Wilfred F Van Gunsteren

List of Publications by Year
in descending order

239	26,652	16437 64	6294 158
papers	citations	h-index	g-index

247	247	247	19230
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A biomolecular force field based on the free enthalpy of hydration and solvation: The GROMOS force-field parameter sets 53A5 and 53A6. Journal of Computational Chemistry, 2004, 25, 1656-1676.	1.5	3,309
2	Definition and testing of the GROMOS force-field versions 54A7 and 54B7. European Biophysics Journal, 2011, 40, 843-856.	1.2	1,902
3	Peptide Folding: When Simulation Meets Experiment. Angewandte Chemie - International Edition, 1999, 38, 236-240.	7.2	1,611
4	The GROMOS Biomolecular Simulation Program Package. Journal of Physical Chemistry A, 1999, 103, 3596-3607.	1.1	1,354
5	Computer Simulation of Molecular Dynamics: Methodology, Applications, and Perspectives in Chemistry. Angewandte Chemie International Edition in English, 1990, 29, 992-1023.	4.4	1,352
6	A generalized reaction field method for molecular dynamics simulations. Journal of Chemical Physics, 1995, 102, 5451-5459.	1.2	1,293
7	A fast SHAKE algorithm to solve distance constraint equations for small molecules in molecular dynamics simulations. Journal of Computational Chemistry, 2001, 22, 501-508.	1.5	959
8	An improved GROMOS96 force field for aliphatic hydrocarbons in the condensed phase. Journal of Computational Chemistry, 2001, 22, 1205-1218.	1.5	814
9	A consistent empirical potential for water-protein interactions. Biopolymers, 1984, 23, 1513-1518.	1.2	759
10	The GROMOS software for biomolecular simulation: GROMOS05. Journal of Computational Chemistry, 2005, 26, 1719-1751.	1.5	592
11	Local elevation: A method for improving the searching properties of molecular dynamics simulation. Journal of Computer-Aided Molecular Design, 1994, 8, 695-708.	1.3	510
12	Biomolecular Modeling: Goals, Problems, Perspectives. Angewandte Chemie - International Edition, 2006, 45, 4064-4092.	7.2	503
13	Validation of the 53A6 GROMOS force field. European Biophysics Journal, 2005, 34, 273-284.	1.2	443
14	Parametrization of aliphatic CHn united atoms of GROMOS96 force field. Journal of Computational Chemistry, 1998, 19, 535-547.	1.5	370
15	Folding-unfolding thermodynamics of a ?-heptapeptide from equilibrium simulations. Proteins: Structure, Function and Bioinformatics, 1999, 34, 269-280.	1.5	370
16	Comparison of four methods to compute the dielectric permittivity of liquids from molecular dynamics simulations. Journal of Chemical Physics, 2001, 115, 1125-1136.	1.2	327
17	Decomposition of the Free Energy of a System in Terms of Specific Interactions. Journal of Molecular Biology, 1994, 240, 167-176.	2.0	314
18	Time-averaged nuclear overhauser effect distance restraints applied to tendamistat. Journal of Molecular Biology, 1990, 214, 223-235.	2.0	288

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19	Basic ingredients of free energy calculations: A review. Journal of Computational Chemistry, 2010, 31, 1569-1582.	1.5	281
20	Architecture, implementation and parallelisation of the GROMOS software for biomolecular simulation. Computer Physics Communications, 2012, 183, 890-903.	3.0	275
21	Time-dependent distance restraints in molecular dynamics simulations. Chemical Physics Letters, 1989, 157, 289-294.	1.2	268
22	A Comparison of Methods to Compute the Potential of Mean Force. ChemPhysChem, 2007, 8, 162-169.	1.0	243
23	Development of a simple, self-consistent polarizable model for liquid water. Journal of Chemical Physics, 2003, 118, 221-234.	1.2	209
