

Publications in the field of Molecular Dynamics and Biomolecular Theory by W.F. van Gunsteren/P.H. Hünenberger (ETH Zürich), A.E. Mark (University of Queensland, AUS), S.J. Marrink/A.H. de Vries (University of Groningen, NL) and co-workers

1977-1981

- 77.01 W.F. van Gunsteren and H.J.C. Berendsen
Algorithms for macromolecular dynamics and constraint dynamics
Mol. Phys. **34** (1977) 1311-1327
- 77.02 J.-P. Ryckaert, G. Ciccotti, H.J.C. Berendsen
Numerical Integration of the Cartesian Equations of Motion of a System with Constraints: Molecular Dynamics of n-Alkanes
J. Comput. Phys. **23** (1977) 327-341
- 78.01 W.G.J. Hol, P.T. van Duijnen and H.J.C. Berendsen
The α -helix dipole and the properties of proteins
Nature **273** (1978) 443-446
- 78.02 W.F. van Gunsteren, H.J.C. Berendsen and J.A.C. Rullmann
Inclusion of Reaction Fields in Molecular Dynamics: Application to Liquid Water
Faraday Disc. Chem. Soc. **66** (1978) 58-70
- 78.03 T. Lee, J. Bisschop, W. van der Lugt and W.F. van Gunsteren
Radial distribution functions of liquid Na and Cs
Physica **93B** (1978) 59-62
- 80.01 P. van der Ploeg and H.J.C. Berendsen
Molecular dynamics of model membranes
Biophys. Struct. Mechanisms **6** Suppl. (1980) 106 (abstract)
- 80.02 W.F. van Gunsteren
Constrained dynamics of flexible molecules
Mol. Phys. **40** (1980) 1015-1019
- 80.03 W.F. van Gunsteren and M. Karplus
A Method for Constrained Energy Minimization of Macromolecules
J. Comput. Chem. **1** (1980) 266-274
- 81.01 H.J.C. Berendsen
Moleculaire dynamica, Perspectief voor complexe systemen (in Dutch)
Chemisch Magazine, juli/aug. 1981, 403 and sept. 1981, 461-464
- 81.02 W.F. van Gunsteren, H.J.C. Berendsen and J.A.C. Rullmann
Stochastic dynamics for molecules with constraints Brownian dynamics of n-alkanes
Mol. Phys. **44** (1981) 69-95
- 81.03 W.F. van Gunsteren and M. Karplus
Effect of constraints, solvent and crystal environment on protein dynamics
Nature **293** (1981) 677-678
- 81.04 H.J.C. Berendsen, J.P.M. Postma, W.F. van Gunsteren and J. Hermans
Interaction models for water in relation to protein hydration
In: "Intermolecular Forces", B. Pullman ed., Reidel, Dordrecht, 1981, p. 331-342

1982

- 82.01 P. van der Ploeg and H.J.C. Berendsen
Molecular dynamics simulation of a bilayer membrane
J. Chem. Phys. **76** (1982) 3271-3276

- 82.02 P. van der Ploeg
 Molecular Dynamics of Membranes
 Thesis, University of Groningen, July 1982
- 82.03 W.F. van Gunsteren and H.J.C. Berendsen
 Algorithms for brownian dynamics
Mol. Phys. **45** (1982) 637-647
- 82.04 W.F. van Gunsteren and H.J.C. Berendsen
 Molecular dynamics: perspective for complex systems
Biochem. Soc. Trans. **10** (1982) 301-305
- 82.05 W.F. van Gunsteren and H.J.C. Berendsen
 On the fluctuation-dissipation theorem for interacting brownian particles
Mol. Phys. **47** (1982) 721-723
- 82.06 J.P.M. Postma, H.J.C. Berendsen and J.R. Haak
 Thermodynamics of Cavity Formation in Water: A Molecular Dynamics Study
Faraday Symp. Chem. Soc. **17** (1982) 55-67
- 82.07 S. Swaminathan, T. Ichiye, W.F. van Gunsteren and M. Karplus
 Time Dependence of Atomic Fluctuations in Proteins: Analysis of Local and Collective Motions in Bovine Pancreatic Trypsin Inhibitor
Biochemistry **21** (1982) 5230-5241
- 82.08 W.F. van Gunsteren and M. Karplus
 Effect of Constraints on the Dynamics of Macromolecules
Macromolecules **15** (1982) 1528-1544
- 82.09 W.F. van Gunsteren and M. Karplus
 Protein Dynamics in Solution and in a Crystalline Environment: A Molecular Dynamics Study
Biochemistry **21** (1982) 2259-2274
- 1983**
- 83.01 P. van der Ploeg and H.J.C. Berendsen
 Molecular dynamics of a bilayer membrane
Mol. Phys. **49** (1983) 233-248
- 83.02 W.F. van Gunsteren, H.J.C. Berendsen, J. Hermans, W.G.J. Hol and J.P.M. Postma
 Computer simulation of the dynamics of hydrated protein crystals and its comparison with X-ray data
Proc. Natl. Acad. Sci USA **80** (1983) 4315-4319
- 83.03 O. Edholm, H.J.C. Berendsen and P. van der Ploeg
 Conformational entropy of a bilayer membrane derived from a molecular dynamics simulation
Mol. Phys. **48** (1983) 379-388
- 83.04 H.J.C. Berendsen and W.F. van Gunsteren
 Molecular dynamics with constraints
 In: "The Physics of Superionic Conductors and Electrode Materials", J.W. Perram, ed., NATO ASI Series **B92** (1983) 221-240 (Plenum Press)
- 83.05 W.F. van Gunsteren and H.J.C. Berendsen
 Stochastic dynamics of polymers
 In: "The Physics of Superionic Conductors and Electrode Materials", J.W. Perram, ed., NATO ASI Series **B92** (1983) 241-256 (Plenum Press)

- 83.06 M. Karplus, S. Swaminathan, T. Ichiye and W.F. van Gunsteren
 Local and collective motions in protein dynamics
 In: "Mobility and function in proteins and nucleic acids", Ciba Symp. **93**, Pitman, London, (1983), pp. 271-290
- 83.07 H.J.C. Berendsen
 Discussion note in "Mobility and function in proteins and nucleic acids", Ciba Symp. **93**, Pitman, London, (1983), pp. 283-284
- 1984**
- 84.01 J. Hermans, H.J.C. Berendsen, W.F. van Gunsteren and J.P.M. Postma
 A Consistent Empirical Potential for Water-Protein Interactions
Biopolymers **23** (1984) 1513-1518
- 84.02 H.J.C. Berendsen, W.F. van Gunsteren and J.P.M. Postma
 Molecular Dynamics on CRAY, CYBER and DAP
 In: "High-Speed Computation", J.S. Kowalik, ed., NATO ASI Series **F7** (1984) 425-438 (Springer, Berlin)
- 84.03 W.F. van Gunsteren, H.J.C. Berendsen, F. Colonna, D. Perahia, J.P. Hollenberg and D. Lellouch
 On Searching Neighbours in Computer Simulations of Macromolecular Systems
J. Comput. Chem. **5** (1984) 272-279
- 84.04 W.F. van Gunsteren and H.J.C. Berendsen
 Computer Simulation as a Tool for Tracing the Conformational Differences between Proteins in Solution and in the Crystalline State
J. Mol. Biol. **176** (1984) 559-564
- 84.05 O. Edholm and H.J.C. Berendsen
 Entropy estimation from simulations of non-diffusive systems
Mol. Phys. **51** (1984) 1011-1028
- 84.06 H.J.C. Berendsen and W.F. van Gunsteren
 Molecular Dynamics Simulations: Techniques and Approaches
 In: "Molecular Liquids - Dynamics and Interactions", A.J. Barnes et al. eds., NATO ASI Series **C135** (1984) 475-500 (Reidel, Dordrecht)
- 84.07 H.J.C. Berendsen
 Survey of Future Developments in Molecular Dynamics
 In: "Molecular Liquids - Dynamics and Interactions", A.J. Barnes et al. eds., NATO ASI Series **C135** (1984) 561-564 (Reidel, Dordrecht)
- 84.08 A. DiNola, H.J.C. Berendsen and O. Edholm
 Free Energy Determination of Polypeptide Conformations Generated by Molecular Dynamics
Macromolecules **17** (1984) 2044-2050
- 84.09 H.J.C. Berendsen, J.P.M. Postma, W.F. van Gunsteren, A. DiNola and J.R. Haak
 Molecular dynamics with coupling to an external bath
J. Chem. Phys. **81** (1984) 3684-3690
- 84.10 K. Remerie, W.F. van Gunsteren, J.P.M. Postma, H.J.C. Berendsen and J.B.F.N. Engberts
 Molecular dynamics computer simulation of the hydration of two simple organic solutes. Comparison with the simulation of an empty cavity
Mol. Phys. **53** (1984) 1517-1526
- 84.11 J.P.M. Postma, H.J.C. Berendsen and T.P. Straatsma
 Intramolecular vibrations from molecular dynamics simulations of liquid water
Journal de Physique C7 (1984) 31-40

- 84.12 W.F. van Gunsteren, R. Kaptein and E.R.P. Zuiderweg
 Use of Molecular Dynamics Computer Simulations When Determining Protein Structure by 2D NMR
 In: "Proceedings NATO/CECAM workshop on nucleic acid conformation and dynamics", W.K. Olson ed., 1984, Orsay, 79-92 (CECAM, France)
- 1985**
- 85.01 R. Kaptein, E.R.P. Zuiderweg, R.M. Scheek, R. Boelens and W.F. van Gunsteren
 A Protein Structure from Nuclear Magnetic Resonance Data lac Repressor Headpiece
J. Mol. Biol. **182** (1985) 179-182
- 85.02 J. Åqvist, W.F. van Gunsteren, M. Leijonmarck and O. Tapia
 A Molecular Dynamics Study of the C-terminal Fragment of the L7/12 Ribosomal Protein Secondary Structure Motion in a 150 Picosecond Trajectory
J. Mol. Biol. **183** (1985) 461-477
- 85.03 E.R.P. Zuiderweg, R.M. Scheek, R. Boelens, W.F. van Gunsteren and R. Kaptein
 Determination of protein structures from nuclear magnetic resonance data using a restrained molecular dynamics approach: The lac repressor DNA binding domain
Biochimie **67** (1985) 707-715
- 85.04 B. Witholt, W.F. van Gunsteren and W.G.J. Hol
 Protein Engineering
 In: "Proceedings of the Third European Congress on Biotechnology" Vol. IV, Verlag Chemie, Weinheim, FRG, 1985, pp. 497-517
- 85.05 W.F. van Gunsteren and H.J.C. Berendsen
 Molecular Dynamics Simulations: Techniques and Applications to Proteins,
 In: "Molecular Dynamics and Protein Structure", J. Hermans ed., Polycrystal Book Service, P.O. Box 27, Western Springs, Ill. 60558, USA, (1985), pp. 5-14
- 85.06 W.F. van Gunsteren, R. Boelens, R. Kaptein, R.M. Scheek and E.R.P. Zuiderweg
 An Improved Restrained Molecular Dynamics Technique to Obtain Protein Tertiary Structure from Nuclear Magnetic Resonance Data
 In: "Molecular Dynamics and Protein Structure", J. Hermans ed., Polycrystal Book Service, P.O. Box 27, Western Springs, Ill. 60558, USA, (1985), pp. 92-99
- 85.07 I. Haneef, I.D. Glover, I.J. Tickle, D.S. Moss, S.P. Wood, T.L. Blundell and W.F. van Gunsteren
 The Dynamics of Pancreatic Polypeptide: A Comparison of X-ray Anisotropic Refinement at 0.98 K Resolution, Molecular Dynamics and Normal Mode Analysis
 In: "Molecular Dynamics and Protein Structure", J. Hermans ed., Polycrystal Book Service, P.O. Box 27, Western Springs, Ill. 60558, USA, (1985), pp. 85-91
- 85.08 J. Åqvist, W.F. van Gunsteren, M. Leijonmarck and O. Tapia
 A Molecular Dynamics Study of the C-terminal Fragment of the L7/L12 Ribosomal Protein
 In: "Molecular Dynamics and Protein Structure", J. Hermans ed., Polycrystal Book Service, P.O. Box 27, Western Springs, Ill. 60558, USA, (1985), pp. 145-147
- 85.09 W.F. van Gunsteren, H.J.C. Berendsen and J.P. Hollenberg
 Prospects for complex molecular systems
Supercomputer **7** (1985) 26-36
- 85.10 R.M. Scheek, E.R.P. Zuiderweg, R. Boelens, W.F. van Gunsteren and R. Kaptein
 The Tertiary Structure of the Lac Repressor Headpiece Derived from Nuclear Magnetic Resonance Spectroscopy
 In: "Magnetic resonance in Biology and Medicine", G. Govil, C.L. Khetrapal, A. Saran eds., McGraw-Hill Publ. Comp., New Delhi, India, (1985), pp. 293-303

