Wilfred F Van Gunsteren

List of Publications by Citations

242 papers	22,938 citations	63 h-index	149 g-index
247 ext. papers	24,791 ext. citations	4.2 avg, IF	6.8 L-index

#	Paper	IF	Citations
242	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, 1656-76	3.5	2844
241	Definition and testing of the GROMOS force-field versions 54A7 and 54B7. *European Biophysics Journal*, **2011**, 40, 843-56	1.9	1326
240	Peptide Folding: When Simulation Meets Experiment. *Angewandte Chemie - International Edition*, **1999**, 38, 236-240	16.4	1258
239	The GROMOS Biomolecular Simulation Program Package. *Journal of Physical Chemistry A*, **1999**, 103, 3596-3607	2.8	1220
238	Computer Simulation of Molecular Dynamics: Methodology, Applications, and Perspectives in Chemistry. *Angewandte Chemie International Edition in English*, **1990**, 29, 992-1023		1180
237	A generalized reaction field method for molecular dynamics simulations. *Journal of Chemical Physics*, **1995**, 102, 5451-5459	3.9	1146
236	An improved GROMOS96 force field for aliphatic hydrocarbons in the condensed phase. *Journal of Computational Chemistry*, **2001**, 22, 1205-1218	3.5	741
235	A consistent empirical potential for water–protein interactions. *Biopolymers*, **1984**, 23, 1513-1518	2.2	693
234	A fast SHAKE algorithm to solve distance constraint equations for small molecules in molecular dynamics simulations. *Journal of Computational Chemistry*, **2001**, 22, 501-508	3.5	647
233	The GROMOS software for biomolecular simulation: GROMOS05. *Journal of Computational Chemistry*, **2005**, 26, 1719-51	3.5	514
232	Local elevation: a method for improving the searching properties of molecular dynamics simulation. *Journal of Computer-Aided Molecular Design*, **1994**, 8, 695-708	4.2	451
231	Biomolecular modeling: Goals, problems, perspectives. *Angewandte Chemie - International Edition*, **2006**, 45, 4064-92	16.4	441
230	Validation of the 53A6 GROMOS force field. *European Biophysics Journal*, **2005**, 34, 273-84	1.9	392
229	Parametrization of aliphatic CHn united atoms of GROMOS96 force field **1998**, 19, 535-547		335
228	Folding-unfolding thermodynamics of a beta-heptapeptide from equilibrium simulations. *Proteins: Structure, Function and Bioinformatics*, **1999**, 34, 269-80	4.2	330
227	Comparison of four methods to compute the dielectric permittivity of liquids from molecular dynamics simulations. *Journal of Chemical Physics*, **2001**, 115, 1125-1136	3.9	303
226	Decomposition of the free energy of a system in terms of specific interactions. Implications for theoretical and experimental studies. *Journal of Molecular Biology*, **1994**, 240, 167-76	6.5	289

225	Time-averaged nuclear Overhauser effect distance restraints applied to tendamistat. *Journal of Molecular Biology*, **1990**, 214, 223-35	6.5	265
224	Architecture, implementation and parallelisation of the GROMOS software for biomolecular simulation. *Computer Physics Communications*, **2012**, 183, 890-903	4.2	246
223	Time-dependent distance restraints in molecular dynamics simulations. *Chemical Physics Letters*, **1989**, 157, 289-294	2.5	245
222	Basic ingredients of free energy calculations: a review. *Journal of Computational Chemistry*, **2010**, 31, 1569-82	3.5	225
221	A comparison of methods to compute the potential of mean force. *ChemPhysChem*, **2007**, 8, 162-9	3.2	203
220	Development of a simple, self-consistent polarizable model for liquid water. *Journal of Chemical Physics*, **2003**, 118, 221-234	3.9	195
219	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	3.9	186
218	Derivation of an improved simple point charge model for liquid water: SPC/A and SPC/L. *Journal of Chemical Physics*, **2002**, 116, 9811-9828	3.9	173
217	GROMOS++ Software for the Analysis of Biomolecular Simulation Trajectories. *Journal of Chemical Theory and Computation*, **2011**, 7, 3379-90	6.4	160
216	Absolute entropies from molecular dynamics simulation trajectories. *Journal of Chemical Physics*, **2000**, 113, 7809-7817	3.9	158
215	Molecular simulation as an aid to experimentalists. *Current Opinion in Structural Biology*, **2008**, 18, 149-53	8.1	150
214	An improved nucleic acid parameter set for the GROMOS force field. *Journal of Computational Chemistry*, **2005**, 26, 725-37	3.5	147
213	Can one derive the conformational preference of a beta-peptide from its CD spectrum?. *Journal of the American Chemical Society*, **2002**, 124, 12972-8	16.4	147
212	Validation of molecular dynamics simulation. *Journal of Chemical Physics*, **1998**, 108, 6109-6116	3.9	139
211	Simulating proteins at constant pH: An approach combining molecular dynamics and Monte Carlo simulation. *Proteins: Structure, Function and Bioinformatics*, **2002**, 47, 469-80	4.2	137
210	Calculating Electrostatic Interactions Using the Particle−Particle Particle−Mesh Method with Nonperiodic Long-Range Interactions. *The Journal of Physical Chemistry*, **1996**, 100, 2581-2587		133
209	On searching in, sampling of, and dynamically moving through conformational space of biomolecular systems: A review. *Journal of Computational Chemistry*, **2008**, 29, 157-66	3.5	125
208	Estimating entropies from molecular dynamics simulations. *Journal of Chemical Physics*, **2004**, 120, 2652-61	3.9	122

