamond. Physical Review B, 2002, 66, .	3.2	38
142	Molecular Dynamics Simulations of Water with Novel Shell-Model Potentials. Journal of Physical Chemistry B, 2001, 105, 2618-2626.	2.6	162
143	<title>Radiation-induced electron cascade in diamond and amorphous carbon</title>. , 2001, , .		0
144	GROMACS 3.0: a package for molecular simulation and trajectory analysis. Journal of Molecular Modeling, 2001, 7, 306-317.	1.8	6,085

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145	Auger-electron cascades in diamond and amorphous carbon. Physical Review B, 2001, 64, .	3.2	53
146	Potential for biomolecular imaging with femtosecond X-ray pulses. Nature, 2000, 406, 752-757.	27.8	1,773
147	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.	2.6	273
148	Ultrafast structural studies on biological molecules by x-rays. , 1999, , .		0
149	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.	2.0	16
150	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.	3.0	581
151	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.	2.0	2
152	Molecular dynamics simulations of Leu-enkephalin in water and DMSO. Biophysical Journal, 1997, 72, 2032-2041.	0.5	108
153	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.	0.5	18
154	Molecular dynamics simulations of N-terminal peptides from a nucleotide binding protein. , 1996, 24, 450-466.		17
155	Molecular dynamics simulations of peptides from BPTI: A closer look at amideâ€”aromatic interactions. Journal of Biomolecular NMR, 1996, 8, 229-238.	2.8	84
156	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.	7.6	6
157	Bending of the calmodulin central helix: A theoretical study. Protein Science, 1996, 5, 2044-2053.	7.6	71
158	GROMACS: A message-passing parallel molecular dynamics implementation. Computer Physics Communications, 1995, 91, 43-56.	7.5	8,250
159	Towards phase transferable potential functions: Methodology and application to nitrogen. Journal of Chemical Physics, 1995, 103, 2272-2285.	3.0	33
160	Molecular Modeling of Inhibitors at Qi and Qo Sites in Cytochromebc1 Complex. , 0, , 110-127.		0