24	Derivation of an improved simple point charge model for liquid water: SPC/A and SPC/L. Journal of Chemical Physics, 2002, 116, 9811-9828.	1.2	203
25	Consistent dielectric properties of the simple point charge and extended simple point charge water models at 277 and 300 K. Journal of Chemical Physics, 1994, 100, 3169-3174.	1.2	201
26	GROMOS++ Software for the Analysis of Biomolecular Simulation Trajectories. Journal of Chemical Theory and Computation, 2011, 7, 3379-3390.	2.3	180
27	Absolute entropies from molecular dynamics simulation trajectories. Journal of Chemical Physics, 2000, 113, 7809-7817.	1.2	171
28	Molecular simulation as an aid to experimentalists. Current Opinion in Structural Biology, 2008, 18, 149-153.	2.6	171
29	Calculating Electrostatic Interactions Using the Particleâˆ'Particle Particleâˆ'Mesh Method with Nonperiodic Long-Range Interactions. The Journal of Physical Chemistry, 1996, 100, 2581-2587.	2.9	164
30	Can One Derive the Conformational Preference of a Î²-Peptide from Its CD Spectrum?. Journal of the American Chemical Society, 2002, 124, 12972-12978.	6.6	162
31	Validation of molecular dynamics simulation. Journal of Chemical Physics, 1998, 108, 6109-6116.	1.2	161
32	An improved nucleic acid parameter set for the GROMOS force field. Journal of Computational Chemistry, 2005, 26, 725-737.	1.5	161
33	Simulating proteins at constant pH: An approach combining molecular dynamics and Monte Carlo simulation. Proteins: Structure, Function and Bioinformatics, 2002, 47, 469-480.	1.5	157
34	On searching in, sampling of, and dynamically moving through conformational space of biomolecular systems: A review. Journal of Computational Chemistry, 2008, 29, 157-166.	1.5	148
35	Estimating entropies from molecular dynamics simulations. Journal of Chemical Physics, 2004, 120, 2652-2661.	1.2	138
36	Structure refinement using time-averaged J-coupling constant restraints. Journal of Biomolecular NMR, 1993, 3, 55-66.	1.6	125

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37	The effect of force-field parameters on properties of liquids: Parametrization of a simple three-site model for methanol. Journal of Chemical Physics, 2000, 112, 10450-10459.	1.2	125
38	The Key to Solving the Protein-Folding Problem Lies in an Accurate Description of the Denatured State. Angewandte Chemie - International Edition, 2001, 40, 351-355.	7.2	124
39	Computer Simulation of Ureaâ^'Water Mixtures:â€‰ A Test of Force Field Parameters for Use in Biomolecular Simulation. Journal of Physical Chemistry B, 2004, 108, 1065-1071.	1.2	123
40	A simple, efficient polarizable coarse-grained water model for molecular dynamics simulations. Journal of Chemical Physics, 2011, 134, 084110.	1.2	121
41	Studying the Stability of a Helical Î²â€Heptapeptide by Molecular Dynamics Simulations. Chemistry - A European Journal, 1997, 3, 1410-1417.	1.7	120
42	On the interpretation of biochemical data by molecular dynamics computer simulation. FEBS Journal, 1992, 204, 947-961.	0.2	117
43	MolekÃ¼ldynamikâ€Computersimulationen; Methodik, Anwendungen und Perspektiven in der Chemie. Angewandte Chemie, 1990, 102, 1020-1055.	1.6	114
44	New Interaction Parameters for Oxygen Compounds in the GROMOS Force Field: Improved Pure-Liquid and Solvation Properties for Alcohols, Ethers, Aldehydes, Ketones, Carboxylic Acids, and Esters. Journal of Chemical Theory and Computation, 2011, 7, 1016-1031.	2.3	112
45	On the Choice of Dihedral Angle Potential Energy Functions forn-Alkanes. Molecular Simulation, 2000, 25, 301-319.	0.9	111