207	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	3.9	120
206	Structure refinement using time-averaged J-coupling constant restraints. *Journal of Biomolecular NMR*, **1993**, 3, 55-66	3	114
205	Studying the Stability of a Helical -Heptapeptide by Molecular Dynamics Simulations. *Chemistry - A European Journal*, **1997**, 3, 1410-1417	4.8	109
204	Computer Simulation of Urea Water Mixtures: A Test of Force Field Parameters for Use in Biomolecular Simulation. *Journal of Physical Chemistry B*, **2004**, 108, 1065-1071	3.4	109
203	A simple, efficient polarizable coarse-grained water model for molecular dynamics simulations. *Journal of Chemical Physics*, **2011**, 134, 084110	3.9	107
202	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	16.4	106
201	On the interpretation of biochemical data by molecular dynamics computer simulation. *FEBS Journal*, **1992**, 204, 947-61		105
200	On the Choice of Dihedral Angle Potential Energy Functions for n-Alkanes. *Molecular Simulation*, **2000**, 25, 301-319	2	101
199	A Comparison of Non-Bonded Scaling Approaches for Free Energy Calculations. *Molecular Simulation*, **2002**, 28, 45-65	2	99
198	Molecular dynamics simulations of liquid methanol and methanol-water mixtures with polarizable models. *Journal of Computational Chemistry*, **2006**, 27, 1494-504	3.5	98
197	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, 1016-31	6.4	93
196	Comparison of thermodynamic properties of coarse-grained and atomic-level simulation models. *ChemPhysChem*, **2007**, 8, 452-61	3.2	92
195	New functionalities in the GROMOS biomolecular simulation software. *Journal of Computational Chemistry*, **2012**, 33, 340-53	3.5	91
194	An Effective Force Field for Molecular Dynamics Simulations of Dimethyl Sulfoxide and Dimethyl Sulfoxide Water Mixtures. *Journal of Physical Chemistry B*, **2004**, 108, 1436-1445	3.4	90
193	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	4.2	85
192	When Are Free Energy Components Meaningful?. *The Journal of Physical Chemistry*, **1994**, 98, 13735-13740		85
191	Calculation of NMR-relaxation parameters for flexible molecules from molecular dynamics simulations. *Journal of Biomolecular NMR*, **2001**, 20, 297-310	3	83
190	The effect of motional averaging on the calculation of NMR-derived structural properties **1999**, 36, 542-555		83

189	Molekldynamik-Computersimulationen; Methodik, Anwendungen und Perspektiven in der Chemie. *Angewandte Chemie*, **1990**, 102, 1020-1055	3.6	83
188	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	4.2	80
187	Algorithms for clustering molecular dynamics configurations. *Journal of Computational Chemistry*, **1994**, 15, 1331-1340	3.5	78
186	Comparing atomistic simulation data with the NMR experiment: how much can NOEs actually tell us?. *Proteins: Structure, Function and Bioinformatics*, **2006**, 63, 210-8	4.2	77
185	On the relative merits of flexible versus rigid models for use in computer simulations of molecular liquids. *Chemical Physics Letters*, **1996**, 250, 19-24	2.5	76
184	A structure refinement method based on molecular dynamics in four spatial dimensions. *Journal of Molecular Biology*, **1993**, 234, 751-62	6.5	75
183	Validation of Molecular Simulation: An Overview of Issues. *Angewandte Chemie - International Edition*, **2018**, 57, 884-902	16.4	74
182	Free energies of binding of polychlorinated biphenyls to the estrogen receptor from a single simulation. *Proteins: Structure, Function and Bioinformatics*, **2004**, 54, 237-46	4.2	74
181	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	3.6	70
180	Calculation of relative free energy via indirect pathways. *Journal of Chemical Physics*, **1991**, 94, 3808-3816	3.9	70
179	Multi-resolution simulation of biomolecular systems: a review of methodological issues. *Angewandte Chemie - International Edition*, **2013**, 52, 2820-34	16.4	63
178	Predictions of free energy differences from a single simulation of the initial state. *Journal of Chemical Physics*, **1994**, 100, 577-585	3.9	63
177	Single-step perturbations to calculate free energy differences from unphysical reference states: limits on size, flexibility, and character. *Journal of Computational Chemistry*, **2003**, 24, 1730-9	3.5	60
176	SWARM-MD: Searching Conformational Space by Cooperative Molecular Dynamics. *Journal of Physical Chemistry A*, **1998**, 102, 5937-5943	2.8	58
175	Structure refinement with molecular dynamics and a Boltzmann-weighted ensemble. *Journal of Biomolecular NMR*, **1995**, 6, 163-70	3	58
174	Entropy calculations on the molten globule state of a protein: side-chain entropies of alpha-lactalbumin. *Proteins: Structure, Function and Bioinformatics*, **2002**, 46, 215-24	4.2	55
173	One-Step Perturbation Methods for Solvation Free Energies of Polar Solutes. *Journal of Physical Chemistry B*, **2001**, 105, 11264-11274	3.4	55
172	Estimating relative free energies from a single ensemble: Hydration free energies. *Journal of Computational Chemistry*, **1999**, 20, 1604-1617	3.5	55

