# 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 | On the use of <scp>intraâ€molecular</scp> distance and angle constraints to lengthen the time step in molecular and stochastic dynamics simulations of proteins. Proteins: Structure, Function and Bioinformatics, 2022, 90, 543-559. | 1.5 | 2 |
| 2 | Molecular dynamics simulation or structure refinement of proteins: are solvent molecules required? A case study using hen lysozyme. European Biophysics Journal, 2022, 51, 265-282. | 1.2 | 6 |
| 3 | A Method to Derive Structural Information on Molecules from Residual Dipolar Coupling NMR Data. Journal of Physical Chemistry B, 2022, 126, 3867-3888. | 1.2 | 1 |
| 4 | A method to apply bondâ€angle constraints in molecular dynamics simulations. Journal of Computational Chemistry, 2021, 42, 418-434. | 1.5 | 4 |
| 5 | On the Use of Sideâ€Chain NMR Relaxation Data to Derive Structural and Dynamical Information on Proteins: A Case Study Using Hen Lysozyme. ChemBioChem, 2021, 22, 1049-1064. | 1.3 | 5 |
| 6 | On the use of 3J-coupling NMR data to derive structural information on proteins. Journal of Biomolecular NMR, 2021, 75, 39-70. | 1.6 | 3 |
| 7 | 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 |
| 8 | Algorithms to apply dihedral-angle constraints in molecular or stochastic dynamics simulations. Journal of Chemical Physics, 2020, 152, 024109. | 1.2 | 5 |
| 9 | A Suite of Advanced Tutorials for the GROMOS Biomolecular Simulation Software [Article v1.0]. Living Journal of Computational Molecular Science, 2020, 2, . | 2.2 | 3 |
| 10 | The Roots of Bioâ€Molecular Simulation: The Eightâ€Week CECAM Workshop â€˜Models for Protein Dynamicsâ€™ of 1976. Helvetica Chimica Acta, 2019, 102, e1800239. | 1.0 | 3 |
| 11 | 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. | 2.5 | 4 |
| 12 | Validierung von molekularen Simulationen: eine Ãœbersicht verschiedener Aspekte. Angewandte Chemie, 2018, 130, 894-915. | 1.6 | 3 |
| 13 | Validation of Molecular Simulation: An Overview of Issues. Angewandte Chemie - International Edition, 2018, 57, 884-902. | 7.2 | 101 |
| 14 | Interpretation of Seemingly Contradictory Data: Low NMR S 2 Order Parameters Observed in Helices and High NMR S 2 Order Parameters in Disordered Loops of the Protein hGH at Low pH. Chemistry - A European Journal, 2017, 23, 9585-9591. | 1.7 | 2 |
| 15 | 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. | 1.2 | 2 |
| 16 | A comparison of pathwayâ€independent and pathwayâ€dependent methods in the calculation of conformational free enthalpy differences. Protein Science, 2016, 25, 184-191. | 3.1 | 1 |
| 17 | Going for a PhD: Joys and Pitfalls. Helvetica Chimica Acta, 2016, 99, 755-759. | 1.0 | 1 |
| 18 | A molecular dynamics simulation investigation of the relative stability of the cyclic peptide octreotide and its deprotonated and its (CF3)-Trp substituted analogs in different solvents. Bioorganic and Medicinal Chemistry, 2016, 24, 4936-4948. | 1.4 | 3 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Bestimmung von Strukturinformation aus experimentellen Messdaten fÃ¼r BiomolekÃ¼le. Angewandte Chemie, 2016, 128, 16222-16244. | 1.6 | 7 |
| 20 | On the use of time-averaging restraints when deriving biomolecular structure from $$^3J$$ 3 J -coupling values obtained from NMR experiments. Journal of Biomolecular NMR, 2016, 66, 69-83. | 1.6 | 1 |
| 21 | Deriving Structural Information from Experimentally Measured Data on Biomolecules. Angewandte Chemie - International Edition, 2016, 55, 15990-16010. | 7.2 | 24 |
| 22 | 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, 5860-5866. | 1.3 | 4 |
| 23 | GROMOS polarisable model for acetone. Molecular Physics, 2016, 114, 845-854. | 0.8 | 7 |
| 24 | Structural and energetic effects of the use of polarisable water to solvate proteins. Molecular Physics, 2015, 113, 2815-2828. | 0.8 | 3 |