46	A Comparison of Non-Bonded Scaling Approaches for Free Energy Calculations. Molecular Simulation, 2002, 28, 45-65.	0.9	109
47	The effect of motional averaging on the calculation of NMR-derived structural properties. , 1999, 36, 542-555.		103
48	Molecular dynamics simulations of liquid methanol and methanolâ€“water mixtures with polarizable models. Journal of Computational Chemistry, 2006, 27, 1494-1504.	1.5	103
49	Comparison of Thermodynamic Properties of Coarse-Grained and Atomic-Level Simulation Models. ChemPhysChem, 2007, 8, 452-461.	1.0	102
50	Validation of Molecular Simulation: An Overview of Issues. Angewandte Chemie - International Edition, 2018, 57, 884-902.	7.2	101
51	New functionalities in the GROMOS biomolecular simulation software. Journal of Computational Chemistry, 2012, 33, 340-353.	1.5	98
52	Entropy calculations on a reversibly folding peptide: Changes in solute free energy cannot explain folding behavior. Proteins: Structure, Function and Bioinformatics, 2001, 43, 45-56.	1.5	97
53	An Effective Force Field for Molecular Dynamics Simulations of Dimethyl Sulfoxide and Dimethyl Sulfoxideâ^'Water Mixtures. Journal of Physical Chemistry B, 2004, 108, 1436-1445.	1.2	97
54	Algorithms for clustering molecular dynamics configurations. Journal of Computational Chemistry, 1994, 15, 1331-1340.	1.5	92

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55	Calculation of NMR-relaxation parameters for flexible molecules from molecular dynamics simulations. Journal of Biomolecular NMR, 2001, 20, 297-310.	1.6	89
56	When Are Free Energy Components Meaningful?. The Journal of Physical Chemistry, 1994, 98, 13735-13740.	2.9	87
57	On the relative merits of flexible versus rigid models for use in computer simulations of molecular liquids. Chemical Physics Letters, 1996, 250, 19-24.	1.2	85
58	A Structure Refinement Method Based on Molecular Dynamics in Four Spatial Dimensions. Journal of Molecular Biology, 1993, 234, 751-762.	2.0	84
59	Molecular dynamics simulation of hen egg white lysozyme: A test of the GROMOS96 force field against nuclear magnetic resonance data. Proteins: Structure, Function and Bioinformatics, 2000, 40, 145-153.	1.5	82
60	Comparing atomistic simulation data with the NMR experiment: How much can NOEs actually tell us?. Proteins: Structure, Function and Bioinformatics, 2006, 63, 210-218.	1.5	82
61	Calculation of relative free energy via indirect pathways. Journal of Chemical Physics, 1991, 94, 3808-3816.	1.2	78
62	Free energies of binding of polychlorinated biphenyls to the estrogen receptor from a single simulation. Proteins: Structure, Function and Bioinformatics, 2003, 54, 237-246.	1.5	77
63	On using a too large integration time step in molecular dynamics simulations of coarse-grained molecular models. Physical Chemistry Chemical Physics, 2009, 11, 1934-41.	1.3	76
64	Predictions of free energy differences from a single simulation of the initial state. Journal of Chemical Physics, 1994, 100, 577-585.	1.2	72
65	Multiâ€Resolution Simulation of Biomolecular Systems: A Review of Methodological Issues. Angewandte Chemie - International Edition, 2013, 52, 2820-2834.	7.2	72
66	Structure refinement with molecular dynamics and a Boltzmann-weighted ensemble. Journal of Biomolecular NMR, 1995, 6, 163-170.	1.6	66
67	SWARM-MD:Â Searching Conformational Space by Cooperative Molecular Dynamics. Journal of Physical Chemistry A, 1998, 102, 5937-5943.	1.1	63
68	Single-step perturbations to calculate free energy differences from unphysical reference states: Limits on size, flexibility, and character. Journal of Computational Chemistry, 2003, 24, 1730-1739.	1.5	62