171	Peptide Folding: When Simulation Meets Experiment **1999**, 38, 236		54
170	Peptidfaltung: Wenn die Simulation das Experiment erreicht. *Angewandte Chemie*, **1999**, 111, 249-253	3.6	51
169	Combined QM/MM Molecular Dynamics Study on a Condensed-Phase SN2 Reaction at Nitrogen: The Effect of Explicitly Including Solvent Polarization. *Journal of Chemical Theory and Computation*, **2007**, 3, 1499-509	6.4	50
168	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, 509-19	4.2	48
167	Energy-entropy compensation in the transfer of nonpolar solutes from water to cosolvent/water mixtures. *ChemPhysChem*, **2004**, 5, 144-7	3.2	47
166	Parametrisation of time-averaged distance restraints in MD simulations. *Journal of Biomolecular NMR*, **1995**, 6, 313-20	3	45
165	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, 1101-18	6.3	43
164	Solvent structure at a hydrophobic protein surface. *Proteins: Structure, Function and Bioinformatics*, **1997**, 27, 395-404	4.2	42
163	Viscosity dependence of protein dynamics. *Proteins: Structure, Function and Bioinformatics*, **2001**, 42, 414-421	4.2	42
162	A combined solid-state NMR and MD characterization of the stability and dynamics of the HET-s(218-289) prion in its amyloid conformation. *ChemBioChem*, **2009**, 10, 1657-65	3.8	41
161	Solvating atomic level fine-grained proteins in supra-molecular level coarse-grained water for molecular dynamics simulations. *European Biophysics Journal*, **2012**, 41, 647-61	1.9	40
160	Molecular dynamics simulations of small peptides: can one derive conformational preferences from ROESY spectra?. *Chemistry - A European Journal*, **2003**, 9, 5838-49	4.8	40
159	Refinement of the application of the GROMOS 54A7 force field to ǂpeptides. *Journal of Computational Chemistry*, **2013**, 34, 2796-805	3.5	39
158	Biomolecular structure refinement using the GROMOS simulation software. *Journal of Biomolecular NMR*, **2011**, 51, 265-81	3	39
157	Molecular-dynamics simulation of the beta domain of metallothionein with a semi-empirical treatment of the metal core. *Proteins: Structure, Function and Bioinformatics*, **2000**, 41, 299-315	4.2	39
156	Biomolecular simulation: historical picture and future perspectives. *Biochemical Society Transactions*, **2008**, 36, 11-5	5.1	38
155	Interpreting NMR data for beta-peptides using molecular dynamics simulations. *Journal of the American Chemical Society*, **2005**, 127, 14320-9	16.4	38
154	Are NMR-derived model structures for beta-peptides representative for the ensemble of structures adopted in solution?. *Angewandte Chemie - International Edition*, **2004**, 43, 6312-6	16.4	36