- 85.11 P. Kruger, W. Strassburger, A. Wollmer and W.F. van Gunsteren
 A comparison of the structure and dynamics of avian pancreatic polypeptide hormone in solution and in the crystal
Eur. Biophys. J. **13** (1985) 77-88
- 85.12 J.P.M. Postma
 MD of H₂O, a molecular dynamics study of water
 Thesis, University of Groningen, 1985
- 85.13 H.J.C. Berendsen
 Treatment of Long-Range Forces in Molecular Dynamics
 In: "Molecular Dynamics and Protein Structure", J. Hermans ed., Polycrystal Book Service, P.O. Box 27, Western Springs, Ill. 60558, USA, (1985), pp. 18-22
- 85.14 H.J.C. Berendsen
 Molecular Dynamics on Vector Processors and Special-Purpose Computers
 In: "Molecular Dynamics and Protein Structure", J. Hermans ed., Polycrystal Book Service, P.O. Box 27, Western Springs, Ill. 60558, USA, (1985), pp. 123-125
- 85.15 H.J.C. Berendsen
 Simuleren: een gebied met toekomst (in Dutch)
Chemisch Magazine, oktober 1985, 688-690
- 85.16 K. Remerie, W.F. van Gunsteren and J.B.F.N. Engberts
 A molecular dynamics computer simulation study of the hydration of bis(methylsulfonyl)methane in water
Mol. Phys. **56** (1985) 1393-1409
- 85.17 K. Remerie, W.F. van Gunsteren and J.B.F.N. Engberts
 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
Recl. Trav. Chim. Pays-Bas **104** (1985) 79-89
- 85.18 H.J.C. Berendsen, J.P.M. Postma and W.F. van Gunsteren
 Statistical Mechanics and Molecular Dynamics: The Calculation of Free Energy
 In: "Molecular Dynamics and Protein Structure", J. Hermans ed., Polycrystal Book Service, P.O. Box 27, Western Springs, Ill. 60558, USA, (1985), pp. 43-46
- 85.19 H. Kessler, B. Kutscher, R. Kerssebaum, A. Klein, J. Lautz, R. Obermeier, H. Muellner, W.F. van Gunsteren, R. Boelens, R. Kaptein
 Design, synthesis and conformation of superactive thymopoietin-analogues
 In: "Peptides, Structure and Function, Proceedings of the Ninth American Peptide Symposium", C.M. Deber, V.J. Hruby and K.D. Kopple eds., Pierce Chemical, (1985) pp. 83-92
- 1986**
- 86.01 W.F. van Gunsteren
 Ontwerpen van medicijnen en gemodificeerde enzymen met behulp van computersimulatie (in Dutch)
Biotechnologie in Nederland **1** (1986) 13-15
- 86.02 R.G. Geurtzen and J.P. Hollenberg
 Vectorization of the calculation of nonbonded interactions
Supercomputer **11** (1986) 15-25
- 86.03 H.J.C. Berendsen and W.G.J. Hol
 Long-Range Electrostatic Forces
Europhysics News **17** (1986) 8-10

- 86.04 K. Remerie, J.B.F.N. Engberts and W.F. van Gunsteren
 A molecular dynamics computer simulation study of the temperature dependence of hydration of 1,4-dioxane and 1,3-dioxane
Chemical Physics **101** (1986) 27-44
- 86.05 T.P. Straatsma, H.J.C. Berendsen and A.J. Stam
 Estimation of statistical errors in molecular simulation calculations
Mol. Phys. **57** (1986) 89-95
- 86.06 P. Sandblom, J. Åqvist, T.A. Jones, M.E. Newcomer, W.F. van Gunsteren and O. Tapia
 Structural Changes in Retinol Binding Protein Induced by Retinol Removal. A Molecular Dynamics Study
Biochem. and Biophys. Research Comm. **139** (1986) 564-570
- 86.07 H.J.C. Berendsen and W.F. van Gunsteren
 Practical Algorithms for Dynamic Simulations
 In: "Molecular-Dynamics Simulation of Statistical-Mechanical Systems", Proceedings of the International School of Physics "Enrico Fermi", course 97, G. Ciccotti and W.G. Hoover eds., (1986), North-Holland, Amsterdam, pp. 43-65
- 86.08 H.J.C. Berendsen
 Biological Molecules and Membranes
 In: "Molecular-Dynamics Simulation of Statistical-Mechanical Systems", Proceedings of the International School of Physics "Enrico Fermi", course 97, G. Ciccotti and W.G. Hoover eds., (1986), North-Holland, Amsterdam, pp. 496-519
- 86.09 T.P. Straatsma, H.J.C. Berendsen and J.P.M. Postma
 Free energy of hydrophobic hydration: A molecular dynamics study of noble gases in water
J. Chem. Phys. **85** (1986) 6720-6727
- 86.10 J. Åqvist, P. Sandblom, T.A. Jones, M.E. Newcomer, W.F. van Gunsteren and O. Tapia
 Molecular Dynamics Simulations of the Holo and Apo Forms of Retinol Binding Protein Structural and Dynamical Changes Induced by Retinol Removal
J. Mol. Biol. **192** (1986) 593-604
- 86.11 H.J.C. Berendsen, W.F. van Gunsteren, H.R.J. Zwinderman and R.G. Geurtsen
 Simulations of Proteins in Water
Ann. New York Acad. Sci. **482** (1986) 269-285
- 86.12 W.F. van Gunsteren, H.J.C. Berendsen, R.G. Geurtsen and H.R.J. Zwinderman
 A Molecular Dynamics Computer Simulation of an Eight-Base-Pair DNA Fragment in Aqueous Solution: Comparison with Experimental Two-Dimensional NMR Data
Ann. New York Acad. Sci. **482** (1986) 287-303
- 86.13 H.J.C. Berendsen and B. Egberts
 Molecular Dynamics of a Bilayer Membrane with Atomic Detail
 In: Springer Series in Biophysics, Vol. 1, "Structure, Dynamics and Function of Biomolecules", A. Ehrenberg, R. Rigler, A. Graslund, L. Nilsson eds., (1986), Springer, pp. 275-280
- 86.14 J. de Vlieg, R. Boelens, R.M. Scheek, R. Kaptein and W.F. van Gunsteren
 Restrained Molecular Dynamics Procedure for Protein Tertiary Structure Determination from NMR Data: A Lac Repressor Headpiece Structure Based on Information on J-coupling and from Presence and Absence of NOE's
Isr. Journal of Chemistry **27** (1986) 181-188
- 1987**
- 87.01 W.F. van Gunsteren
 Molecular dynamics of proteins and nucleic acids
Fres. Z. Anal. Chem. **327** (1987) 69-70

- 87.02 W.F. van Gunsteren and H.J.C. Berendsen
Thermodynamic cycle integration by computer simulation as a tool for obtaining free energy differences in molecular chemistry
J. Computer-Aided Mol. Design **1** (1987) 171-176
- 87.03 P. Kruger, W. Strassburger, A. Wollmer, W.F. van Gunsteren and G.G. Dodson
The simulated dynamics of the insulin monomer and their relationship to the molecule's structure
Eur. Biophys. J. **14** (1987) 449-459
- 87.04 H.J.C. Berendsen
Biophysical applications of molecular dynamics
Comput Phys. Comm. **44** (1987) 233-242
- 87.05 H.J.C. Berendsen, J.R. Grigera and T.P. Straatsma
The Missing Term in Effective Pair Potentials
J. Phys. Chem. **91** (1987) 6269-6271
- 87.06 J. Koehler, W. Saenger and W.F. van Gunsteren
A molecular dynamics simulation of crystalline α -cyclodextrin hexahydrate
Eur. Biophys. J. **15** (1987) 197-210
- 87.07 J. Koehler, W. Saenger and W.F. van Gunsteren
Molecular dynamics simulation of crystalline β -cyclodextrin dodecahydrate at 293 K and 120 K
Eur. Biophys. J. **15** (1987) 211-224
- 87.08 J. Lautz, H. Kessler, R. Boelens, R. Kaptein and W.F. van Gunsteren
Conformational analysis of a cyclic thymopoietin-analogue by ^1H n.m.r. spectroscopy and restrained molecular dynamics simulations
Int. J. Peptide Protein Res. **30** (1987) 404-414
- 87.09 H.J.C. Berendsen, W.F. van Gunsteren, E. Egberts and J. de Vlieg
Dynamic Simulation of Complex Molecular Systems
ACS Symposium Series 353, "Supercomputer Research in Chemistry and Chemical Engineering", K.F. Jensen and D.G. Truhlar eds., Am. Chem. Soc., Washington D.C., 1987, pp. 106-122
- 87.10 T.P. Straatsma
Free energy evaluation by molecular dynamics simulations
Thesis, University of Groningen, December 1987
- 87.11 P. Kollman and W.F. van Gunsteren
Molecular Mechanics and Dynamics in Protein Design
Methods in Enzymology Vol 154, Recombinant DNA, Part E, R. Wu and L. Grossman eds.,(1987), pp. 430-449 (Academic Press)
- 87.12 J. Lautz, H. Kessler, R. Kaptein and W.F. van Gunsteren
Molecular dynamics simulations of cyclosporin A: The crystal structure and dynamic modelling of a structure in apolar solution based on NMR data
J. Computer-Aided Mol. Design **1** (1987) 219-241
- 87.13 W.F. van Gunsteren, J.E.H. Koehler and W. Saenger
On the Difference between Molecular Conformation and Hydrogen Bonding in Solution and in Crystalline State
Proceedings of the XXXV-th Colloquium Protides of the Biological Fluids, Brussels, April 1987, Pergamon, Oxford, 35 (1987) 489-492