| 25 | On the use of a weak-coupling thermostat in replica-exchange molecular dynamics simulations. Journal of Chemical Physics, 2015, 143, 034110. | 1.2 | 10 |
| 26 | On the pitfalls of peer review. F1000Research, 2015, 4, 1244. | 0.8 | 2 |
| 27 | 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 |
| 28 | Polarizable coarseâ€grained models for molecular dynamics simulation of liquid cyclohexane. Journal of Computational Chemistry, 2015, 36, 1311-1321. | 1.5 | 7 |
| 29 | Challenge of Representing Entropy at Different Levels of Resolution in Molecular Simulation. Journal of Physical Chemistry B, 2015, 119, 753-763. | 1.2 | 6 |
| 30 | On the compatibility of polarisable and non-polarisable models for liquid water. Molecular Physics, 2014, 112, 2761-2780. | 0.8 | 11 |
| 31 | A polarizable empirical force field for molecular dynamics simulation of liquid hydrocarbons. Journal of Computational Chemistry, 2014, 35, 789-801. | 1.5 | 24 |
| 32 | On the Use of a Supramolecular Coarseâ€Grained Model for the Solvent in Simulations of the Folding Equilibrium of an Octaâ€Î²â€peptide in MeOH and H<sub>2</sub>O. Helvetica Chimica Acta, 2014, 97, 1591-1605. | 1.0 | 5 |
| 33 | Time-averaged order parameter restraints in molecular dynamics simulations. Journal of Biomolecular NMR, 2014, 60, 169-187. | 1.6 | 20 |
| 34 | Using enveloping distribution sampling to compute the folding free enthalpy of a Î²-peptide with a very unstable folded conformation in solution: The advantage of focused sampling using EDS. Chemical Physics, 2014, 428, 156-163. | 0.9 | 3 |
| 35 | On the use of one-step perturbation to investigate the dependence of NOE-derived atomâ€“atom distance bound violations of peptides upon a variation of force-field parameters. European Biophysics Journal, 2014, 43, 113-119. | 1.2 | 7 |
| 36 | An improved simple polarisable water model for use in biomolecular simulation. Journal of Chemical Physics, 2014, 141, 22D515. | 1.2 | 19 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | 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. | 2.3 | 3 |
| 38 | 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 |
| 39 | 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. | 0.9 | 4 |
| 40 | 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 simulationâ€. Molecular Physics, 2013, 111, 2334-2344. | 0.8 | 2 |
| 41 | The Seven Sins in Academic Behavior in the Natural Sciences. Angewandte Chemie - International Edition, 2013, 52, 118-122. | 7.2 | 24 |
| 42 | Multiâ€Resolution Simulation of Biomolecular Systems: A Review of Methodological Issues. Angewandte Chemie - International Edition, 2013, 52, 2820-2834. | 7.2 | 72 |
| 43 | On the choice of a reference state for oneâ€step perturbation calculations between polar and nonpolar molecules in a polar environment. Journal of Computational Chemistry, 2013, 34, 387-393. | 1.5 | 5 |
| 44 | Multiple binding modes for palmitate to barley lipid transfer protein facilitated by the presence of proline 12. Protein Science, 2013, 22, 56-64. | 3.1 | 9 |
| 45 | Conformational Preferences of a Î²â€Octapeptide as Function of Solvent and Forceâ€Field Parameters. Helvetica Chimica Acta, 2013, 96, 189-200. | 1.0 | 5 |
| 46 | Refinement of the application of the GROMOS 54A7 force field to Î²-peptides. Journal of Computational Chemistry, 2013, 34, 2796-2805. | 1.5 | 51 |
| 47 | Influence of variation of a side chain on the folding equilibrium of a Î²â€peptide: Limitations of oneâ€step perturbation. Journal of Computational Chemistry, 2013, 34, 1899-1906. | 1.5 | 1 |
| 48 | 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. | 0.8 | 2 |
| 49 | Free enthalpies of replacing water molecules in protein binding pockets. Journal of Computer-Aided Molecular Design, 2012, 26, 1293-1309. | 1.3 | 23 |