153	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, 1664-79	3.5	34
152	Dynamical studies of peptide motifs in the Plasmodium falciparum circumsporozoite surface protein by restrained and unrestrained MD simulations. *Journal of Molecular Biology*, **1997**, 267, 1012-25	6.5	34
151	Calculating zeros: Non-equilibrium free energy calculations. *Chemical Physics*, **2006**, 323, 102-108	2.3	34
150	Backbone folding of the polypeptide cardiac stimulant anthopleurin-A determined by nuclear magnetic resonance, distance geometry and molecular dynamics. *FEBS Letters*, **1988**, 239, 266-70	3.8	34
149	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, 363-78	3.5	33
148	Efficient calculation of many stacking and pairing free energies in DNA from a few molecular dynamics simulations. *Chemistry - A European Journal*, **2005**, 11, 4340-8	4.8	33
147	Peptide folding simulations: no solvent required?. *Computer Physics Communications*, **1999**, 123, 97-102	4.2	32
146	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, 588-99	6.5	32
145	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, 255-67	1.9	31
144	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, 221-35	3	30
143	Biomolekulare Modellierung: Ziele, Probleme, Perspektiven. *Angewandte Chemie*, **2006**, 118, 4168-4198	3.6	29
142	Force field evaluation for biomolecular simulation: free enthalpies of solvation of polar and apolar compounds in various solvents. *ChemPhysChem*, **2006**, 7, 671-8	3.2	28
141	Sampling of rare events using hidden restraints. *Journal of Physical Chemistry B*, **2006**, 110, 8488-98	3.4	27
140	Protein under pressure: molecular dynamics simulation of the arc repressor. *Proteins: Structure, Function and Bioinformatics*, **2006**, 65, 136-44	4.2	27
139	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	2	27
138	Molecular dynamics simulations of human alpha-lactalbumin: changes to the structural and dynamical properties of the protein at low pH. *Proteins: Structure, Function and Bioinformatics*, **1999** , 36, 77-86	4.2	27
137	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, 2544-51	6.3	26
136	A strategy for analysis of (molecular) equilibrium simulations: Configuration space density estimation, clustering, and visualization. *Journal of Chemical Physics*, **2001**, 114, 2079-2089	3.9	26

135	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, 1032-44	6.4	25
134	On using time-averaging restraints in molecular dynamics simulation. *Journal of Biomolecular NMR*, **1998**, 12, 501-8	3	25
133	The Photoisomerization of cis-Stilbene Does Not Follow the Minimum Energy Path. *Angewandte Chemie - International Edition*, **1999**, 38, 2609-2611	16.4	25
132	A polarizable empirical force field for molecular dynamics simulation of liquid hydrocarbons. *Journal of Computational Chemistry*, **2014**, 35, 789-801	3.5	24
131	Accessibility and order of water sites in and around proteins: A crystallographic time-averaging study **1999**, 36, 501-511		24
130	On the Conformational Properties of Amylose and Cellulose Oligomers in Solution. *International Journal of Carbohydrate Chemistry*, **2009**, 2009, 1-8		23
129	A method to explore protein side chain conformational variability using experimental data. *ChemPhysChem*, **2009**, 10, 3213-28	3.2	23
128	Amine hydration: a united-atom force-field solution. *ChemPhysChem*, **2005**, 6, 1800-4	3.2	23
127	On the influence of charged side chains on the folding-unfolding equilibrium of beta-peptides: a molecular dynamics simulation study. *Chemistry - A European Journal*, **2005**, 11, 7276-93	4.8	23
126	Free enthalpies of replacing water molecules in protein binding pockets. *Journal of Computer-Aided Molecular Design*, **2012**, 26, 1293-309	4.2	22
125	A novel approach for designing simple point charge models for liquid water with three interaction sites. *Journal of Computational Chemistry*, **2003**, 24, 1087-96	3.5	22
124	Molecular dynamics simulation of n-dodecyl phosphate aggregate structures. *European Biophysics Journal*, **2001**, 30, 330-43	1.9	22
123	Further investigation on the validity of StokesEinstein behaviour at the molecular level. *Chemical Physics Letters*, **2001**, 334, 337-342	2.5	22
122	Deriving Structural Information from Experimentally Measured Data on Biomolecules. *Angewandte Chemie - International Edition*, **2016**, 55, 15990-16010	16.4	21
121	Assessment of enveloping distribution sampling to calculate relative free enthalpies of binding for eight netropsin-DNA duplex complexes in aqueous solution. *Journal of Computational Chemistry*, **2012**, 33, 640-51	3.5	21
120	The seven sins in academic behavior in the natural sciences. *Angewandte Chemie - International Edition*, **2013**, 52, 118-22	16.4	21
119	On the calculation of □J□coupling constants for side chains in proteins. *Journal of Biomolecular NMR*, **2012**, 53, 223-46	3	21
118	Biomolecular structure refinement based on adaptive restraints using local-elevation simulation. *Journal of Biomolecular NMR*, **2007**, 39, 265-73	3	20