1988

- 88.01 H. Pepermans, D. Tourwe, G. van Binst, R. Boelens, R.M. Scheek, W.F. van Gunsteren and R. Kaptein
The Combined Use of NMR, Distance Geometry, and Restrained Molecular Dynamics for the Conformational Study of a Cyclic Somatostatin Analogue
Biopolymers **27** (1988) 323-338
- 88.02 W.F. van Gunsteren and H.J.C. Berendsen
A leap-frog algorithm for stochastic dynamics
Molecular Simulation **1** (1988) 173-185
- 88.03 W.F. van Gunsteren
The role of computer simulation techniques in protein engineering
Protein Engineering **2** (1988) 5-13
- 88.04 Y.Y. Shi, R.H. Yun and W.F. van Gunsteren
Molecular Dynamics Simulation of Despentapeptide Insulin in a Crystalline Environment
J. Mol. Biol. **200** (1988) 571-577
- 88.05 H. Kessler, C. Griesinger, J. Lautz, A. Mueller, W.F. van Gunsteren and H.J.C. Berendsen
Conformational Dynamics Detected by Nuclear Magnetic Resonance NOE Values and J-Coupling Constants
J.Am.Chem.Soc. **110** (1988) 3393-3396
- 88.06 J. de Vlieg, R.M. Scheek, W.F. van Gunsteren, H.J.C. Berendsen, R. Kaptein and J. Thomason
Combined Procedure of Distance Geometry and Restrained Molecular Dynamics Techniques for Protein Structure Determination From Nuclear Magnetic Resonance Data: Application to the DNA Binding Domain of Lac Repressor From Escherichia Coli
Proteins: Struct. Funct. Genet. **3** (1988) 209-218
- 88.07 J.E.H. Koehler, W. Saenger and W.F. van Gunsteren
On the Occurrence of Three-Center Hydrogen Bonds in Cyclodextrins in Crystalline Form and in Aqueous Solution: Comparison of Neutron Diffraction and Molecular Dynamics Results
J. Biomol. Struct. Dyn. **6** (1988) 181-198
- 88.08 W. Soppe, C. van der Marel, W.F. van Gunsteren and H.W. den Hartog
New insights into the structure of B_2O_3 glass
J. of Non-Crystalline Solids **103** (1988) 201-209
- 88.09 R. Kaptein, R. Boelens, R.M. Scheek and W.F. van Gunsteren
Protein Structures from NMR
Biochemistry **27** (1988) 5389-5395
- 88.10 J.E.H. Koehler, W. Saenger and W.F. van Gunsteren
The flip-flop hydrogen bonding phenomenon Molecular dynamics simulation of crystalline β -cyclodextrin
Eur. Biophys. J. **16** (1988) 153-168
- 88.11 J.E.H. Koehler, W. Saenger and W.F. van Gunsteren
Conformational Differences Between α -Cyclodextrin in Aqueous Solution and in Crystalline Form: A Molecular Dynamics Study
J. Mol. Biol. **203** (1988) 241-250
- 88.12 E. Egberts and H.J.C. Berendsen
Molecular dynamics simulation of a smectic liquid crystal with atomic detail
J. Chem. Phys. **89** (1988) 3718-3732
- 88.13 H.J.C. Berendsen
Dynamic simulation as an essential tool in molecular modeling
J. Computer-Aided Mol. Design **2** (1988) 217-221

- 88.14 Y.Y. Shi, L. Wang and W.F. van Gunsteren
On the approximation of solvent effects on the conformation and dynamics of cyclosporin A by stochastic dynamics simulation techniques
Molecular Simulation **1** (1988) 369-383
- 88.15 W.F. van Gunsteren
Classical molecular dynamics simulations: algorithms and applications, stochastic dynamics, and free energies
In: "Mathematical Frontiers in Computational Chemical Physics", D.G. Truhlar ed., The IMA Volumes in Mathematics and its Applications, Vol. 15 (1988) Springer, New York, pp. 136-156
- 88.16 T.P. Straatsma and H.J.C. Berendsen
Free energy of ionic hydration: Analysis of a thermodynamic integration technique to evaluate free energy differences by molecular dynamics simulations
J. Chem. Phys. **89** (1988) 5876-5886
- 88.17 A.E. Torda, B.C. Mabbott, W.F. van Gunsteren and R.S. Norton
Backbone folding of the polypeptide cardiac stimulant anthopleurin-A determined by nuclear magnetic resonance, distance geometry and molecular dynamics
FEBS Letters **239** (1988) 266-270
- 88.18 E. Egberts
Molecular Dynamics Simulation of Multibilayer Membranes
Thesis, University of Groningen, November 1988
- 1989**
- 89.01 W.F. van Gunsteren
Methods for calculation of free energies and binding constants: Successes and problems
In: "Computer Simulation of Biomolecular Systems, Theoretical and Experimental Applications", W.F. van Gunsteren and P.K. Weiner eds., Escom Science Publishers, Leiden, The Netherlands, (1989), pp. 27-59
- 89.02 M. Fujinaga, P. Gros and W.F. van Gunsteren
Testing the Method of Crystallographic Refinement Using Molecular Dynamics
J. Appl. Cryst. **22** (1989) 1-8
- 89.03 P. Gros, M. Fujinaga, B.W. Dijkstra, K.H. Kalk and W.G.J. Hol
Molecular dynamics refinement of the X-ray structure of thermitase complexed with egin-c
In: "Computer Simulation of Biomolecular Systems, Theoretical and Experimental Applications", W.F. van Gunsteren and P.K. Weiner eds., Escom Science Publishers, Leiden, The Netherlands, (1989), pp. 190-193
- 89.04 A.E. Torda, R.M. Scheek and W.F. van Gunsteren
Time-dependent distance restraints in molecular dynamics simulations
Chem. Phys. Letters **157** (1989) 289-294
- 89.05 J. Lautz, H. Kessler, J.M. Blaney, R.M. Scheek and W.F. van Gunsteren
On calculating three-dimensional molecular structure from atom-atom distance information: cyclosporin A
Int. J. Peptide Protein Res. **33** (1989) 281-288
- 89.06 J. de Vlieg
Molecular Dynamics Computer Simulations based on NMR Data: Application to the DNA binding domain of lac repressor and its operator
Thesis, University of Groningen, May 1989
- 89.07 W.F. van Gunsteren
Computer simulation by molecular dynamics as a tool for modelling of molecular systems
Molecular Simulation **3** (1989) 187-200

- 89.08 M.W. Makinen, J.M. Troyer, H. van der Werff, H.J.C. Berendsen and W.F. van Gunsteren
 Dynamical Structure of Carboxypeptidase A
J. Mol. Biol. **207** (1989) 201-216
- 89.09 P. Gros, M. Fujinaga, A. Mattevi, F.M.D. Vellieux, W.F. van Gunsteren and W.G.J. Hol
 Protein Structure Refinement by Molecular Dynamics Techniques
 In: "Molecular Simulation and Protein Crystallography, Proceedings of the Joint CCP4/CCP5 Study Weekend 27-28 January, 1989, J. Goodfellow, K. Henrick and R. Hubbard eds., SERC, Daresbury, 1989
- 89.10 S.J. Picken, W.F. van Gunsteren, P.Th. van Duijnen and W.H. de Jeu
 A molecular dynamics study of the nematic phase of 4-n-pentyl-4'-cyanobiphenyl
Liquid Crystals **6** (1989) 357-371
- 89.11 J. de Vlieg, H.J.C. Berendsen and W.F. van Gunsteren
 An NMR Based Molecular Dynamics Simulation of the Interaction of the lac Repressor Headpiece and Its Operator in Aqueous Solution
Proteins: Struct. Funct. Genet. **6** (1989) 104-127
- 89.12 P. Gros, M. Fujinaga, B.W. Dijkstra, K.H. Kalk and W.G.J. Hol
 Crystallographic Refinement by Incorporation of Molecular Dynamics: Thermostable Serine Protease Thermitase Complexed with Eglin c
Acta Cryst. B **45** (1989) 488-499
- 89.13 R.M. Scheek, W.F. van Gunsteren and R. Kaptein
 Molecular Dynamics Simulation Techniques for Determination of Molecular Structures from Nuclear Magnetic Resonance Data
 In: Methods in Enzymology, Vol. 177, "Nuclear Magnetic Resonance, Part B: Structure and Mechanism", N.J. Oppenheimer and T.L. James eds., (1989) 204-218 (Academic Press)
- 89.14 J. Lautz, H. Kessler, W.F. van Gunsteren, H.J.C. Berendsen, R.M. Scheek, R. Kaptein and J.M. Blaney
 Restrained Molecular Dynamics Simulations of Cyclic Peptides
 In: "Proceedings of the 20-th European Peptide Symposium (1988)", G. Jung and E. Bayer eds., (1989), pp. 438-440
- 1990**
- 90.01 W.F. van Gunsteren
 On testing theoretical models by comparison of calculated with experimental data
 In: Studies in Physical and Theoretical Chemistry, Vol 71, Modelling of Molecular Structures and Properties, J.-L. Rivail ed., Elsevier, Amsterdam, 1990, pp. 463-478
- 90.02 A.E. Torda, R.M. Scheek and W.F. van Gunsteren
 Time-averaged Nuclear Overhauser Effect Distance Restraints Applied to Tendamistat
J. Mol. Biol. **214** (1990) 223-235
- 90.03 J. Lautz, H. Kessler, W.F. van Gunsteren, H.-P. Weber and R.M. Wenger
 On the Dependence of Molecular Conformation on the Type of Solvent Environment: A Molecular Dynamics Study of Cyclosporin A
Biopolymers **29** (1990) 1669-1687
- 90.04 P. Gros
 Studies in Protein Crystallography & Dynamics: On Membrane Protein Crystallization, the Structure of Thermitase - Eglin and the Application of Molecular Dynamics
 Thesis, University of Groningen, August 1990
- 90.05 P. Gros, W.F. van Gunsteren and W.G.J. Hol
 Inclusion of Thermal Motion in Crystallographic Structures by Restrained Molecular Dynamics
Science **249** (1990) 1149-1152

- 90.06 W.F. van Gunsteren and H.J.C. Berendsen
 Computer Simulation of Molecular Dynamics: Methodology, Applications and Perspectives in Chemistry
Angew. Chem. Int. Ed. Engl. **29** (1990) 992-1023
Angew. Chem. **102** (1990) 1020--1055
- 90.07 J. de Vlieg, H.J.C. Berendsen and W.F. van Gunsteren
 Structure of lac Repressor Headpiece-Operator Complex in Aqueous Solution
 In: "Frontiers in Drug Research", Alfred Benzon Symposium 28, B. Jensen, F.S. Jorgensen, H. Kofod eds., Munksgaard, Copenhagen, (1990), pp. 362-368
- 90.08 O. Nilsson, O. Tapia and W.F. van Gunsteren
 Structure and Fluctuations of Bacteriophage T4 Glutaredoxin Modelled by Molecular Dynamics
Biochem. and Biophys. Research Comm. **171** (1990) 581-588
- 90.09 C.P.M. van Mierlo, P. Lijnzaad, J. Vervoort, F. Mueller, H.J.C. Berendsen and J. de Vlieg
 Tertiary C structure of two-electron reduced *Megasphaera elsdonii* flavodoxin and some implications, as determined by two-dimensional ^1H NMR and restrained molecular dynamics
Eur. J. Biochem. **194** (1991) 185-198
- 1991**
- 91.01 A.E. Torda and W.F. van Gunsteren
 The Refinement of NMR structures by Molecular Dynamics Simulation
Computer Phys. Comm. **62** (1991) 289-296
- 91.02 A.E. Mark, W.F. van Gunsteren and H.J.C. Berendsen
 Calculation of Relative Free Energy via Indirect Pathways
J. Chem. Phys. **94** (1991) 3808-3816
- 91.03 A.E. Mark, H.J.C. Berendsen, A.P. Heiner and W.F. van Gunsteren
 Calculation of Relative Free Energy by Molecular Dynamics
 Proc. 7th Intl. Symp. on "Metabolism and Enzymology of Nucleic Acids including Gene and Protein Engineering", J. Balan, ed., Inst. of Mol. Biol., Slovak Academy of Sciences, Bratislava (1991) pp. 25-38
- 91.04 H.J.C. Berendsen
 Incomplete equilibration: A source of error in free energy calculations
 in: "Proteins: Structure, Dynamics and Design"
 V. Renugopalakrishnan, P.R. Carey, I.C.P. Smith, S.G. Huang and A.C. Storer eds., ESCOM, Leiden (1991) pp. 384-392
- 91.05 H.J.C. Berendsen
 Molecular Dynamic studies of proteins and nucleic acids
Current Opinion in Struct. Biol. **1** (1991) 191-195
- 91.06 H.J.C. Berendsen
 Transport Properties computed by Linear Response through weak coupling to a bath
 in: "Computer Simulation in Materials Science", M. Meyer and V. Pontikis, eds., Kluwer Academic Publishers (1991) pp. 139-155
- 91.07 A.H. Juffer, E.F.F. Botta, B.A.M. van Keulen, A. van der Ploeg and H.J.C. Berendsen
 The Electric Potential of a Macromolecule in a Solvent: A Fundamental Approach
J. Comput. Phys. **97** (1991) 144-171