| 50 | Validation of the GROMOS 54A7 Force Field Regarding Mixed Î±/Î²â€Peptide Molecules. Helvetica Chimica Acta, 2012, 95, 2562-2577. | 1.0 | 11 |
| 51 | Thirty-five years of biomolecular simulation: development of methodology, force fields and software. Molecular Simulation, 2012, 38, 1271-1281. | 0.9 | 20 |
| 52 | 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, 1672-1681. | 3.1 | 3 |
| 53 | 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 |
| 54 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | Molecular dynamics simulation of thionated hen egg white lysozyme. Protein Science, 2012, 21, 1153-1161. | 3.1 | 5 |
| 56 | Calculation of the relative free energy of oxidation of azurin at pH 5 and pH 9. Journal of Computational Chemistry, 2012, 33, 1467-1477. | 1.5 | 1 |
| 57 | Interfacing the GROMOS (bio)molecular simulation software to quantumâ€chemical program packages. Journal of Computational Chemistry, 2012, 33, 2108-2117. | 1.5 | 13 |
| 58 | Architecture, implementation and parallelisation of the GROMOS software for biomolecular simulation. Computer Physics Communications, 2012, 183, 890-903. | 3.0 | 275 |
| 59 | Helical Content of a Î²<sup>3</sup>â€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 |
| 60 | New functionalities in the GROMOS biomolecular simulation software. Journal of Computational Chemistry, 2012, 33, 340-353. | 1.5 | 98 |
| 61 | 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 |
| 62 | 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 |
| 63 | A simple, efficient polarizable molecular model for liquid carbon tetrachloride. Molecular Physics, 2011, 109, 365-372. | 0.8 | 15 |
| 64 | 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 |
| 65 | GROMOS++ Software for the Analysis of Biomolecular Simulation Trajectories. Journal of Chemical Theory and Computation, 2011, 7, 3379-3390. | 2.3 | 180 |
| 66 | An effective force field for molecular dynamics simulations of dimethyl sulfone. Molecular Physics, 2011, 109, 2593-2605. | 0.8 | 4 |
| 67 | 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 |
| 68 | 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 |
| 69 | Biomolecular structure refinement using the GROMOS simulation software. Journal of Biomolecular NMR, 2011, 51, 265-281. | 1.6 | 41 |
| 70 | 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 |
| 71 | Definition and testing of the GROMOS force-field versions 54A7 and 54B7. European Biophysics Journal, 2011, 40, 843-856. | 1.2 | 1,902 |
| 72 | A Method for Conformational Sampling of Loops in Proteins Based on Adiabatic Decoupling and Temperature or Force Scaling. ChemPhysChem, 2011, 12, 2609-2614. | 1.0 | 3 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | Influence of Variation of a Side Chain on the Folding Equilibrium of a Î²â€Peptide. Helvetica Chimica Acta, 2011, 94, 597-610. | 1.0 | 5 |
| 74 | Calculation of binding free energies of inhibitors to plasmepsin II. Journal of Computational Chemistry, 2011, 32, 1801-1812. | 1.5 | 18 |
| 75 | 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 |
| 76 | A simple, efficient polarizable coarse-grained water model for molecular dynamics simulations. Journal of Chemical Physics, 2011, 134, 084110. | 1.2 | 121 |
| 77 | Basic ingredients of free energy calculations: A review. Journal of Computational Chemistry, 2010, 31, 1569-1582. | 1.5 | 281 |
| 78 | 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 |
| 79 | Structure Determination of a Flexible Cyclic Peptide Based on NMR and MD Simulation 3Jâ€Coupling. ChemPhysChem, 2010, 11, 830-835. | 1.0 | 13 |
| 80 | Molecular Dynamics Simulation of Esterâ€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. | 1.0 | 8 |