69	One-Step Perturbation Methods for Solvation Free Energies of Polar Solutes. Journal of Physical Chemistry B, 2001, 105, 11264-11274.	1.2	59
70	Entropy calculations on the molten globule state of a protein: Side-chain entropies of Î±-lactalbumin. Proteins: Structure, Function and Bioinformatics, 2002, 46, 215-224.	1.5	58
71	Estimating relative free energies from a single ensemble: Hydration free energies. Journal of Computational Chemistry, 1999, 20, 1604-1617.	1.5	57
72	Peptide Folding: When Simulation Meets Experiment. Angewandte Chemie - International Edition, 1999, 38, 236-240.	7.2	57

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73	Combined QM/MM Molecular Dynamics Study on a Condensed-Phase SN2 Reaction at Nitrogen:â€‰ The Effect of Explicitly Including Solvent Polarization. Journal of Chemical Theory and Computation, 2007, 3, 1499-1509.	2.3	52
74	Comparison of different schemes to treat long-range electrostatic interactions in molecular dynamics simulations of a protein crystal. Proteins: Structure, Function and Bioinformatics, 2001, 43, 509-519.	1.5	51
75	Molecular dynamics simulations of the native and partially folded states of ubiquitin: Influence of methanol cosolvent, pH, and temperature on the protein structure and dynamics. Protein Science, 2007, 16, 1101-1118.	3.1	51
76	Refinement of the application of the GROMOS 54A7 force field to Î²-peptides. Journal of Computational Chemistry, 2013, 34, 2796-2805.	1.5	51
77	Energyâ€“Entropy Compensation in the Transfer of Nonpolar Solutes from Water to Cosolvent/Water Mixtures. ChemPhysChem, 2004, 5, 144-147.	1.0	49
78	Biomolecular simulation: historical picture and future perspectives. Biochemical Society Transactions, 2008, 36, 11-15.	1.6	48
79	Viscosity dependence of protein dynamics. Proteins: Structure, Function and Bioinformatics, 2001, 42, 414-421.	1.5	47
80	Parametrisation of time-averaged distance restraints in MD simulations. Journal of Biomolecular NMR, 1995, 6, 313-320.	1.6	46
81	Solvating atomic level fine-grained proteins in supra-molecular level coarse-grained water for molecular dynamics simulations. European Biophysics Journal, 2012, 41, 647-661.	1.2	45
82	Solvent structure at a hydrophobic protein surface. , 1997, 27, 395-404.		43
83	Molecular-dynamics simulation of the ? domain of metallothionein with a semi-empirical treatment of the metal core. Proteins: Structure, Function and Bioinformatics, 2000, 41, 299-315.	1.5	43
84	A Combined Solidâ€State NMR and MD Characterization of the Stability and Dynamics of the HETâ€s(218â€289) Prion in its Amyloid Conformation. ChemBioChem, 2009, 10, 1657-1665.	1.3	43
85	Molecular Dynamics Simulations of Small Peptides: Can One Derive Conformational Preferences from ROESY Spectra?. Chemistry - A European Journal, 2003, 9, 5838-5849.	1.7	41
86	Biomolecular structure refinement using the GROMOS simulation software. Journal of Biomolecular NMR, 2011, 51, 265-281.	1.6	41
87	Backbone folding of the polypeptide cardiac stimulant anthopleurin-A determined by nuclear magnetic resonance, distance geometry and molecular dynamics. FEBS Letters, 1988, 239, 266-270.	1.3	39
88	Interpreting NMR Data for Î²-Peptides Using Molecular Dynamics Simulations. Journal of the American Chemical Society, 2005, 127, 14320-14329.	6.6	39
89	Are NMR-Derived Model Structures for Î²-Peptides Representative for the Ensemble of Structures Adopted in Solution?. Angewandte Chemie - International Edition, 2004, 43, 6312-6316.	7.2	38