- 91.08 W.F. van Gunsteren
 Computer Simulation of Biomolecular Systems: Overview of time-saving techniques
 in: "Advances in Biomolecular Simulations", R. Lavery, J.-L. Rivail and J. Smith, eds., 1991, American Inst. of Physics (A.I.P.) Conference Proceedings, Vol. **239**, New York, pp. 131-146
- 91.09 W.F. van Gunsteren, P. Gros, A.E. Torda, H.J.C. Berendsen and R.C. van Schaik
 On deriving spatial structure from NMR or X-ray diffraction data
 In: "Protein Conformation", 1991, Wiley-Interscience, Ciba Foundation Symposium **161**, pp. 150-159
- 91.10 A.E. Mark, H.J.C. Berendsen and W.F. van Gunsteren
 Conformational flexibility of aqueous monomeric and dimeric insulin: A molecular dynamics study
Biochemistry **30** (1991) 10866-10872
- 91.11 J. de Vlieg and W.F. van Gunsteren
 Combined Procedures of Distance Geometry and Molecular Dynamics for Determining Protein Structure from Nuclear Magnetic Resonance Data
 In: "Molecular Design and Modeling: Concepts and Applications, Part A: Proteins, Peptides and Enzymes", J.J. Langone ed., 1991, Academic Press Inc., Methods in Enzymology, Vol. **202**, pp. 268-285
- 91.12 R.M. Scheek, A.E. Torda, J. Kemmink and W.F. van Gunsteren
 Structure Determination by NMR: The Modelling of NMR Parameters as Ensemble Averages
 In: Computational Aspects of the Study of Biological Macromolecules by Nuclear Magnetic Resonance Spectroscopy, J.C. Hoch, F.M. Poulsen and C. Redfield, eds., NATO ASI Series **A225**, Plenum Press, New York, 1991, pp. 209-217
- 91.13 A.E. Torda, R.M. Scheek and W.F. van Gunsteren
 Time Averaged Distance Restraints in NMR based Structural Refinement
 In: Computational Aspects of the Study of Biological Macromolecules by Nuclear Magnetic Resonance Spectroscopy, J.C. Hoch, F.M. Poulsen and C. Redfield, eds., NATO ASI Series **A225**, Plenum Press, New York, 1991, pp. 219-225
- 1992**
- 92.01 W.F. van Gunsteren and A.E. Mark
 On the interpretation of biochemical data by molecular dynamics computer simulation
Eur. J. Biochem. **204** (1992) 947-961
- 92.02 S.P. van Helden
 Structure and Stability of Cyclodextrin Complexes
 thesis, University of Utrecht, April 1992
- 92.03 T. Vorherr, O. Kessler, A. Mark and E. Carafoli
 Construction and molecular dynamics simulation of calmodulin in the extended and in a bent conformation
Eur. J. Biochem. **204** (1992) 931-937
- 92.04 R.C. van Schaik, W.F. van Gunsteren and H.J.C. Berendsen
 Conformational Search by Potential Energy Annealing: Algorithm and Application to Cyclosporin A
J. of Computer-Aided Mol. Design **6** (1992) 97-112

- 92.05 W.F. van Gunsteren
 Molecular Dynamics Simulation in Practice
 in: *Les Cahiers IMABIO*, no. 4, CNRS, April 1992, pp. 27-29
- 92.06 R.M. Spycher, P.M. King and A. Bauder
 Rotational spectrum and structure of a furan-(argon)₂ van der Waals complex
Chem. Phys. Lett. **191** (1992) 102-106
- 92.07 F. Müller-Plathe and W.F. van Gunsteren
 Molecular Simulation of Polymer-Penetrant Systems
Polymer Preprints, ACS, 1992, 633-634
- 92.08 W.F. van Gunsteren, R.M. Brunne, A.E. Mark and S.P. van Helden
 Computer Simulation of Biomolecules: Comparison with Experimental Data
 in: *Molecular Aspects of Biotechnology: Computational Models and Theories*, J. Bertran, ed., NATO ASI Series **C368**, Kluwer Academic Publishers, Dordrecht, 1992, pp. 105-122
- 92.09 A.P. Heiner
 Predictive Aspects of Molecular Dynamics Simulations for Proteins: Application to subtilisin BPN thesis, University of Groningen, August 1992
- 92.10 R.M. Sok, H.J.C. Berendsen and W.F. van Gunsteren
 Molecular Dynamics Simulation of the Transport of Small Molecules across a Polymer Membrane
J. Chem. Phys. **96** (6) (1992) 4699-4704
- 92.11 K.E. Edgecombe, R.O. Esquivel, V.H. Smith, Jr. and F. Müller-Plathe
 Pseudoatoms of the electron density
J. Chem. Phys. **97** (4) (1992) 2593-2599
- 92.12 W.F. van Gunsteren and A.E. Mark
 Prediction of the Activity and Stability Effects of Site-directed Mutagenesis on a Protein Core
J. Mol. Biol. **227** (1992) 389-395
- 92.13 A.E. Mark and W.F. van Gunsteren
 Simulation of the Thermal Denaturation of Hen Egg White Lysozyme: Trapping the Molten Globule State
Biochemistry **31** (34) (1992) 7745-7748
- 92.14 F. Müller-Plathe, S.C. Rogers and W.F. van Gunsteren
 Computational Evidence for Anomalous Diffusion of Small Molecules in Amorphous Polymers
Chem. Phys. Letters **199** (3,4) (1992) 237-243
- 92.15 M.A. Castro, S. Canuto and F. Müller-Plathe
 Many-body-perturbation-theory calculations of the microwave and vibrational constants of CaC
Physical Review A **46** 7 (1992) 4415-4417, The American Physical Society, 1992.
- 92.16 H.J.C. Berendsen, B. Egberts, S.-J. Marrink and P. Ahlström
 Molecular Dynamics Simulations of Phospholipid Membranes and their Interaction with Phospholipase A₂
 in: *Membrane Proteins: Structures, Interactions and Models*, A. Pullman et al. (eds.), Kluwer Academic Publishers, 1992, pp. 457-470
- 92.17 H.J.C. Berendsen
 Rationale for using NMR to study water relations in foods and biological tissues
Trends in Food Science & Technology **3** (1992) 202-205

- 92.18 F. Müller-Plathe, S.C. Rogers and W.F. van Gunsteren
 Diffusion Coefficients of Penetrant Gases in Polyisobutylene Can Be Calculated Correctly by Molecular Dynamics Simulations
Macromolecules **25** (1992) 6722-6724
- 92.19 A.P. Heiner, H.J.C. Berendsen and W.F. van Gunsteren
 MD Simulation of Subtilisin BPN' in a Crystal Environment
Proteins: Struct. Funct. Genet. **14** (1992) 451-464
- 92.20 A.E. Torda and W.F. van Gunsteren
 Molecular Modeling Using Nuclear Magnetic Resonance Data
 in: *Reviews in Computational Chemistry, Volume III*, K.B. Lipkowitz, D.B. Boyd eds., VCH Publishers, Inc.
 New York, 1992, pp. 143-172
- 92.21 A. Gunzinger, U. Müller, W. Scott, B. Bäumle, P. Kohler and W.F. van Gunsteren
 Architecture and Realization of a Multi Signalprocessor System
IEEE Computer Society Press Reprint, Los Alamitos, 1992, pp. 327-340
- 92.22 F. Müller-Plathe, W. Scott and W.F. van Gunsteren
 Molecular Dynamics on Supercomputers: Implementations and Applications
SPEEDUP Journal **6** (1992) 33-38
- 92.23 A. Gunzinger, U.A. Müller, W. Scott, B. Bäumle, P. Kohler, H.R. vonder Mühl,
 F. Müller-Plathe, W.F. van Gunsteren, W. Guggenbühl
 Achieving Super Computer Performance with a DSP Array Processor
IEEE Computer Society Press Reprint, Los Alamitos, 1992, pp. 543-550
- 92.24 S.P. van Helden, B.P. van Eijck, A.E. Mark, W.F. van Gunsteren and L.H.M. Janssen
 Molecular Dynamics and free energy perturbation calculations on complexes of α -cyclodextrins with p-substituted phenols. A comparison between experiment and simulation
 In: "Minutes of the 6th International Symposium on Cyclodextrins", A.R. Hedges ed., Editions de Santé, Paris, (1992), pp. 170-175
- 1993**
- 93.01 A.E. Torda, R.M. Brunne, T. Huber, H. Kessler and W.F. van Gunsteren
 Structure refinement using time-averaged J-coupling constant restraints
J. Biomol. NMR **3** (1993) 55-66
- 93.02 P.M. King, R.M. Spycher and W.F. van Gunsteren
 Structure elucidation from rotation spectra: a penalty function approach
Chem. Phys. Letters **203** (1993) 88-92
- 93.03 P.E. Smith, R.M. Brunne, A.E. Mark and W.F. van Gunsteren
 Dielectric Properties of Trypsin Inhibitor and Lysozyme Calculated from
 Molecular Dynamics Simulations
J. Phys. Chem. **97** (1993) 2009-2014
- 93.04 W.F. van Gunsteren
 Molecular dynamics studies of proteins
Current Opinion in Structural Biology **3** (1993) 277-281
- 93.05 W. Scott, A. Gunzinger, B. Bäumle, P. Kohler, U.A. Müller, H-R. Vonder Mühl, A. Eichenberger,
 W. Guggenbühl, N. Ironmonger, F. Müller-Plathe and W.F. van Gunsteren
 Parallel molecular dynamics on a multi signalprocessor system
Computer Physics Communications **75** (1993) 65-86