117	Carbopeptoid folding: effects of stereochemistry, chain length, and solvent. *Angewandte Chemie - International Edition*, **2004**, 43, 4055-9	16.4	20
116	Fundamentals of drug design from a biophysical viewpoint. *Quarterly Reviews of Biophysics*, **1994**, 27, 435-81	7	20
115	Time-averaged order parameter restraints in molecular dynamics simulations. *Journal of Biomolecular NMR*, **2014**, 60, 169-87	3	19
114	Numerical simulation of the effect of solvent viscosity on the motions of a beta-peptide heptamer. *Chemistry - A European Journal*, **2005**, 12, 72-5	4.8	19
113	Alpha- and beta-polypeptides show a different stability of helical secondary structure. *Tetrahedron*, **2004**, 60, 7775-7780	2.4	19
112	Thirty-five years of biomolecular simulation: development of methodology, force fields and software. *Molecular Simulation*, **2012**, 38, 1271-1281	2	18
111	Calculation of binding free energies of inhibitors to plasmepsin II. *Journal of Computational Chemistry*, **2011**, 32, 1801-12	3.5	18
110	Folding and unfolding of two mixed alpha/beta peptides. *ChemBioChem*, **2009**, 10, 2032-41	3.8	18
109	The effect of using a polarizable solvent model upon the folding equilibrium of different peptides. *Molecular Physics*, **2011**, 109, 493-506	1.7	18
108	A GPU solvent-solvent interaction calculation accelerator for biomolecular simulations using the GROMOS software. *Journal of Computational Chemistry*, **2010**, 31, 1636-43	3.5	18
107	Structure and dynamics of two beta-peptides in solution from molecular dynamics simulations validated against experiment. *European Biophysics Journal*, **2008**, 37, 903-12	1.9	18
106	Principles of carbopeptoid folding: a molecular dynamics simulation study. *Journal of Peptide Science*, **2005**, 11, 74-84	2.1	18
105	Reversible peptide folding: Dependence on molecular force field used. *Journal of Computational Chemistry*, **2000**, 21, 774-787	3.5	18
104	Conformational transitions of a dipeptide in water: Effects of imposed pathways using umbrella sampling techniques. *Biopolymers*, **1994**, 34, 347-355	2.2	18
103	An improved simple polarisable water model for use in biomolecular simulation. *Journal of Chemical Physics*, **2014**, 141, 22D515	3.9	16
102	Simulating the Physiological Phase of Hydrated DPPC Bilayers: The Ester Moiety. *Soft Materials*, **2004**, 2, 27-45	1.7	16
101	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, 504-20	1.9	16
100	Molecular dynamics simulations of peptides containing an unnatural amino acid: dimerization, folding, and protein binding. *Proteins: Structure, Function and Bioinformatics*, **2004**, 54, 116-27	4.2	16

99	Der Schlüssel zum Verständnis des Proteinfaltungsproblems liegt in der richtigen Beschreibung des denaturierten Zustandes. *Angewandte Chemie*, **2001**, 113, 363-367	3.6	16
98	Interpreting experimental data by using molecular simulation instead of model building. *Chemistry - A European Journal*, **2009**, 15, 6389-98	4.8	15
97	Terminal-group effects on the folding behavior of selected beta-peptides. *Proteins: Structure, Function and Bioinformatics*, **2006**, 63, 136-43	4.2	15
96	Comparison of properties of Aib-rich peptides in crystal and solution: a molecular dynamics study. *ChemPhysChem*, **2004**, 5, 633-41	3.2	15
95	MD simulation of subtilisin BPN' in a crystal environment. *Proteins: Structure, Function and Bioinformatics*, **1992**, 14, 451-64	4.2	15
94	Peptide Folding: When Simulation Meets Experiment **1999**, 38, 236		15
93	Helical content of a (β)-octapeptide in methanol: molecular dynamics simulations explain a seeming discrepancy between conclusions derived from CD and NMR data. *Chemistry - A European Journal*, **2012**, 18, 586-93	4.8	14
92	On using oscillating time-dependent restraints in MD simulation. *Journal of Biomolecular NMR*, **2007**, 37, 1-14	3	14
91	Optimization methods for conformational sampling using a Boltzmann-weighted mean field approach. *Biopolymers*, **1998**, 39, 103-114	2.2	14
90	Crystallographic Refinement and Structure-Factor Time-Averaging by Molecular Dynamics in the Absence of a Physical Force Field. *Molecular Simulation*, **1993**, 10, 377-395	2	14
89	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	1.9	13
88	A simple, efficient polarizable molecular model for liquid carbon tetrachloride. *Molecular Physics*, **2011**, 109, 365-372	1.7	13
87	Simulation of beta-depsipeptides: the effect of missing hydrogen-bond donors on their folding equilibria. *Biopolymers*, **2007**, 85, 318-32	2.2	13
86	Interfacing the GROMOS (bio)molecular simulation software to quantum-chemical program packages. *Journal of Computational Chemistry*, **2012**, 33, 2108-17	3.5	12
85	A one-site polarizable model for liquid chloroform: COS/C. *Molecular Physics*, **2010**, 108, 1749-1757	1.7	12
84	A comparison of the different helices adopted by α and β peptides suggests different reasons for their stability. *Protein Science*, **2010**, 19, 2186-95	6.3	12
83	Are NMR-Derived Model Structures for β-Peptides Representative for the Ensemble of Structures Adopted in Solution?. *Angewandte Chemie*, **2004**, 116, 6472-6476	3.6	12
82	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, 339-53	3	11