| 81 | The Effect of Fluoro Substitution upon the Î²â€Hairpin Fold of a Î²â€Tetrapeptide in Methanol. Helvetica Chimica Acta, 2010, 93, 1870-1881. | 1.0 | 2 |
| 82 | Î±â€Cyclodextrin Hostâ€“Guest Binding: A Computational Study of the Different Driving Forces. Helvetica Chimica Acta, 2010, 93, 2318-2325. | 1.0 | 2 |
| 83 | 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 |
| 84 | 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 |
| 85 | 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 |
| 86 | 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 |
| 87 | A one-site polarizable model for liquid chloroform: COS/C. Molecular Physics, 2010, 108, 1749-1757. | 0.8 | 12 |
| 88 | 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. | 0.9 | 6 |
| 89 | 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 |
| 90 | The thermal isomerization of the GFP chromophore: A computational study. Physical Chemistry Chemical Physics, 2010, 12, 11051. | 1.3 | 9 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | On the Conformational Properties of Amylose and Cellulose Oligomers in Solution. International Journal of Carbohydrate Chemistry, 2009, 2009, 1-8. | 1.5 | 25 |
| 92 | Interpreting Experimental Data by Using Molecular Simulation Instead of Model Building. Chemistry - A European Journal, 2009, 15, 6389-6398. | 1.7 | 16 |
| 93 | 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 |
| 94 | Folding and Unfolding of Two Mixed Î±/Î² Peptides. ChemBioChem, 2009, 10, 2032-2041. | 1.3 | 18 |
| 95 | A Method to Explore Protein Side Chain Conformational Variability Using Experimental Data. ChemPhysChem, 2009, 10, 3213-3228. | 1.0 | 25 |
| 96 | On the direct calculation of the free energy of quantization for molecular systems in the condensed phase. Journal of Computational Chemistry, 2009, 30, 514-523. | 1.5 | 6 |
| 97 | 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 |
| 98 | 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 |
| 99 | 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 |
| 100 | A Molecular Dynamics Study of the ASC and NALP1 Pyrin Domains at Neutral and Low pH. ChemBioChem, 2008, 9, 923-933. | 1.3 | 6 |
| 101 | Exploring the Conserved Water Site and Hydration of a Coiledâ€Coil Trimerisation Motif: A MD Simulation Study. ChemBioChem, 2008, 9, 1749-1756. | 1.3 | 7 |
| 102 | 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 |
| 103 | Molecular simulation as an aid to experimentalists. Current Opinion in Structural Biology, 2008, 18, 149-153. | 2.6 | 171 |
| 104 | Biomolecular simulation: historical picture and future perspectives. Biochemical Society Transactions, 2008, 36, 11-15. | 1.6 | 48 |
| 105 | Molecular Modeling Using Nuclear Magnetic Resonance Data. Reviews in Computational Chemistry, 2007, , 143-172. | 1.5 | 10 |
| 106 | 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 |
| 107 | Simulation ofÎ²-depsipeptides: The effect of missing hydrogen-bond donors on their folding equilibria. Biopolymers, 2007, 85, 318-332. | 1.2 | 13 |
| 108 | A Comparison of Methods to Compute the Potential of Mean Force. ChemPhysChem, 2007, 8, 162-169. | 1.0 | 243 |

| # | Article | IF | Citations |
|---|---|---|---|
| 109 | Comparison of Thermodynamic Properties of Coarse-Grained and Atomic-Level Simulation Models. ChemPhysChem, 2007, 8, 452-461. | 1.0 | 102 |
| 110 | Free Energy Calculations Using Flexible-Constrained, Hard-Constrained and Non-Constrained Molecular Dynamics Simulations. ChemPhysChem, 2007, 8, 1557-1564. | 1.0 | 7 |
| 111 | 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 |
| 112 | On using oscillating time-dependent restraints in MD simulation. Journal of Biomolecular NMR, 2007, 37, 1-14. | 1.6 | 15 |
| 113 | Biomolecular structure refinement based on adaptive restraints using local-elevation simulation. Journal of Biomolecular NMR, 2007, 39, 265-273. | 1.6 | 22 |