- 93.06 A.H. Juffer
On the Modelling of Solvent Mean Force Potentials. From Liquid Argon to Solvated Macromolecules
thesis, University of Groningen, April 1993
- 93.07 Y.Y. Shi, A.E. Mark, C.X. Wang, F. Huang, H.J.C. Berendsen and W.F. van Gunsteren
Can the stability of protein mutants be predicted by free energy calculations ?
Protein Engineering **6** (1993) 289-295
- 93.08 S.T. Jones, P. Ahlström, H.J.C. Berendsen and R.W. Pickersgill
Molecular dynamics simulation of a phospholipase A₂ - substrate complex
Biochimica et Biophysica Acta **1162** (1993) 135-142
- 93.09 K.E. Edgecombe, V.H. Smith, Jr. and F. Müller-Plathe
Nonnuclear Maxima in the Charge Density
Z. Naturforsch. **48a** (1993) 127-133
- 93.10 R.M. Brunne and W.F. van Gunsteren
Dynamical properties of bovine pancreatic trypsin inhibitor from
a molecular dynamics simulation at 5000 atm
FEBS Letters **323** (1993) 215-217
- 93.11 R.M. Brunne, W.F. van Gunsteren, R. Brüschweiler and R.R. Ernst
Molecular Dynamics Simulation of the Proline Conformational Equilibrium
and Dynamics in Antamanide Using the GROMOS Force Field
J. Am. Chem. Soc. **115** (1993) 4764-4768
- 93.12 F. Müller-Plathe, S.C. Rogers and W.F. van Gunsteren
Gas sorption and transport in polyisobutylene: Equilibrium
and nonequilibrium molecular dynamics simulations
J. Chem. Phys. **98** (1993) 9895-9904
- 93.13 T.S. Harvey and W.F. van Gunsteren
The Application of Chemical Shift Calculation to Protein Structure Determination by NMR
Techniques in Protein Chemistry IV (1993), Academic Press, pp. 615-622
- 93.14 P.R. Gerber, A.E. Mark and W.F. van Gunsteren
An approximate but efficient method to calculate free energy trends by computer simulation: Application
to dihydrofolate reductase-inhibitor complexes
J. Computer-Aided Molecular Design **7** (1993) 305-323
- 93.15 A.P. Heiner, H.J.C. Berendsen and W.F. van Gunsteren
Structure prediction of Subtilisin BPN' mutants using molecular dynamics methods
Protein Engineering **6** (1993) 397-408
- 93.16 A.H. Juffer and H.J.C. Berendsen
Dynamic surface boundary conditions. A simple boundary model for molecular dynamics simulations
Mol. Phys. **79** (1993) 623-644
- 93.17 R.M. Brunne, E. Liepinsh, G. Otting, K. Wüthrich and W.F. van Gunsteren
Hydration of Proteins: A Comparison of Experimental Residence Times of Water Molecules Solvating the
Bovine Pancreatic Trypsin Inhibitor with Theoretical Model Calculations
J. Mol. Biol. **231** (1993) 1040-1048
- 93.18 P. Gros and W.F. van Gunsteren
Crystallographic Refinement and Structure-Factor Time-Averaging by Molecular Dynamics in the Absence
of a Physical Force Field
Molecular Simulation **10** (1993) 377-395

- 93.19 C.K. Kuhn and W.F. van Gunsteren
 Dynamics of solitons in polyacetylene in the step-potential model
Solid State Commun. **87** (1993) 203-207
- 93.20 F. Müller-Plathe, L. Laaksonen and W.F. van Gunsteren
 Cooperative effects in the transport of small molecules through an amorphous polymer matrix
J. Mol. Graphics **11** (1993) 118-126
- 93.21 A.R. van Buuren, S.-J. Marrink and H.J.C. Berendsen
 A Molecular Dynamics Study of the Decane/Water Interface
J. Phys. Chem. **97** (1993) 9206-9212
- 93.22 P.E. Smith and W.F. van Gunsteren
 The viscosity of SPC and SPC/E water at 277 and 300K
Chem. Phys. Letters **215** (1993) 315-318
- 93.23 A. Amadei, A.B.M. Linssen and H.J.C. Berendsen
 Essential Dynamics of Proteins
Proteins: Struct. Funct. Genet. **17** (1993) 412-425
- 93.24 S.-J. Marrink, M. Berkowitz and H.J.C. Berendsen
 Molecular Dynamics Simulation of a Membrane/Water Interface:
 The Ordering of Water and Its Relation to the Hydration Force
Langmuir **9** (1993) 3122-3131
- 93.25 F. Müller-Plathe
 YASP: A molecular simulation package
Comput. Phys. Commun. **78** (1993) 77-94
- 93.26 R.C. van Schaik, H.J.C. Berendsen, A.E. Torda and W.F. van Gunsteren
 A Structure Refinement Method Based on Molecular Dynamics in Four Spatial Dimensions
J. Mol. Biol. **234** (1993) 751-762
- 93.27 N. El Tayar, A.E. Mark, P. Vallat, R.M. Brunne, B. Testa and W.F. van Gunsteren
 Solvent-Dependent Conformation and Hydrogen-Bonding Capacity of Cyclosporin A: Evidence From Partition Coefficients and Molecular Dynamics Simulations
J. Med. Chem. **36** (1993) 3757-3764
- 93.28 W.F. van Gunsteren
 Molecular dynamics and stochastic dynamics simulation: A primer
 In: "Computer Simulation of Biomolecular Systems, Theoretical and Experimental Applications", Vol. 2,
 W.F. van Gunsteren, P.K. Weiner, A.J. Wilkinson eds., Escom Science Publishers, Leiden, The Netherlands,
 (1993), pp. 3-36
- 93.29 W.F. van Gunsteren, T.C. Beutler, F. Fraternali, P.M. King, A.E. Mark and P.E. Smith
 Computation of free energy in practice: choice of approximations and accuracy limiting factors
 In: "Computer Simulation of Biomolecular Systems, Theoretical and Experimental Applications", Vol. 2,
 W.F. van Gunsteren, P.K. Weiner, A.J. Wilkinson eds., Escom Science Publishers, Leiden, The Netherlands,
 (1993), pp. 315-348
- 93.30 P.M. King
 Free Energy via molecular simulation: A primer
 In: "Computer Simulation of Biomolecular Systems, Theoretical and Experimental Applications", Vol. 2,
 W.F. van Gunsteren, P.K. Weiner, A.J. Wilkinson eds., Escom Science Publishers, Leiden, The Netherlands,
 (1993), pp. 267-314

- 93.31 P.E. Smith and W.F. van Gunsteren
 Methods for the evaluation of long-range electrostatic forces in computer simulations of molecular systems
 In: "Computer Simulation of Biomolecular Systems, Theoretical and Experimental Applications", Vol. 2,
 W.F. van Gunsteren, P.K. Weiner, A.J. Wilkinson eds., Escom Science Publishers, Leiden, The Netherlands,
 (1993), pp. 182-212
- 93.32 J. Mavri, H.J.C. Berendsen and W.F. van Gunsteren
 Influence of Solvent on Intramolecular Proton Transfer in Hydrogen Malonate. Molecular Dynamics
 Simulation Study of Tunneling by Density Matrix Evolution and Nonequilibrium Solvation
J. Phys. Chem. **97** (1993) 13469-13476
- 93.33 P. Ahlström and H.J.C. Berendsen
 A Molecular Dynamics Study of Lecithin Monolayers
J. Phys. Chem. **97** (1993) 13691-13702
- 93.34 H.J.C. Berendsen and J. Mavri
 Quantum Simulation of Reaction Dynamics by Density Matrix Evolution
J. Phys. Chem. **97** (1993) 13464-13468
- 93.35 H.J.C. Berendsen
 Electrostatic interactions
 In: "Computer Simulation of Biomolecular Systems, Theoretical and Experimental Applications", Vol. 2,
 W.F. van Gunsteren, P.K. Weiner, A.J. Wilkinson eds., Escom Science Publishers, Leiden, The Netherlands,
 (1993), pp. 161-181
- 93.36 H.J.C. Berendsen and S.-J. Marrink
 Molecular dynamics of water transport through membranes: Water from solvent to solute
Pure & Appl. Chem. **65** (1993) 2513-2520
- 93.37 H. Bekker, E.J. Dijkstra and H.J.C. Berendsen
 Molecular Dynamics simulation on an i860 based ring architecture
Supercomputer **54** (1993) 4-10
- 93.38 A.R. van Buuren and H.J.C. Berendsen
 Molecular Dynamics Simulation of the Stability of a 22-Residue α -Helix in Water and 30% Trifluoroethanol
Biopolymers **33** (1993) 1159-1166
- 93.39 H. Bekker, H.J.C. Berendsen, E.J. Dijkstra, S. Achterop, R. v. Drunen, D. v.d. Spoel,
 A. Sijbers, H. Keegstra, B. Reitsma and M.K.R. Renardus
 GROMACS: a Parallel Computer for Molecular Dynamics Simulations
 In: Proceedings of the 4th Intl. Conference Physics Computing '92, R.A. de Groot and J. Nadchal eds.,
 World Scientific Publishing Company, Singapore, 1993, pp. 252-256
- 93.40 H. Bekker, H.J.C. Berendsen, E.J. Dijkstra, S. Achterop, R. v. Drunen, D. v.d. Spoel,
 A. Sijbers, H. Keegstra, B. Reitsma and M.K.R. Renardus
 GROMACS Method of Virial Calculation Using a Single Sum
 In: Proceedings of the 4th Intl. Conference Physics Computing '92, R.A. de Groot and J. Nadchal eds.,
 World Scientific Publishing Company, Singapore, 1993, pp. 257-261
- 1994**
- 94.01 P.E. Smith and W.F. van Gunsteren
 Predictions of free energy differences from a single simulation of the initial state
J. Chem. Phys. **100** (1994) 577-585
- 94.02 T.C. Beutler and W.F. van Gunsteren
 The computation of a potential of mean force: Choice of the biasing
 potential in the umbrella sampling technique
J. Chem. Phys. **100** (1994) 1492-1497

- 94.03 R.C. van Schaik
 Novel Search Algorithms for Biomolecular Structure Refinement
 thesis, University of Groningen, March 1994
- 94.04 E. Egberts, S.-J. Marrink and H.J.C. Berendsen
 Molecular dynamics simulation of a phospholipid membrane
Eur. Biophys. J. **22** (1994) 423-436
- 94.05 P.E. Smith and W.F. van Gunsteren
 Consistent dielectric properties of the simple point charge and extended
 simple point charge water models at 277 and 300 K
J. Chem. Phys. **100** (1994) 3169-3174
- 94.06 P.E. Smith and W.F. van Gunsteren
 Translational and Rotational Diffusion of Proteins
J. Mol. Biol. **236** (1994) 629-636
- 94.07 R. Leenders, W.F. van Gunsteren, H.J.C. Berendsen and A.J.W.G. Visser
 Molecular Dynamics Simulations of Oxidized and Reduced *Clostridium beijerinckii* Flavodoxin
Biophysical Journal **66** (1994) 634-645
- 94.08 X. de la Cruz, A.E. Mark, J. Tormo, I. Fita and W.F. van Gunsteren
 Investigation of Shape Variations in the Antibody Binding Site by
 Molecular Dynamics Computer Simulation
J. Mol. Biol. **236** (1994) 1186-1195
- 94.09 S.R. Billeter, P.M. King and W.F. van Gunsteren
 Can the density maximum of water be found by computer simulation ?
J. Chem. Phys. **100** (1994) 6692-6699
- 94.10 F. Fraternali and W.F. van Gunsteren
 Conformational Transitions of a Dipeptide in Water: Effects of Imposed Pathways
 Using Umbrella Sampling Techniques
Biopolymers **34** (1994) 347-355
- 94.11 T. Mordasini Denti, W.F. van Gunsteren and F. Diederich
 Studies toward computer liquid phase simulations of the solvent-dependency of apolar association strength:
 conformational analysis of a cyclophane-pyrene complex by pseudo Monte Carlo and molecular dynamics
 methods
 In: "Computational Approaches in Supramolecular Chemistry", G. Wipff ed.,
 Kluwer Academic Publishers, The Netherlands, (1994), pp. 11-136
- 94.12 T.C. Beutler, A.E. Mark, R.C. van Schaik, P.R. Gerber and W.F. van Gunsteren
 Avoiding singularities and numerical instabilities in free energy calculations
 based on molecular simulations
Chem. Phys. Letters **222** (1994) 529-539
- 94.13 N.A.J. van Nuland, I.W. Hangyi, R.C. van Schaik, H.J.C. Berendsen,
 W.F. van Gunsteren, R.M. Scheek and G.T. Robillard
 The High-resolution Structure of the Histidine-containing Phosphocarrier Protein HPr
 from *Escherichia coli* Determined by Restrained Molecular Dynamics from
 Nuclear Magnetic Resonance Nuclear Overhauser Effect Data
J. Mol. Biol. **237** (1994) 544-559
- 94.14 W.F. van Gunsteren, F.J. Luque, D. Timms and A.E. Torda
 MOLECULAR MECHANICS IN BIOLOGY: From Structure to Function, Taking Account of Solvation
Ann. Rev. Biophys. Biomol. Structure **23** (1994) 847-863
- 94.15 A.E. Mark and W.F. van Gunsteren
 Decomposition of the Free Energy of a System in Terms of Specific Interactions:
 Implications for Theoretical and Experimental Studies
J. Mol. Biol. **240** (1994) 167-176