81	On the compatibility of polarisable and non-polarisable models for liquid water. *Molecular Physics*, **2014**, 112, 2761-2780	1.7	11
80	Validation of the GROMOS 54A7 Force Field Regarding Mixed Peptide Molecules. *Helvetica Chimica Acta*, **2012**, 95, 2562-2577	2	11
79	Exploring the trigger sequence of the GCN4 coiled-coil: biased molecular dynamics resolves apparent inconsistencies in NMR measurements. *Protein Science*, **2010**, 19, 2462-74	6.3	11
78	On the use of a weak-coupling thermostat in replica-exchange molecular dynamics simulations. *Journal of Chemical Physics*, **2015**, 143, 034110	3.9	10
77	Free energy calculations offer insights into the influence of receptor flexibility on ligand-receptor binding affinities. *Journal of Computer-Aided Molecular Design*, **2011**, 25, 709-16	4.2	10
76	Reply to the Comment on On using a too large integration time step in molecular dynamics simulations of coarse-grained molecular models 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	3.6	10
75	Structure determination of a flexible cyclic peptide based on NMR and MD simulation 3J-coupling. *ChemPhysChem*, **2010**, 11, 830-5	3.2	10
74	Factor Xa: simulation studies with an eye to inhibitor design. *Journal of Computer-Aided Molecular Design*, **2000**, 14, 507-29	4.2	10
73	An improved GROMOS96 force field for aliphatic hydrocarbons in the condensed phase **2001**, 22, 1205		10
72	Die sieben Todsünden akademischen Handelns in der naturwissenschaftlichen Forschung. *Angewandte Chemie*, **2013**, 125, 128-132	3.6	9
71	The thermal isomerization of the GFP chromophore: A computational study. *Physical Chemistry Chemical Physics*, **2010**, 12, 11051-61	3.6	9
70	Using one-step perturbation to predict the effect of changing force-field parameters on the simulated folding equilibrium of a beta-peptide in solution. *Journal of Computational Chemistry*, **2010**, 31, 2419-27	3.5	9
69	Free energy barrier estimation of unfolding the alpha-helical surfactant-associated polypeptide C. *Proteins: Structure, Function and Bioinformatics*, **2001**, 43, 395-402	4.2	9
68	Reply. *Angewandte Chemie - International Edition*, **2001**, 40, 4616-4618	16.4	9
67	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, 453-76	3	9
66	Multiple binding modes for palmitate to barley lipid transfer protein facilitated by the presence of proline 12. *Protein Science*, **2013**, 22, 56-64	6.3	8
65	Molecular Dynamics Simulation of Ester-Linked Hen Egg White Lysozyme Reveals the Effect of Missing Backbone Hydrogen Bond Donors on the Protein Structure. *Helvetica Chimica Acta*, **2010**, 93, 1857-1869	2	8
64	Polarizable coarse-grained models for molecular dynamics simulation of liquid cyclohexane. *Journal of Computational Chemistry*, **2015**, 36, 1311-21	3.5	7

63	Bestimmung von Strukturinformation aus experimentellen Messdaten f Biomolek e. *Angewandte Chemie*, **2016**, 128, 16222-16244	3.6	7
62	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	4	7
61	Molecular dynamics computer simulation as a tool for the analysis of solvation: A study of dilute aqueous solutions of 1,4-dioxane and 1,3-dioxane. *Recueil Des Travaux Chimiques Des Pays-Bas*, **2010**, 104, 79-89		7
60	Free energy calculations using flexible-constrained, hard-constrained and non-constrained molecular dynamics simulations. *ChemPhysChem*, **2007**, 8, 1557-64	3.2	7
59	The Application of Chemical Shift Calculation to Protein Structure Determination by NMR **1993**, 615-622		7
58	Challenge of representing entropy at different levels of resolution in molecular simulation. *Journal of Physical Chemistry B*, **2015**, 119, 753-63	3.4	6
57	On the use of one-step perturbation to investigate the dependence of NOE-derived atom-atom distance bound violations of peptides upon a variation of force-field parameters. *European Biophysics Journal*, **2014**, 43, 113-9	1.9	6
56	Biomolekulare Simulationen mit mehreren Aufl sungsniveaus: ein berblick ber methodische Aspekte. *Angewandte Chemie*, **2013**, 125, 2888-2904	3.6	6
55	Molecular dynamics simulations of the interaction between polyhydroxylated compounds and Lennard-Jones walls: preferential affinity/exclusion effects and their relevance for bioprotection. *Molecular Simulation*, **2010**, 36, 708-728	2	6
54	On the direct calculation of the free energy of quantization for molecular systems in the condensed phase. *Journal of Computational Chemistry*, **2009**, 30, 514-23	3.5	6
53	A molecular dynamics study of the ASC and NALP1 pyrin domains at neutral and low pH. *ChemBioChem*, **2008**, 9, 923-33	3.8	6
52	Exploring the conserved water site and hydration of a coiled-coil trimerisation motif: a MD simulation study. *ChemBioChem*, **2008**, 9, 1749-56	3.8	6
51	Optimization methods for conformational sampling using a Boltzmann-weighted mean field approach **1996**, 39, 103		6
50	GROMOS polarisable model for acetone. *Molecular Physics*, **2016**, 114, 845-854	1.7	5
49	On the choice of a reference state for one-step perturbation calculations between polar and nonpolar molecules in a polar environment. *Journal of Computational Chemistry*, **2013**, 34, 387-93	3.5	5
48	Conformational Preferences of a Octapeptide as Function of Solvent and Force-Field Parameters. *Helvetica Chimica Acta*, **2013**, 96, 189-200	2	5
47	Influence of Variation of a Side Chain on the Folding Equilibrium of a Peptide. *Helvetica Chimica Acta*, **2011**, 94, 597-610	2	5
46	Simulation of an all-beta 3-icosapeptide containing the 20 proteinogenic side chains: effect of temperature, pH, counterions, solvent, and force field on helix stability. *Biopolymers*, **2006**, 83, 636-45	2.2	5