90	A molecular dynamics study of the bee venom melittin in aqueous solution, in methanol, and inserted in a phospholipid bilayer. European Biophysics Journal, 2006, 35, 255-267.	1.2	36

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91	Comparison of three enveloping distribution sampling Hamiltonians for the estimation of multiple free energy differences from a single simulation. Journal of Computational Chemistry, 2009, 30, 1664-1679.	1.5	36
92	On the effect of a variation of the force field, spatial boundary condition and size of the QM region in QM/MM MD simulations. Journal of Computational Chemistry, 2012, 33, 363-378.	1.5	36
93	Peptide folding simulations: no solvent required?. Computer Physics Communications, 1999, 123, 97-102.	3.0	35
94	Calculating zeros: Non-equilibrium free energy calculations. Chemical Physics, 2006, 323, 102-108.	0.9	35
95	Simultaneous Refinement of the Structure of BPTI Against NMR Data Measured in Solution and X-ray Diffraction Data Measured in Single Crystals. Journal of Molecular Biology, 1994, 241, 588-599.	2.0	34
96	Dynamical studies of peptide motifs in the Plasmodium falciparum circumsporozoite surface protein by restrained and unrestrained MD simulations. Journal of Molecular Biology, 1997, 267, 1012-1025.	2.0	34
97	Efficient Calculation of Many Stacking and Pairing Free Energies in DNA from a Few Molecular Dynamics Simulations. Chemistry - A European Journal, 2005, 11, 4340-4348.	1.7	33
98	Force Field Evaluation for Biomolecular Simulation: Free Enthalpies of Solvation of Polar and Apolar Compounds in Various Solvents. ChemPhysChem, 2006, 7, 671-678.	1.0	32
99	Increasing the Time Step and Efficiency of Molecular Dynamics Simulations: Optimal Solutions for Equilibrium Simulations or Structure Refinement of Large Biomolecules. Molecular Simulation, 2003, 29, 123-138.	0.9	31
100	Protein under pressure: Molecular dynamics simulation of the arc repressor. Proteins: Structure, Function and Bioinformatics, 2006, 65, 136-144.	1.5	31
101	Methods of NMR structure refinement: molecular dynamics simulations improve the agreement with measured NMR data of a C-terminal peptide of GCN4-p1. Journal of Biomolecular NMR, 2010, 47, 221-235.	1.6	31
102	Sampling of Rare Events Using Hidden Restraints. Journal of Physical Chemistry B, 2006, 110, 8488-8498.	1.2	30
103	Catalytic mechanism of cyclophilin as observed in molecular dynamics simulations: Pathway prediction and reconciliation of X-ray crystallographic and NMR solution data. Protein Science, 2006, 15, 2544-2551.	3.1	29
104	Molecular dynamics simulations of human ?-lactalbumin: Changes to the structural and dynamical properties of the protein at low pH. , 1999, 36, 77-86.		28
105	A strategy for analysis of (molecular) equilibrium simulations: Configuration space density estimation, clustering, and visualization. Journal of Chemical Physics, 2001, 114, 2079-2089.	1.2	28
106	Further investigation on the validity of Stokesâ€“Einstein behaviour at the molecular level. Chemical Physics Letters, 2001, 334, 337-342.	1.2	27
107	Accessibility and order of water sites in and around proteins: A crystallographic time-averaging study. , 1999, 36, 501-511.		26
108	On using time-averaging restraints in molecular dynamics simulation. Journal of Biomolecular NMR, 1998, 12, 501-508.	1.6	25

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109	The Photoisomerization ofcis-Stilbene Does Not Follow the Minimum Energy Path. Angewandte Chemie - International Edition, 1999, 38, 2609-2611.	7.2	25
110	Amine Hydration: A United-Atom Force-Field Solution. ChemPhysChem, 2005, 6, 1800-1804.	1.0	25