- 94.16 A.E. Mark, S.P. van Helden, P.E. Smith, L.H.M. Janssen and W.F. van Gunsteren
Convergence Properties of Free Energy Calculations: α -Cyclodextrin Complexes as a Case Study
J. Am. Chem. Soc. **116** (1994) 6293-6302
- 94.17 A.A. Gusev, F. Müller-Plathe, W.F. van Gunsteren and U.W. Suter
Dynamics of Small Molecules in Bulk Polymers
Adv. Polym. Sci. **116** (1994) 207-247
- 94.18 T.C. Beutler and W.F. van Gunsteren
Molecular dynamics free energy calculation in four dimensions
J. Chem. Phys. **101** (1994) 1417-1422
- 94.19 W. Scott, F. Müller-Plathe and W.F. van Gunsteren
Molecular dynamics study of the mixing and demixing of a binary Lennard-Jones fluid
Mol. Phys. **82** (1994) 1049-1062
- 94.20 F. Müller-Plathe
Permeation of polymers: A computational approach
Acta Polymer **45** (1994) 259-293
- 94.21 J. Mavri and H.J.C. Berendsen
Dynamical simulation of a quantum harmonic oscillator in a noble-gas bath by density-matrix evolution
Phys. Rev. E, **50** (1994) 198-204
- 94.22 A.R. van Buuren and H.J.C. Berendsen
Molecular Dynamics Simulations of Carbohydrate-Based Surfactants in Surfactant/Water/Oil Systems
Langmuir **10** (1994) 1703-1713
- 94.23 A.R. van Buuren and H.J.C. Berendsen
Molecular Dynamics Simulations of Molecular Systems
in: "Crossing Over in Chemistry", A.R. van Buuren ed., Proceedings of the
2nd Annual Advanced Research Workshop, 15-17 January 1994, Eischoll, Switzerland
- 94.24 S.-J. Marrink and H.J.C. Berendsen
Simulation of Water Transport through a Lipid Membrane
J. Phys. Chem. **98** (1994) 4155-4168
- 94.25 J. Mavri and H.J.C. Berendsen
Treatment of nonadiabatic transitions by density matrix evolution and molecular dynamics simulations
J. Molecular Structure **322** (1994) 1-7
- 94.26 W.F. van Gunsteren, R.M. Brunne, P. Gros, R.C. van Schaik, C.A. Schiffer and A.E. Torda
Accounting for Molecular Mobility in Structure Determination Based on Nuclear
Magnetic Resonance Spectroscopic and X-Ray Diffraction Data
in: "Methods in Enzymology: Nuclear Magnetic Resonance", Vol. **239**, T.L. James,
N.J. Oppenheimer eds., Academic Press, New York, (1994), pp. 619-654
- 94.27 C.A. Schiffer, R. Huber, K. Wüthrich and W.F. van Gunsteren
Simultaneous Refinement of the Structure of BPTI Against NMR Data Measured
in Solution and X-ray Diffraction Data Measured in Single Crystals
J. Mol. Biol. **241** (1994) 588-599
- 94.28 F. Müller-Plathe and W.F. van Gunsteren
Can Simple Quantum-Chemical Continuum Models Explain the Gauche Effect in Poly(ethylene oxide)?
Macromolecules **27** (1994) 6040-6045
- 94.29 A.E. Torda and W.F. van Gunsteren
Algorithms For Clustering Molecular Dynamics Configurations
J. Comput. Chem. **15** (1994) 1331-1340
- 94.30 A.P. Nanzer, F.M. Poulsen, W.F. van Gunsteren and A.E. Torda
A Reassessment of the Structure of Chymotrypsin Inhibitor 2 (CI-2)
Using Time-Averaged NMR restraints
Biochemistry **33** (1994) 14503-14511

- 94.31 A. Di Nola, D. Roccatano and H.J.C. Berendsen
 Molecular Dynamics simulation of the docking of substrates to proteins
Proteins: Struct. Funct. Genet. **19** (1994) 174-182
- 94.32 S.J. Marrink
 Permeation of Small Molecules Across Lipid Membranes
 thesis, University of Groningen, November 1994
- 94.33 M. Yoneya and H.J.C. Berendsen
 Molecular Dynamics Simulations of Chiral Nematic Liquid Crystals
J. Phys. Soc. Japan **63** (1994) 1025-1030
- 94.34 J. Mavri, M. Lensink and H.J.C. Berendsen
 Treatment of inelastic collisions of a particle with a quantum harmonic oscillator by density matrix evolution
Mol. Phys. **82** (1994) 1249-1257
- 94.35 F. Müller-Plathe, W. Scott and W.F. van Gunsteren
 PARALLACS: A benchmark for parallel molecular dynamics
Computer Physics Communications **84** (1994) 102-114
- 94.36 I.G. Tironi and W.F. van Gunsteren
 A molecular dynamics simulation study of chloroform
Mol. Phys. **83** (1994) 381-403
- 94.37 R.M. Sok
 Permeation of Small Molecules across a Polymer Membrane: a Computer Simulation Study
 thesis, University of Groningen, November 1994
- 94.38 T. Huber, A.E. Torda and W.F. van Gunsteren
 Local elevation: A method for improving the searching properties of molecular dynamics simulation
J. Comput.-Aided Mol. Design **8** (1994) 695-708
- 94.39 H. Bekker and P. Ahlström
 The Virial of Angle Dependent Potentials in Molecular Dynamics Simulations
Molecular Simulation **13** (1994) 367-374
- 94.40 M. Yoneya, H.J.C. Berendsen and K. Hirasawa
 A Non-Iterative Matrix Method for Constraint Molecular Dynamics Simulations
Molecular Simulation **13** (1994) 395-405
- 94.41 P.E. Smith and W.F. van Gunsteren
 When are Free Energy Components Meaningful?
J. Phys. Chem. **98** (1994) 13735-13740
- 94.42 T.C. Beutler
 Thermodynamic properties derived from molecular dynamics computer simulations:
 Improved methods for the application to biomolecular systems
 thesis, ETH Zürich, December 1994
- 94.43 T.C. Beutler and W.F. van Gunsteren
 Molecular dynamics simulations with first order coupling to a bath of constant chemical potential
Molecular Simulation **14** (1994) 21-34
- 94.44 B.A. Luty, M.E. Davis, I.G. Tironi and W.F. van Gunsteren
 A Comparison of Particle-Particle Particle-Mesh and Ewald Methods for Calculating Electrostatic Interactions in Periodic Molecular Systems
Molecular Simulation **14** (1994) 11-20
- 94.45 F. Müller-Plathe
 How good are molecular local-density methods? Case studies: The quadrupole moment of benzene, geometry and electrostatics of dimethyl sulfoxide, and the conformations of dimethoxy ethane
Brazilian Journal of Physics **24** (1994) 965-976

- 94.46 W.F. van Gunsteren, P.M. King and A.E. Mark
Fundamentals of drug design from a biophysical viewpoint
Quart. Rev. Biophysics **27** (1994) 435-481
- 94.47 P. Ulrich, W. Scott, W.F. van Gunsteren and A.E. Torda
Newtonian Dynamics in Unusual Places: Parameterising a Low Resolution Force Field
In: "Annual Report 1993/1994 of the Competence Center for Computational Chemistry", F. Müller-Plathe and W. Korosec eds., ETH Zürich, Zürich, Switzerland (1994) pp. 17-25
- 1995**
- 95.01 K. Esselink
Large-Scale Simulations of Many-Particles Systems
thesis, University of Groningen, January 1995
- 95.02 C.A. Schiffer, P. Gros and W.F. van Gunsteren
Time-Averaging Crystallographic Refinement: Possibilities and Limitations
Using α -Cyclodextrin as a Test System
Acta Cryst. D **51** (1995) 85-92
- 95.03 C.D. Berweger, W.F. van Gunsteren and F. Müller-Plathe
Force field parametrisation by weak coupling. Re-engineering SPC water
Chem. Phys. Letters **232** (1995) 429-436
- 95.04 H. Liu, F. Müller-Plathe and W.F. van Gunsteren
A molecular dynamics simulation study with a combined quantum mechanical
and molecular mechanical potential energy function: Solvation effects on
the conformational equilibrium of dimethoxyethane
J. Chem. Phys. **102** (1995) 1722-1730
- 95.05 P.E. Smith, R.C. van Schaik, T. Szyperski, K. Wüthrich and W.F. van Gunsteren
Internal Mobility of the Basic Pancreatic Trypsin Inhibitor in Solution:
A Comparison of NMR Spin Relaxation Measurements and Molecular Dynamics Simulations
J. Mol. Biol. **246** (1995) 356-365
- 95.06 T.C. Beutler, D.R. Béguelin and W.F. van Gunsteren
Free energy of cavity formation in solvent: Computational, methodological and physical aspects
J. Chem. Phys. **102** (1995) 3787-3793
- 95.07 P.H. Hünenerger, A.E. Mark and W.F. van Gunsteren
Computational Approaches to Study Protein Unfolding: Hen Egg White Lysozyme as a Case Study
Proteins: Struct. Funct. Genet. **21** (1995) 196-213
- 95.08 A.E. Mark and W.F. van Gunsteren
Free Energy Calculations in Drug Design: A Practical Guide
In: "New Perspectives in Drug Design", Proceedings of the 9th Intl. Roundtable, 11-13 April 1994, Turnberry,
Scotland, P.M. Dean, G. Jolles, C.G. Newton eds., Academic Press Ltd, (1995), pp. 185-200
- 95.09 H. Kovacs, A.E. Mark, J. Johansson and W.F. van Gunsteren
The Effect of Environment on the Stability of an Integral Membrane Helix:
Molecular Dynamics Simulations of Surfactant Protein C in Chloroform, Methanol and Water
J. Mol. Biol. **247** (1995) 808-822
- 95.10 H. Bekker, H.J.C. Berendsen and W.F. van Gunsteren
Force and virial of torsional-angle dependent potentials
J. Comput. Chem. **16** (1995) 527-533
- 95.11 H. Bekker, E.J. Dijkstra, H.J.C. Berendsen and M.K.R. Renardus
An efficient, box shape independent non-bonded force and virial algorithm for Molecular Dynamics
Molecular Simulation **14** (1995) 137-151
- 95.12 H. Liu, F. Müller-Plathe and W.F. van Gunsteren
A Force Field for Liquid Dimethyl Sulfoxide and Physical Properties of Liquid
Dimethyl Sulfoxide Calculated Using Molecular Dynamics Simulation
J. Am. Chem. Soc. **117** (1995) 4363-4366