| 114 | Sampling of Rare Events Using Hidden Restraints. Journal of Physical Chemistry B, 2006, 110, 8488-8498. | 1.2 | 30 |
| 115 | Terminal-group effects on the folding behavior of selected beta-peptides. Proteins: Structure, Function and Bioinformatics, 2006, 63, 136-143. | 1.5 | 17 |
| 116 | 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 |
| 117 | Protein under pressure: Molecular dynamics simulation of the arc repressor. Proteins: Structure, Function and Bioinformatics, 2006, 65, 136-144. | 1.5 | 31 |
| 118 | Calculating zeros: Non-equilibrium free energy calculations. Chemical Physics, 2006, 323, 102-108. | 0.9 | 35 |
| 119 | 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 |
| 120 | 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 |
| 121 | Pathway dependence of the efficiency of calculating free energy and entropy of soluteâ€“solute association in water. Chemical Physics, 2006, 330, 410-416. | 0.9 | 4 |
| 122 | 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 |
| 123 | Simulation of an all-Î²3-icosapeptide containing the 20 proteinogenic side chains: Effect of temperature, pH, counterions, solvent, and force field on helix stability. Biopolymers, 2006, 83, 636-645. | 1.2 | 5 |
| 124 | Biomolecular Modeling: Goals, Problems, Perspectives. Angewandte Chemie - International Edition, 2006, 45, 4064-4092. | 7.2 | 503 |
| 125 | Molecular dynamics simulations of liquid methanol and methanolâ€“water mixtures with polarizable models. Journal of Computational Chemistry, 2006, 27, 1494-1504. | 1.5 | 103 |
| 126 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 127 | 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 |
| 128 | An improved nucleic acid parameter set for the GROMOS force field. Journal of Computational Chemistry, 2005, 26, 725-737. | 1.5 | 161 |
| 129 | The GROMOS software for biomolecular simulation: GROMOS05. Journal of Computational Chemistry, 2005, 26, 1719-1751. | 1.5 | 592 |
| 130 | Amine Hydration: A United-Atom Force-Field Solution. ChemPhysChem, 2005, 6, 1800-1804. | 1.0 | 25 |
| 131 | Energy-Entropy Compensation in the Transfer of Nonpolar Solutes from Water to Cosolvent/Water Mixtures. ChemPhysChem, 2005, 6, 1010-1010. | 1.0 | 0 |
| 132 | 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 |
| 133 | Validation of the 53A6 GROMOS force field. European Biophysics Journal, 2005, 34, 273-284. | 1.2 | 443 |
| 134 | Principles of carbopeptoid folding: a molecular dynamics simulation study. Journal of Peptide Science, 2005, 11, 74-84. | 0.8 | 19 |
| 135 | Interpreting NMR Data for Î²-Peptides Using Molecular Dynamics Simulations. Journal of the American Chemical Society, 2005, 127, 14320-14329. | 6.6 | 39 |
| 136 | Simulating the Physiological Phase of Hydrated DPPC Bilayers: The Ester Moiety. Soft Materials, 2004, 2, 27-45. | 0.8 | 16 |
| 137 | Carbopeptoid Folding: Effects of Stereochemistry, Chain Length, and Solvent. Angewandte Chemie - International Edition, 2004, 43, 4055-4059. | 7.2 | 24 |
| 138 | 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 |
| 139 | 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 |
| 140 | Energyâ€“Entropy Compensation in the Transfer of Nonpolar Solutes from Water to Cosolvent/Water Mixtures. ChemPhysChem, 2004, 5, 144-147. | 1.0 | 49 |
| 141 | Comparison of Properties of Aib-Rich Peptides in Crystal and Solution: A Molecular Dynamics Study. ChemPhysChem, 2004, 5, 633-641. | 1.0 | 15 |
| 142 | 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 |
| 143 | Alpha- and beta-polypeptides show a different stability of helical secondary structure. Tetrahedron, 2004, 60, 7775-7780. | 1.0 | 20 |
| 144 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 145 | Estimating entropies from molecular dynamics simulations. Journal of Chemical Physics, 2004, 120, 2652-2661. | 1.2 | 138 |