45	Molecular Modeling Using Nuclear Magnetic Resonance Data. *Reviews in Computational Chemistry*, **2007**, 143-172		5
44	A Comparison of Seven Fast but Approximate Methods to Compute the Free Energy of Deprotonation for Amino Acids in Aqueous Solution. *Molecular Simulation*, **2001**, 27, 215-236	2	5
43	Investigation of the structural preference and flexibility of the loop residues in amyloid fibrils of the HET-s prion. *Physical Chemistry Chemical Physics*, **2016**, 18, 5860-6	3.6	4
42	On the use of advanced modelling techniques to investigate the conformational discrepancy between two X-ray structures of the AppA BLUF domain. *Molecular Simulation*, **2013**, 39, 472-486	2	4
41	On the Use of a Supramolecular Coarse-Grained Model for the Solvent in Simulations of the Folding Equilibrium of an Octa-peptide in MeOH and H2O. *Helvetica Chimica Acta*, **2014**, 97, 1591-1605	2	4
40	Molecular dynamics simulation of thionated hen egg white lysozyme. *Protein Science*, **2012**, 21, 1153-61	6.3	4
39	Generation of pseudonative protein structures for threading. *Proteins: Structure, Function and Bioinformatics*, **1997**, 28, 522-529	4.2	4
38	Pathway dependence of the efficiency of calculating free energy and entropy of solute solute association in water. *Chemical Physics*, **2006**, 330, 410-416	2.3	4
37	A molecular dynamics computer simulation study of the hydration of bis(methylsulphonyl)methane in water. *Molecular Physics*, **1985**, 56, 1393-1409	1.7	4
36	On the Use of Side-Chain NMR Relaxation Data to Derive Structural and Dynamical Information on Proteins: A Case Study Using Hen Lysozyme. *ChemBioChem*, **2021**, 22, 1049-1064	3.8	4
35	Molecular dynamics simulation of hen egg white lysozyme: A test of the GROMOS96 force field against nuclear magnetic resonance data **2000**, 40, 145		4
34	Algorithms to apply dihedral-angle constraints in molecular or stochastic dynamics simulations. *Journal of Chemical Physics*, **2020**, 152, 024109	3.9	3
33	Validierung von molekularen Simulationen: eine bersicht verschiedener Aspekte. *Angewandte Chemie*, **2018**, 130, 894-915	3.6	3
32	Using enveloping distribution sampling to compute the folding free enthalpy of a peptide with a very unstable folded conformation in solution: The advantage of focused sampling using EDS. *Chemical Physics*, **2014**, 428, 156-163	2.3	3
31	An effective force field for molecular dynamics simulations of dimethyl sulfone. *Molecular Physics*, **2011**, 109, 2593-2605	1.7	3
30	A method for conformational sampling of loops in proteins based on adiabatic decoupling and temperature or force scaling. *ChemPhysChem*, **2011**, 12, 2609-14	3.2	3
29	Carbopeptoid Folding: Effects of Stereochemistry, Chain Length, and Solvent. *Angewandte Chemie*, **2004**, 116, 4147-4151	3.6	3
28	Interpretation of Seemingly Contradictory Data: Low NMR S Order Parameters Observed in Helices and High NMR S Order Parameters in Disordered Loops of the Protein hGH at Low pH. *Chemistry - A European Journal*, **2017**, 23, 9585-9591	4.8	2