- 95.13 W.F. van Gunsteren, P.H. Hünenberger, H. Kovacs, A.E. Mark and C.A. Schiffer
 Investigation of protein unfolding and stability by computer simulation
Phil. Trans. R. Soc. Lond. B **348** (1995) 49-59
- 95.14 S.L. Njo, W.F. van Gunsteren and F. Müller-Plathe
 Determination of force field parameters for molecular simulation by molecular simulation:
 An application of the weak-coupling method
J. Chem. Phys. **102** (1995) 6199-6207
- 95.15 I.G. Tironi, R. Sperb, P.E. Smith and W.F. van Gunsteren
 A generalized reaction field method for molecular dynamics simulations
J. Chem. Phys. **102** (1995) 5451-5459
- 95.16 T.C. Beutler and W.F. van Gunsteren
 Umbrella sampling along linear combinations of generalized coordinates.
 Theory and application to a glycine dipeptide
Chem. Phys. Letters **237** (1995) 308-316
- 95.17 P. Ahlström, J. Lausmaa, P. Löfgren and H.J.C. Berendsen
Biomolecules and Phase Boundaries
 Kluwer Academic Publishers, The Netherlands, (1995), pp. 371-379
- 95.18 S.-J. Marrink and M. Berkowitz
 Water and Membranes
 In: "Permeability and stability of lipid bilayers", E. Anibal Disalvo
 and S.A. Simon eds., CRC Press, Inc., (1995), pp. 21-48
- 95.19 D. van der Spoel and H.C.J. Berendsen
 MD simulation, Section 6.5
 In: "Aspects of computational science", A.J. van der Steen ed., Stichting
 Nationale Computer Fac., s-Gravenhage, The Netherlands, (1995), pp. 367-378
- 95.20 A.R. van Buuren
 Characterization of Oil/Water Interfaces:A Molecular Dynamics Study
 thesis, University of Groningen, September 1995
- 95.21 P.C. Jordan, P.J. van Maaren, J. Mavri, D. van der Spoel and H.J.C. Berendsen
 Towards phase transferable potential functions: Methodology and application to nitrogen
J. Chem. Phys. **103** (1995) 2272-2285
- 95.22 C. Bisang, C. Weber, J. Inglis, C.A. Schiffer, W.F. van Gunsteren,
 I. Jelesarov, H.R. Bosshard and J.A. Robinson
 Stabilization of Type-I β -Turn Conformations in Peptides Containing the NPNA-Repeat Motif
 of the *Plasmodium falciparum* Circumsporozoite Protein by Substituting Proline for (*S*)- α -Methylproline
J. Am. Chem. Soc. **117** (1995) 7904-7915
- 95.23 L.J. Smith, A.E. Mark, C.M. Dobson and W.F. van Gunsteren
 Comparison of MD simulations and NMR experiments for hen lysozyme:
 Analysis of local fluctuations, cooperative motions and global changes
Biochemistry **34** (1995) 10918-10931
- 95.24 B.A. Luty, I.G. Tironi and W.F. van Gunsteren
 Lattice-sum Methods for Calculating Electrostatic Interactions in Molecular Simulations
J. Chem. Phys. **103** (1995) 3014-3021
- 95.25 W.F. van Gunsteren, T. Huber and A.E. Torda
 Biomolecular Modelling: Overview of Types of Methods to Search and Sample Conformational Space
 European Conference on Computational Chemistry (E.C.C.C 1), American Institute of Physics
 Conference Proceedings **330** (1995) 253-268
- 95.26 R.M. Brunne, K.D. Berndt, P. Güntert, K. Wüthrich and W.F. van Gunsteren
 Structure and Internal Dynamics of the Bovine Pancreatic Trypsin Inhibitor in
 Aqueous Solution from Long-time Molecular Dynamics Simulations
Proteins: Struct. Funct. Genet. **23** (1995) 49-62

- 95.27 J. Fennen, A.E. Torda and W.F. van Gunsteren
Structure refinement with molecular dynamics and a Boltzmann-weighted ensemble
J. Biomol. NMR **6** (1995) 163-170
- 95.28 F. Müller-Plathe
Unexpected diffusion behaviour of gas molecules in crystalline poly(4-methyl-1-pentene)
J. Chem. Phys. **103** (1995) 4346-4351
- 95.29 W.F. van Gunsteren, P.H. Hünenberger, A.E. Mark, P.E. Smith and I.G. Tironi
Computer simulation of protein motion
Computer Phys. Communications **91** (1995) 305-319
- 95.30 F. Müller-Plathe, H. Liu and W.F. van Gunsteren
Conceptual Hierarchies in Polymer Electrolyte Simulations - From Quantum Chemistry to Molecular Dynamics
Comput. Theor. Polymer Science **5** (1995) 89-98
- 95.31 P.E. Smith and W.F. van Gunsteren
Reaction field effects on the simulated properties of liquid water
Molecular Simulation **15** (1995) 233-245
- 95.32 P.H. Hünenberger, A.E. Mark and W.F. van Gunsteren
Fluctuation and Cross-Correlation Analysis of Protein Motions
Observed in Nanosecond Molecular Dynamics Simulations
J. Mol. Biol. **252** (1995) 492-503
- 95.33 A.P. Nanzer, W.F. van Gunsteren and A.E. Torda
Parametrisation of time-averaged distance restraints in MD simulations
J. Biomol. NMR **6** (1995) 313-320
- 95.34 F. Müller-Plathe and W.F. van Gunsteren
Computer simulation of a polymer electrolyte: Lithium iodide in amorphous poly(ethylene oxide)
J. Chem. Phys. **103** (1995) 4745-4756
- 95.35 W.R.P. Scott and W.F. van Gunsteren
The GROMOS software package for biomolecular simulations
In: "Methods and Techniques in Computational Chemistry: METECC-95", E. Clementi and G. Corongiu eds., STEF, Cagliari, Italy (1995), pp. 397-434
- 95.36 D.G. Green, K.E. Meecham, M. Surridge, F. van Hoesel and H.J.C. Berendsen
Parallelization of molecular dynamics code. GROMOS87 parallelization for distributed memory architectures
In: "Methods and Techniques in Computational Chemistry: METECC-95", E. Clementi and G. Corongiu eds., STEF, Cagliari, Italy (1995), pp. 435-463
- 95.37 A.R. van Buuren, S.J. Marrink and H.J.C. Berendsen
Characterisation of aqueous interfaces with different hydrophobicities by molecular dynamics
Colloids and Surfaces **102** (1995) 143-157
- 95.38 J. Mavri and H.J.C. Berendsen
Calculation of the Proton Transfer Rate Using Density Matrix Evolution
and Molecular Dynamics Simulations: Inclusion of the Proton Excited States
J. Phys. Chem. **99** (1995) 12711-12717
- 95.39 D.M.F. van Aalten, A. Amadei, A.B.M. Linssen, V.G.H. Eijsink, G. Vriend and H.J.C. Berendsen
The Essential Dynamics of Thermolysin: Confirmation of the Hinge-Bending Motion and Comparison
of Simulations in Vacuum and Water
Proteins: Struct. Funct. Genet. **22** (1995) 45-54
- 95.40 H.J.C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Computer Phys. Communications **91** (1995) 43-56

- 95.41 A.R. van Buuren, J. de Vlieg and H.J.C. Berendsen
 Structural Properties of 1,2-Diacyl-*sn*-glycerol in Bulk and
 at the Water Interface by Molecular Dynamics
Langmuir **11** (1995) 2957-2965
- 95.42 A. Amadei, A.B.M. Linssen, B.L. de Groot and H.J.C. Berendsen
 Essential Degrees of Freedom of Proteins
 In: "Modelling of Biomolecular Structures and Mechanisms", A. Pullman
 et al. eds., Kluwer Academic Publishers, The Netherlands, (1995), pp. 85-93
- 95.43 C.A. Schiffer, V. Dötsch, K. Wüthrich and W.F. van Gunsteren
 Exploring the Role of the Solvent in the Denaturation of a Protein: A Molecular Dynamics
 Study of the DNA Binding Domain of the 434 Repressor
Biochemistry **34** (1995) 15057-15067
- 95.44 S.R. Billeter and W.F. van Gunsteren
 A comparison of different numerical propagation schemes for solving the
 time-dependent Schrödinger equation in the position representation
Molecular Simulation **15** (1995) 301-322
- 95.45 A.E. Mark, Y. Xu, H. Liu and W.F. van Gunsteren
 Rapid non-empirical approaches for estimating relative binding free energies
Acta Biochim. Polonica **42** (1995) 525-536
- 95.46 D. van der Spoel and H.J.C. Berendsen
 Determination of proton transfer rate constants using *ab initio*,
 molecular dynamics and density matrix evolution calculations
 In: "Pacific Symposium of Bio-Computing", World Scientific Singapore (1995) 624-637
- 95.47 D.M.F. van Aalten, J.B.C. Findlay, A. Amadei and H.J.C. Berendsen
 Essential dynamics of the cellular retinol-binding protein - evidence for
 ligand-induced conformational changes
Protein Eng. **8** (1995) 1129-1135
- 1996**
- 96.01 H. Liu, F. Müller-Plathe and W.F. van Gunsteren
 Molecular Dynamics with a Quantum-Chemical Potential: Solvent Effects on
 an S_N2 Reaction at Nitrogen
Chem. Eur. J. **2** (1996) 191-195
- 96.02 H.J.C. Berendsen and J. Mavri
 Quantum dynamics simulation of a small quantum system embedded in a classical environment
 In: "Quantum Mechanical Simulation Methods for Studying Biological Systems", Proceedings of Les Houches
 Workshop, 2-7 May, 1995, Les Houches, France, D. Bicout and M. Field eds., Springer-Verlag and Les
 Editions de Physique Les Ulis, France, (1996), pp. 157-179
- 96.03 A. Amadei, M.E.F. Apol, A. Di Nola and H.J.C. Berendsen
 The quasi-Gaussian entropy theory: Free energy calculations based
 on the potential energy distribution function
J. Chem. Phys. **104** (1996) 1560-1574
- 96.04 B.A. Luty and W.F. van Gunsteren
 Calculating Electrostatic Interactions Using the Particle-Particle Particle-Mesh
 Method with Nonperiodic Long-Range Interactions
J. Phys. Chem. **100** (1996) 2581-2587
- 96.05 T.C. Beutler, T. Bremi, R.R. Ernst and W.F. van Gunsteren
 Motion and Conformation of Side Chains in Peptides. A Comparison
 of 2D Umbrella-Sampling Molecular Dynamics and NMR Results
J. Phys. Chem. **100** (1996) 2637-2645
- 96.06 F. Müller-Plathe
 Simulation grosser Systeme. Trendbericht Theoretische Chemie 1996
Nachr. Chem. Techn. Lab. **44** (1996) 188-190