| 146 | 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 |
| 147 | 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 |
| 148 | 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 |
| 149 | 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 |
| 150 | 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 |
| 151 | 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 |
| 152 | Development of a simple, self-consistent polarizable model for liquid water. Journal of Chemical Physics, 2003, 118, 221-234. | 1.2 | 209 |
| 153 | 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 |
| 154 | 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 |
| 155 | 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 |
| 156 | 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 |
| 157 | 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 |
| 158 | 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 |
| 159 | A Comparison of Non-Bonded Scaling Approaches for Free Energy Calculations. Molecular Simulation, 2002, 28, 45-65. | 0.9 | 109 |
| 160 | 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 |
| 161 | One-Step Perturbation Methods for Solvation Free Energies of Polar Solutes. Journal of Physical Chemistry B, 2001, 105, 11264-11274. | 1.2 | 59 |
| 162 | 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. | 0.9 | 6 |

| # | Article | IF | Citations |
|---|---|---|---|
| 163 | Molecular dynamics simulation of n -dodecyl phosphate aggregate structures. European Biophysics Journal, 2001, 30, 330-343. | 1.2 | 24 |
| 164 | Free energy barrier estimation of unfolding the ?-helical surfactant-associated polypeptide C. Proteins: Structure, Function and Bioinformatics, 2001, 43, 395-402. | 1.5 | 10 |
| 165 | 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 |
| 166 | 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 |
| 167 | Viscosity dependence of protein dynamics. Proteins: Structure, Function and Bioinformatics, 2001, 42, 414-421. | 1.5 | 47 |
| 168 | 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 |
| 169 | An improved GROMOS96 force field for aliphatic hydrocarbons in the condensed phase. Journal of Computational Chemistry, 2001, 22, 1205-1218. | 1.5 | 814 |
| 170 | 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 |
| 171 | Reply. Angewandte Chemie - International Edition, 2001, 40, 4616-4618. | 7.2 | 13 |
| 172 | Further investigation on the validity of Stokesâ€“Einstein behaviour at the molecular level. Chemical Physics Letters, 2001, 334, 337-342. | 1.2 | 27 |
| 173 | Calculation of NMR-relaxation parameters for flexible molecules from molecular dynamics simulations. Journal of Biomolecular NMR, 2001, 20, 297-310. | 1.6 | 89 |
| 174 | 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 |
| 175 | Viscosity dependence of protein dynamics. Proteins: Structure, Function and Bioinformatics, 2001, 42, 414-421. | 1.5 | 2 |
| 176 | Entropy calculations on a reversibly folding peptide: Changes in solute free energy cannot explain folding behavior. , 2001, 43, 45. | | 1 |
| 177 | An improved GROMOS96 force field for aliphatic hydrocarbons in the condensed phase. Journal of Computational Chemistry, 2001, 22, 1205-1218. | 1.5 | 13 |
| 178 | Reversible peptide folding: Dependence on molecular force field used. Journal of Computational Chemistry, 2000, 21, 774-787. | 1.5 | 19 |
| 179 | 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 |
| 180 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 181 | Factor Xa: simulation studies with an eye to inhibitor design. Journal of Computer-Aided Molecular Design, 2000, 14, 507-529. | 1.3 | 11 |
| 182 | On the Choice of Dihedral Angle Potential Energy Functions forn-Alkanes. Molecular Simulation, 2000, 25, 301-319. | 0.9 | 111 |