111	On the Conformational Properties of Amylose and Cellulose Oligomers in Solution. International Journal of Carbohydrate Chemistry, 2009, 2009, 1-8.	1.5	25
112	A Method to Explore Protein Side Chain Conformational Variability Using Experimental Data. ChemPhysChem, 2009, 10, 3213-3228.	1.0	25
113	An Analysis of the Validity of Markov State Models for Emulating the Dynamics of Classical Molecular Systems and Ensembles. Journal of Chemical Theory and Computation, 2011, 7, 1032-1044.	2.3	25
114	Molecular dynamics simulation of n -dodecyl phosphate aggregate structures. European Biophysics Journal, 2001, 30, 330-343.	1.2	24
115	A novel approach for designing simple point charge models for liquid water with three interaction sites. Journal of Computational Chemistry, 2003, 24, 1087-1096.	1.5	24
116	Carbopeptoid Folding: Effects of Stereochemistry, Chain Length, and Solvent. Angewandte Chemie - International Edition, 2004, 43, 4055-4059.	7.2	24
117	The Seven Sins in Academic Behavior in the Natural Sciences. Angewandte Chemie - International Edition, 2013, 52, 118-122.	7.2	24
118	A polarizable empirical force field for molecular dynamics simulation of liquid hydrocarbons. Journal of Computational Chemistry, 2014, 35, 789-801.	1.5	24
119	Deriving Structural Information from Experimentally Measured Data on Biomolecules. Angewandte Chemie - International Edition, 2016, 55, 15990-16010.	7.2	24
120	Fundamentals of drug design from a biophysical viewpoint. Quarterly Reviews of Biophysics, 1994, 27, 435-481.	2.4	23
121	On the Influence of Charged Side Chains on the Foldingâ€“Unfolding Equilibrium of Î²-Peptides: A Molecular Dynamics Simulation Study. Chemistry - A European Journal, 2005, 11, 7276-7293.	1.7	23
122	Free enthalpies of replacing water molecules in protein binding pockets. Journal of Computer-Aided Molecular Design, 2012, 26, 1293-1309.	1.3	23
123	Biomolecular structure refinement based on adaptive restraints using local-elevation simulation. Journal of Biomolecular NMR, 2007, 39, 265-273.	1.6	22
124	On the calculation of 3 J Î±Î²-coupling constants for side chains in proteins. Journal of Biomolecular NMR, 2012, 53, 223-246.	1.6	22
125	A GPU solventâ€“solvent interaction calculation accelerator for biomolecular simulations using the GROMOS software. Journal of Computational Chemistry, 2010, 31, 1636-1643.	1.5	21
126	Assessment of enveloping distribution sampling to calculate relative free enthalpies of binding for eight netropsinâ€“DNA duplex complexes in aqueous solution. Journal of Computational Chemistry, 2012, 33, 640-651.	1.5	21

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127	Alpha- and beta-polypeptides show a different stability of helical secondary structure. Tetrahedron, 2004, 60, 7775-7780.	1.0	20
128	Numerical Simulation of the Effect of Solvent Viscosity on the Motions of a Î²-Peptide Heptamer. Chemistry - A European Journal, 2006, 12, 72-75.	1.7	20
129	Structure and dynamics of two Î²-peptides in solution from molecular dynamics simulations validated against experiment. European Biophysics Journal, 2008, 37, 903-912.	1.2	20
130	Thirty-five years of biomolecular simulation: development of methodology, force fields and software. Molecular Simulation, 2012, 38, 1271-1281.	0.9	20
131	Time-averaged order parameter restraints in molecular dynamics simulations. Journal of Biomolecular NMR, 2014, 60, 169-187.	1.6	20
132	Reversible peptide folding: Dependence on molecular force field used. Journal of Computational Chemistry, 2000, 21, 774-787.	1.5	19