27	Using Complementary NMR Data Sets To Detect Inconsistencies and Model Flaws in the Structure Determination of Human Interleukin-4. *Journal of Physical Chemistry B*, **2017**, 121, 7055-7063	3.4	2
26	Conformational Properties of the Chemotherapeutic Drug Analogue Epothilone A: How to Model a Flexible Protein Ligand Using Scarcely Available Experimental Data. *Journal of Chemical Information and Modeling*, **2019**, 59, 2218-2230	6.1	2
25	A molecular dynamics simulation investigation of the relative stability of the cyclic peptide octreotide and its deprotonated and its (CF)-Trp substituted analogs in different solvents. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 4936-4948	3.4	2
24	On the Sensitivity of Peptide Nucleic Acid Duplex Formation and Crystal Dissolution to a Variation of Force-Field Parameters. *Journal of Chemical Theory and Computation*, **2014**, 10, 391-400	6.4	2
23	On the use of one-step perturbation to investigate the dependence of different properties of liquid water on a variation of model parameters from a single simulation *Molecular Physics*, **2013**, 111, 2334-2344	1.7	2
22	Structural and energetic effects of the use of polarisable water to solvate proteins. *Molecular Physics*, **2015**, 113, 2815-2828	1.7	2
21	On the pitfalls of peer review. *F1000Research*, **2015**, 4, 1244	3.6	2
20	Molecular dynamics simulation of the last step of a catalytic cycle: product release from the active site of the enzyme chorismate mutase from Mycobacterium tuberculosis. *Protein Science*, **2012**, 21, 1672-81	6.3	2
19	Test of a method for sampling the internal degrees of freedom of a flexible solute molecule based on adiabatic decoupling and temperature or force scaling. *Molecular Physics*, **2012**, 110, 407-417	1.7	2
18	Cyclodextrin Host Guest Binding: A Computational Study of the Different Driving Forces. *Helvetica Chimica Acta*, **2010**, 93, 2318-2325	2	2
17	Die Photoisomerisierung von cis-Stilben folgt nicht dem Weg minimaler Energie. *Angewandte Chemie*, **1999**, 111, 2771-2773	3.6	2
16	A method to apply bond-angle constraints in molecular dynamics simulations. *Journal of Computational Chemistry*, **2021**, 42, 418-434	3.5	2
15	On the use of J-coupling NMR data to derive structural information on proteins. *Journal of Biomolecular NMR*, **2021**, 75, 39-70	3	2
14	Parametrization of aliphatic CHn united atoms of GROMOS96 force field **1998**, 19, 535		2
13	Viscosity dependence of protein dynamics **2001**, 42, 414		2
12	On the Effect of the Various Assumptions and Approximations used in Molecular Simulations on the Properties of Bio-Molecular Systems: Overview and Perspective on Issues. *ChemPhysChem*, **2021**, 22, 264-282	3.2	2
11	On the use of time-averaging restraints when deriving biomolecular structure from -coupling values obtained from NMR experiments. *Journal of Biomolecular NMR*, **2016**, 66, 69-83	3	1
10	The Roots of Bio-Molecular Simulation: The Eight-Week CECAM Workshop Models for Protein Dynamics of 1976. *Helvetica Chimica Acta*, **2019**, 102, e1800239	2	1

List of Publications

9	Influence of variation of a side chain on the folding equilibrium of a peptide: limitations of one-step perturbation. *Journal of Computational Chemistry*, **2013**, 34, 1899-906	3.5	1
8	The Effect of Fluoro Substitution upon the Hairpin Fold of a Tetrapeptide in Methanol. *Helvetica Chimica Acta*, **2010**, 93, 1870-1881	2	1
7	A comparison of pathway-independent and pathway-dependent methods in the calculation of conformational free enthalpy differences. *Protein Science*, **2016**, 25, 184-91	6.3	1
6	Folding–unfolding thermodynamics of a heptapeptide from equilibrium simulations **1999**, 34, 269		1
5	Molecular dynamics simulation of hen egg white lysozyme: A test of the GROMOS96 force field against nuclear magnetic resonance data **2000**, 40, 145		1
4	Entropy calculations on a reversibly folding peptide: Changes in solute free energy cannot explain folding behavior **2001**, 43, 45		1
3	Molecular dynamics simulation or structure refinement of proteins: are solvent molecules required? A case study using hen lysozyme.. *European Biophysics Journal*, **2022**, 1	1.9	0
2	Calculation of the relative free energy of oxidation of Azurin at pH 5 and pH 9. *Journal of Computational Chemistry*, **2012**, 33, 1467-77	3.5	
1	Energy–Entropy Compensation in the Transfer of Nonpolar Solutes from Water to Cosolvent/Water Mixtures. *ChemPhysChem*, **2005**, 6, 1010-1010	3.2	