| 183 | Absolute entropies from molecular dynamics simulation trajectories. Journal of Chemical Physics, 2000, 113, 7809-7817. | 1.2 | 171 |
| 184 | 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 |
| 185 | Molecular dynamics simulation of hen egg white lysozyme: A test of the GROMOS96 force field against nuclear magnetic resonance data. , 2000, 40, 145. | | 1 |
| 186 | Molecular dynamics simulation of hen egg white lysozyme: A test of the GROMOS96 force field against nuclear magnetic resonance data. , 2000, 40, 145. | | 4 |
| 187 | Peptide folding simulations: no solvent required?. Computer Physics Communications, 1999, 123, 97-102. | 3.0 | 35 |
| 188 | Estimating relative free energies from a single ensemble: Hydration free energies. Journal of Computational Chemistry, 1999, 20, 1604-1617. | 1.5 | 57 |
| 189 | Folding-unfolding thermodynamics of a ?-heptapeptide from equilibrium simulations. Proteins: Structure, Function and Bioinformatics, 1999, 34, 269-280. | 1.5 | 370 |
| 190 | Molecular dynamics simulations of human ?-lactalbumin: Changes to the structural and dynamical properties of the protein at low pH. , 1999, 36, 77-86. | | 28 |
| 191 | Accessibility and order of water sites in and around proteins: A crystallographic time-averaging study. , 1999, 36, 501-511. | | 26 |
| 192 | The effect of motional averaging on the calculation of NMR-derived structural properties. , 1999, 36, 542-555. | | 103 |
| 193 | Peptide Folding: When Simulation Meets Experiment. Angewandte Chemie - International Edition, 1999, 38, 236-240. | 7.2 | 1,611 |
| 194 | The Photoisomerization ofcis-Stilbene Does Not Follow the Minimum Energy Path. Angewandte Chemie - International Edition, 1999, 38, 2609-2611. | 7.2 | 25 |
| 195 | The GROMOS Biomolecular Simulation Program Package. Journal of Physical Chemistry A, 1999, 103, 3596-3607. | 1.1 | 1,354 |
| 196 | Foldingâ€“unfolding thermodynamics of a Î²-heptapeptide from equilibrium simulations. , 1999, 34, 269. | | 1 |
| 197 | Peptide Folding: When Simulation Meets Experiment. , 1999, 38, 236. | | 16 |
| 198 | Peptide Folding: When Simulation Meets Experiment. Angewandte Chemie - International Edition, 1999, 38, 236-240. | 7.2 | 57 |

| # | Article | IF | Citations |
|---|---|---|---|
| 199 | On using time-averaging restraints in molecular dynamics simulation. Journal of Biomolecular NMR, 1998, 12, 501-508. | 1.6 | 25 |
| 200 | Parametrization of aliphatic CHn united atoms of GROMOS96 force field. Journal of Computational Chemistry, 1998, 19, 535-547. | 1.5 | 370 |
| 201 | SWARM-MD:Â Searching Conformational Space by Cooperative Molecular Dynamics. Journal of Physical Chemistry A, 1998, 102, 5937-5943. | 1.1 | 63 |
| 202 | Validation of molecular dynamics simulation. Journal of Chemical Physics, 1998, 108, 6109-6116. | 1.2 | 161 |
| 203 | Optimization methods for conformational sampling using a Boltzmann-weighted mean field approach. Biopolymers, 1998, 39, 103-114. | 1.2 | 14 |
| 204 | Parametrization of aliphatic CHn united atoms of GROMOS96 force field. , 1998, 19, 535. | | 2 |
| 205 | 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 |
| 206 | Studying the Stability of a Helical Î²â€Heptapeptide by Molecular Dynamics Simulations. Chemistry - A European Journal, 1997, 3, 1410-1417. | 1.7 | 120 |
| 207 | Solvent structure at a hydrophobic protein surface. , 1997, 27, 395-404. | | 43 |
| 208 | Generation of pseudonative protein structures for threading. Proteins: Structure, Function and Bioinformatics, 1997, 28, 522-529. | 1.5 | 4 |
| 209 | Calculating Electrostatic Interactions Using the Particleâ^'Particle Particleâ^'Mesh Method with Nonperiodic Long-Range Interactions. The Journal of Physical Chemistry, 1996, 100, 2581-2587. | 2.9 | 164 |
| 210 | 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 |