133	Principles of carbopeptoid folding: a molecular dynamics simulation study. Journal of Peptide Science, 2005, 11, 74-84.	0.8	19
134	An improved simple polarisable water model for use in biomolecular simulation. Journal of Chemical Physics, 2014, 141, 22D515.	1.2	19
135	Conformational transitions of a dipeptide in water: Effects of imposed pathways using umbrella sampling techniques. Biopolymers, 1994, 34, 347-355.	1.2	18
136	Folding and Unfolding of Two Mixed Î±/Î² Peptides. ChemBioChem, 2009, 10, 2032-2041.	1.3	18
137	Calculation of binding free energies of inhibitors to plasmepsin II. Journal of Computational Chemistry, 2011, 32, 1801-1812.	1.5	18
138	The effect of using a polarizable solvent model upon the folding equilibrium of different Î²-peptides. Molecular Physics, 2011, 109, 493-506.	0.8	18
139	Molecular dynamics simulations of photoactive yellow protein (PYP) in three states of its photocycle: a comparison with X-ray and NMR data and analysis of the effects of Glu46 deprotonation and mutation. European Biophysics Journal, 2002, 31, 504-520.	1.2	17
140	Molecular dynamics simulations of peptides containing an unnatural amino acid: Dimerization, folding, and protein binding. Proteins: Structure, Function and Bioinformatics, 2003, 54, 116-127.	1.5	17
141	Terminal-group effects on the folding behavior of selected beta-peptides. Proteins: Structure, Function and Bioinformatics, 2006, 63, 136-143.	1.5	17
142	Simulating the Physiological Phase of Hydrated DPPC Bilayers: The Ester Moiety. Soft Materials, 2004, 2, 27-45.	0.8	16
143	Interpreting Experimental Data by Using Molecular Simulation Instead of Model Building. Chemistry - A European Journal, 2009, 15, 6389-6398.	1.7	16
144	Peptide Folding: When Simulation Meets Experiment. , 1999, 38, 236.		16

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145	MD simulation of subtilisin BPNâ€² in a crystal environment. Proteins: Structure, Function and Bioinformatics, 1992, 14, 451-464.	1.5	15
146	Crystallographic Refinement and Structure-Factor Time-Averaging by Molecular Dynamics in the Absence of a Physical Force Field. Molecular Simulation, 1993, 10, 377-395.	0.9	15
147	Comparison of Properties of Aib-Rich Peptides in Crystal and Solution: A Molecular Dynamics Study. ChemPhysChem, 2004, 5, 633-641.	1.0	15
148	On using oscillating time-dependent restraints in MD simulation. Journal of Biomolecular NMR, 2007, 37, 1-14.	1.6	15
149	A simple, efficient polarizable molecular model for liquid carbon tetrachloride. Molecular Physics, 2011, 109, 365-372.	0.8	15
150	Optimization methods for conformational sampling using a Boltzmann-weighted mean field approach. Biopolymers, 1998, 39, 103-114.	1.2	14
151	Membrane protein dynamics in different environments: simulation study of the outer membrane protein X in a lipid bilayer and in a micelle. European Biophysics Journal, 2011, 40, 39-58.	1.2	14
152	Helical Content of a Î²³â€Octapeptide in Methanol: Molecular Dynamics Simulations Explain a Seeming Discrepancy between Conclusions Derived from CD and NMR Data. Chemistry - A European Journal, 2012, 18, 586-593.	1.7	14
153	Reply. Angewandte Chemie - International Edition, 2001, 40, 4616-4618.	7.2	13
154	Are NMR-Derived Model Structures for Î²-Peptides Representative for the Ensemble of Structures Adopted in Solution?. Angewandte Chemie, 2004, 116, 6472-6476.	1.6	13
155	Simulation ofÎ²-depsipeptides: The effect of missing hydrogen-bond donors on their folding equilibria. Biopolymers, 2007, 85, 318-332.	1.2	13