| 211 | 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 |
| 212 | Optimization methods for conformational sampling using a Boltzmannâ€weighted mean field approach. Biopolymers, 1996, 39, 103-114. | 1.2 | 6 |
| 213 | Parametrisation of time-averaged distance restraints in MD simulations. Journal of Biomolecular NMR, 1995, 6, 313-320. | 1.6 | 46 |
| 214 | Structure refinement with molecular dynamics and a Boltzmann-weighted ensemble. Journal of Biomolecular NMR, 1995, 6, 163-170. | 1.6 | 66 |
| 215 | A generalized reaction field method for molecular dynamics simulations. Journal of Chemical Physics, 1995, 102, 5451-5459. | 1.2 | 1,293 |
| 216 | Fundamentals of drug design from a biophysical viewpoint. Quarterly Reviews of Biophysics, 1994, 27, 435-481. | 2.4 | 23 |

| # | Article | IF | Citations |
|---|---|---|---|
| 217 | 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 |
| 218 | Predictions of free energy differences from a single simulation of the initial state. Journal of Chemical Physics, 1994, 100, 577-585. | 1.2 | 72 |
| 219 | 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 |
| 220 | Algorithms for clustering molecular dynamics configurations. Journal of Computational Chemistry, 1994, 15, 1331-1340. | 1.5 | 92 |
| 221 | Conformational transitions of a dipeptide in water: Effects of imposed pathways using umbrella sampling techniques. Biopolymers, 1994, 34, 347-355. | 1.2 | 18 |
| 222 | Decomposition of the Free Energy of a System in Terms of Specific Interactions. Journal of Molecular Biology, 1994, 240, 167-176. | 2.0 | 314 |
| 223 | 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 |
| 224 | When Are Free Energy Components Meaningful?. The Journal of Physical Chemistry, 1994, 98, 13735-13740. | 2.9 | 87 |
| 225 | Structure refinement using time-averaged J-coupling constant restraints. Journal of Biomolecular NMR, 1993, 3, 55-66. | 1.6 | 125 |
| 226 | A Structure Refinement Method Based on Molecular Dynamics in Four Spatial Dimensions. Journal of Molecular Biology, 1993, 234, 751-762. | 2.0 | 84 |
| 227 | 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 |
| 228 | The Application of Chemical Shift Calculation to Protein Structure Determination by NMR. , 1993, , 615-622. | | 8 |
| 229 | MD simulation of subtilisin BPNâ€² in a crystal environment. Proteins: Structure, Function and Bioinformatics, 1992, 14, 451-464. | 1.5 | 15 |
| 230 | On the interpretation of biochemical data by molecular dynamics computer simulation. FEBS Journal, 1992, 204, 947-961. | 0.2 | 117 |
| 231 | Calculation of relative free energy via indirect pathways. Journal of Chemical Physics, 1991, 94, 3808-3816. | 1.2 | 78 |
| 232 | 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 |
| 233 | MolekÃ¼ldynamikâ€Computersimulationen; Methodik, Anwendungen und Perspektiven in der Chemie. Angewandte Chemie, 1990, 102, 1020-1055. | 1.6 | 114 |
| 234 | Time-averaged nuclear overhauser effect distance restraints applied to tendamistat. Journal of Molecular Biology, 1990, 214, 223-235. | 2.0 | 288 |

| # | Article | IF | Citations |
|---|---|---|---|
| 235 | Time-dependent distance restraints in molecular dynamics simulations. Chemical Physics Letters, 1989, 157, 289-294. | 1.2 | 268 |
| 236 | 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 |
| 237 | A molecular dynamics computer simulation study of the hydration of bis(methylsulphonyl)methane in water. Molecular Physics, 1985, 56, 1393-1409. | 0.8 | 5 |
| 238 | Molecular dynamics computer simulation as a tool for the analysis of solvation: A study of dilute aqueous solutions of 1,4â€dioxane and 1,3â€dioxane. Recueil Des Travaux Chimiques Des Pays-Bas, 1985, 104, 79-89. | 0.0 | 8 |
| 239 | A consistent empirical potential for water-protein interactions. Biopolymers, 1984, 23, 1513-1518. | 1.2 | 759 |