156	Structure Determination of a Flexible Cyclic Peptide Based on NMR and MD Simulation 3Jâ€Coupling. ChemPhysChem, 2010, 11, 830-835.	1.0	13
157	A comparison of the different helices adopted by Î±â€•and Î²â€peptides suggests different reasons for their stability. Protein Science, 2010, 19, 2186-2195.	3.1	13
158	Interfacing the GROMOS (bio)molecular simulation software to quantumâ€chemical program packages. Journal of Computational Chemistry, 2012, 33, 2108-2117.	1.5	13
159	An improved GROMOS96 force field for aliphatic hydrocarbons in the condensed phase. Journal of Computational Chemistry, 2001, 22, 1205-1218.	1.5	13
160	A one-site polarizable model for liquid chloroform: COS/C. Molecular Physics, 2010, 108, 1749-1757.	0.8	12
161	On the Effect of the Various Assumptions and Approximations used in Molecular Simulations on the Properties of Bioâ€Molecular Systems: Overview and Perspective on Issues. ChemPhysChem, 2021, 22, 264-282.	1.0	12
162	Factor Xa: simulation studies with an eye to inhibitor design. Journal of Computer-Aided Molecular Design, 2000, 14, 507-529.	1.3	11

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163	Exploring the trigger sequence of the GCN4 coiledâ€coil: Biased molecular dynamics resolves apparent inconsistencies in NMR measurements. Protein Science, 2010, 19, 2462-2474.	3.1	11
164	Validation of the GROMOS 54A7 Force Field Regarding Mixed Î±/Î²â€Peptide Molecules. Helvetica Chimica Acta, 2012, 95, 2562-2577.	1.0	11
165	Structure of hen egg-white lysozyme solvated in TFE/water: a molecular dynamics simulation study based on NMR data. Journal of Biomolecular NMR, 2013, 55, 339-353.	1.6	11
166	On the compatibility of polarisable and non-polarisable models for liquid water. Molecular Physics, 2014, 112, 2761-2780.	0.8	11
167	Free energy barrier estimation of unfolding the ?-helical surfactant-associated polypeptide C. Proteins: Structure, Function and Bioinformatics, 2001, 43, 395-402.	1.5	10
168	Molecular Modeling Using Nuclear Magnetic Resonance Data. Reviews in Computational Chemistry, 2007, , 143-172.	1.5	10
169	Reply to the â€˜Comment on â€œOn using a too large integration time step in molecular dynamics simulations of coarse-grained molecular modelsâ€â€™ by S. J. Marrink, X. Periole, D. Peter Tieleman and Alex H. de Vries, Phys. Chem. Chem. Phys., 2010, 12, DOI: 10.1039/b915293h. Physical Chemistry Chemical Physics, 2010, 12, 2257.	1.3	10
170	Free energy calculations offer insights into the influence of receptor flexibility on ligandâ€“receptor binding affinities. Journal of Computer-Aided Molecular Design, 2011, 25, 709-716.	1.3	10
171	On the use of a weak-coupling thermostat in replica-exchange molecular dynamics simulations. Journal of Chemical Physics, 2015, 143, 034110.	1.2	10
172	The key to predicting the stability of protein mutants lies in an accurate description and proper configurational sampling of the folded and denatured states. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 983-995.	1.1	10
173	Investigations of peptide hydration using NMR and molecular dynamics simulations: A study of effects of water on the conformation and dynamics of antamanide. Journal of Biomolecular NMR, 1996, 8, 453-476.	1.6	9
174	Using oneâ€step perturbation to predict the effect of changing forceâ€field parameters on the simulated folding equilibrium of a Î²â€peptide in solution. Journal of Computational Chemistry, 2010, 31, 2419-2427.	1.5	9
175	The thermal isomerization of the GFP chromophore: A computational study. Physical Chemistry Chemical Physics, 2010, 12, 11051.	1.3	9
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