- 96.07 I.G. Tironi, R.M. Brunne and W.F. van Gunsteren
 On the relative merits of flexible versus rigid models for use
 in computer simulations of molecular liquids
Chem. Phys. Letters **250** (1996) 19-24
- 96.08 F. Fraternali and W.F. van Gunsteren
 An Efficient Mean Solvation Force Model for Use in Molecular Dynamics
 Simulations of Proteins in Aqueous Solution
J. Mol. Biol. **256** (1996) 939-948
- 96.09 J.J. Lopéz Cascales, J. Garcia de la Torre, S.J. Marrink and H.J.C. Berendsen
 Molecular dynamics simulation of a charged biological membrane
J. Chem. Phys. **104** (1996) 2713-2720
- 96.10 T.Z. Mordasini Denti, T.C. Beutler, W.F. van Gunsteren and F. Diederich
 Computation of Gibbs Free Energies of Hydration for Simple Aromatic Molecules:
 A Comparative Study Using Monte Carlo and Molecular Dynamics Computer Simulation Techniques
J. Phys. Chem. **100** (1996) 4256-4260
- 96.11 F. Müller-Plathe
 Solvent dynamics in swollen polymers
Chem. Phys. Letters **252** (1996) 419-424
- 96.12 M.E.F. Apol, A. Amadei and H.J.C. Berendsen
 Application of the quasi-Gaussian entropy theory to the calculation of thermodynamic properties of water
 and methane in the liquid and gas phase
J. Chem. Phys. **104** (1996) 6665-6678
- 96.13 H. Bekker
 Molecular Dynamics Simulation Methods Revised
 thesis, University of Groningen, June 1996
- 96.14 W.F. van Gunsteren, A.P. Nanzer and A.E. Torda
 Molecular simulation methods for generating ensembles or trajectories consistent with experimental data
 In: "Monte Carlo and Molecular Dynamics of Condensed Matter Systems", Proceedings of the
 Euroconference, 3-28 July 1995, Como, Italy, Vol. **49**, K. Binder and G. Ciccotti eds., SIF, Bologna, Italy, (1996),
 pp. 777-788
- 96.15 H. Liu, A.E. Mark and W.F. van Gunsteren
 Estimating the Relative Free Energy of Different Molecular States
 with Respect to a Single Reference State
J. Phys. Chem. **100** (1996) 9485-9494
- 96.16 H.J.C. Berendsen and J. Mavri
 Approach to Nonadiabatic Transitions by Density Matrix Evolution
 and Molecular Dynamics Simulations
Int. J. Quantum Chem. **57** (1996) 965-983
- 96.17 D. van der Spoel, H.J. Vogel and H.J.C. Berendsen
 Molecular Dynamics Simulations of N-Terminal Peptides From a Nucleotide Binding Protein
Proteins: Struct. Funct. Genet. **24** (1996) 450-466
- 96.18 A.R. van Buuren, D.P. Tielemans, J. de Vlieg and H.J.C. Berendsen
 Cosurfactants Lower Surface Tension of the Diglyceride/Water Interface:
 A Molecular Dynamics Study
Langmuir **12** (1996) 2570-2579
- 96.19 H.J.C. Berendsen
 Bio-Molecular Dynamics Comes of Age
Science **271** (1996) 954-955

- 96.20 A. Amadei, A.B.M. Linssen, B.L. de Groot, D.M.F. van Aalten and H.J.C. Berendsen
 An Efficient Method for Sampling the Essential Subspace of Proteins
J. Biomol. Structure & Dynamics **13** (1996) 615-625
- 96.21 B.L. de Groot, A. Amadei, D.M.F. van Aalten and H.J.C. Berendsen
 Towards an Exhaustive Sampling of the Configurational Spaces of the Two Forms of the Peptide Hormone Guanylin
J. Biomol. Structure & Dynamics **13** (1996) 741-751
- 96.22 S.J. Marrink, R.M. Sok and H.J.C. Berendsen
 Free volume properties of a simulated lipid membrane
J. Chem. Phys. **104** (1996) 9090-9099
- 96.23 J.J. Lopéz Cascales, H.J.C. Berendsen and J. Garcia de la Torre
 Molecular Dynamics Simulation of Water between Two Charged Layers of Dipalmitoyl-phosphatidylserine
J. Phys. Chem. **100** (1996) 8621-8627
- 96.24 T.Z. Mordasini Denti, W.F. van Gunsteren and F. Diederich
 Computer Simulations of the Solvent Dependence of Apolar Association Strength: Gibbs Free Energy Calculations on a Cyclophane-Pyrene Complex in Water and Chloroform
J. Am. Chem. Soc. **118** (1996) 6044-6051
- 96.25 F. Müller-Plathe
 Local Structure and Dynamics in Solvent-Swollen Polymers
Macromolecules **29** (1996) 4782-4791
- 96.26 T. Huber, A.E. Torda and W.F. van Gunsteren
 Optimization Methods for Conformational Sampling Using a Boltzmann-Weighted Mean Field Approach
Biopolymers **39** (1996) 103-114
- 96.27 X. Daura, P.H. Hünenberger, A.E. Mark, E. Querol, F.X. Avilés and W.F. van Gunsteren
 Free Energies of Transfer of Trp Analogs from Chloroform to Water: Comparison of Theory and Experiment and the Importance of Adequate Treatment of Electrostatic and Internal Interactions
J. Am. Chem. Soc. **118** (1996) 6285-6294
- 96.28 H. Liu, F. Müller-Plathe and W.F. van Gunsteren
 A Combined Quantum/Classical Molecular Dynamics Study of the Catalytic Mechanism of HIV-Protease
J. Mol. Biol. **261** (1996) 454-469
- 96.29 C.A. Schiffer and W.F. van Gunsteren
 Structural Stability of Disulfide Mutants of Basic Pancreatic Trypsin Inhibitor: A Molecular Dynamics Study
Proteins: Struct. Funct. Genet. **26** (1996) 66-71
- 96.30 M.E.F. Apol, A. Amadei and H.J.C. Berendsen
 Derivation of a thermodynamic closure relation in the isothermal-isobaric ensemble using quasi-Gaussian entropy theory
Chem. Phys. Letters **256** (1996) 172-178
- 96.31 S.J. Marrink, F. Jähnig and H.J.C. Berendsen
 Proton Transport across Transient Single-Fit Water Pores in a Lipid Membrane Studied by Molecular Dynamics Simulations
Biophys. J. **71** (1996) 632-647
- 96.32 F. Müller-Plathe
 An All-atom Force Field for Liquid Ethanol - Properties of Ethanol-Water Mixtures
Molecular Simulation **18** (1996) 133-143
- 96.33 I.G. Tironi, P. Fontana and W.F. van Gunsteren
 A molecular dynamics simulation study of liquid carbon tetrachloride
Mol. Simulation **18** (1996) 1-11

- 96.34 S.J. Marrink and H.J.C. Berendsen
 Permeation Process of Small Molecules across Lipid Membranes Studied
 by Molecular Dynamics Simulations
J. Phys. Chem. **100** (1996) 16729-16738
- 96.35 D.P. Tieleman and H.J.C. Berendsen
 Molecular dynamics simulations of a fully hydrated dipalmitoylphosphatidylcholine bilayer with different
 macroscopic boundary conditions and parameters
J. Chem. Phys. **105** (1996) 4871-4880
- 96.36 B.L. de Groot, D.M.F. van Aalten, A. Amadei and H.J.C. Berendsen
 The Consistency of Large Concerted Motions in Proteins in Molecular Dynamics Simulations
Biophysical Journal **71** (1996) 1707-1713
- 96.37 A. Amadei, D. Roccatano, M.E.F. Apol, H.J.C. Berendsen and A. Di Nola
 Prediction of the liquid-vapor equilibrium pressure using the quasi-Gaussian entropy theory
J. Chem. Phys. **105** (1996) 7022-7025
- 96.38 D. van der Spoel, A.R. van Buuren, D.P. Tieleman and H.J.C. Berendsen
 Molecular dynamics simulations of peptides from BPTI: A closer look at amide-aromatic interactions
J. Biomol. NMR **8** (1996) 229-238
- 96.39 A.P. Nanzer, T. Huber, A.E. Torda and W.F. van Gunsteren
 Molecular dynamics simulation using weak-coupling NOE distance restraining
J. Biomol. NMR **8** (1996) 285-291
- 96.40 W.F. van Gunsteren, S.R. Billeter, A.A. Eising, P.H. Hünenberger, P. Krüger,
 A.E. Mark, W.R.P. Scott, I.G. Tironi
Biomolecular Simulation: The GROMOS96 Manual and User Guide
 Vdf Hochschulverlag AG an der ETH Zürich, Zürich, Switzerland (1996) pp. 1-1042
- 96.41 P.R. Ulrich
 Development of a novel protein structure prediction force field
 thesis, ETH Zürich, November 1996
- 96.42 J.W. Peng, C.A. Schiffer, P. Xu, W.F. van Gunsteren and R.R. Ernst
 Investigations of peptide hydration using NMR and molecular dynamics simulations:
 A study of effects of water on the conformation and dynamics of antamanide
J. Biomol. NMR **8** (1996) 453-476
- 96.43 B.L. de Groot, A. Amadei, R.M. Scheek, N.A.J. van Nuland and H.J.C. Berendsen
 An Extended Sampling of the Configurational Space of HPr from *E. coli*
Proteins: Struct. Funct. Genet. **26** (1996) 314-322
- 96.44 D. van der Spoel, B.L. de Groot, S. Hayward, H.J.C. Berendsen and H.J. Vogel
 Bending of the calmodulin central helix: A theoretical study
Protein Science **5** (1996) 2044-2053
- 96.45 D. van der Spoel, K.A. Feenstra, M.A. Hemminga and H.J.C. Berendsen
 Molecular Modeling of the RNA Binding N-Terminal Part of Cowpea Chlorotic
 Mottle Virus Coat Protein in Solution with Phosphate Ions
Biophys. J. **71** (1996) 2920-2932
- 96.46 D. van der Spoel
 Structure and Dynamics of Peptides: Theoretical Aspects of Protein Folding
 thesis, University of Groningen, The Netherlands, December 1996
- 96.47 P. Lijnzaad, H.J.C. Berendsen and P. Argos
 Hydrophobic Patches on the Surfaces of Protein Structures
Proteins: Struct. Funct. Genet. **25** (1996) 389-397
- 96.48 P. Lijnzaad, H.J.C. Berendsen and P. Argos
 A Method for Detecting Hydrophobic Patches on Protein Surfaces
Proteins: Struct. Funct. Genet. **26** (1996) 192-203

- 96.49 A.P. Nanzer
 Molecular dynamics simulations to determine structure and dynamics of biomolecules using nuclear magnetic resonance data
 thesis, ETH Zürich, July 1996
- 96.50 A.C. Bach, II, S.X. Tang, J.R. Espina, P.F.W. Stouten, W.F. deGrado, J. Fennen, A.E. Torda, A.P. Nanzer and W.F. van Gunsteren
 Restrained molecular dynamics of RGD-containing cyclic peptides using time-averaged NOEs
 In: "Peptides: Chemistry, Structure and Biology", Proceedings of the 14th American Peptide Symposium, 18-23 June 1995, Columbus, Ohio, USA, P.T.P. Kaumaya and R.S. Hodges eds., Mayflower Scientific Ltd., England, (1996) pp. 489-490
- 96.51 M.F. Lensink, J. Mavri and H.J.C. Berendsen
 Simultaneous Integration of Mixed Quantum-Classical Systems by Density Matrix Evolution Equations Using Interaction Representation and Adaptive Time Step Integrator
J. Comp. Chem. **17** (1996) 1287-1295
- 96.52 D.M.F. van Aalten, A. Amadei, R. Bywater, J.B.C. Findlay, H.J.C. Berendsen, C. Sander and P.F.W. Stouten
 A Comparison of Structural and Dynamic Properties of Different Simulation Methods Applied to SH3
Biophys. J. **70** (1996) 684-692
- 1997**
- 97.01 I.G. Tironi
 Treatment of electrostatic interactions in molecular systems: development of methodology and application to liquids
 thesis, ETH Zürich, January 1997
- 97.02 P.H. Hünenberger
 Molecular dynamics simulations using empirical force fields: Principles and applications to selected systems of chemical and biochemical interest
 thesis, ETH Zürich, January 1997
- 97.03 A. Amadei, M.E.F. Apol and H.J.C. Berendsen
 Extensions of the quasi-Gaussian entropy theory
J. Chem. Phys. **106** (1997) 1893-1912
- 97.04 F. Müller-Plathe
 Combining quantum chemistry and molecular simulation
 In: "Advances in Quantum Chemistry", Vol 28, P.O. Löwdin, J.R. Sabin and M.C. Zerner eds., Academic Press, New York (1997) pp. 81-87
- 97.05 P. Ulrich, W.R.P. Scott, W.F. van Gunsteren and A.E. Torda
 Protein Structure Prediction Force Fields: Parametrization With Quasi-Newtonian Dynamics
Proteins: Struct. Funct. Genet. **27** (1997) 367-384
- 97.06 H. Kovacs, A.E. Mark and W.F. van Gunsteren
 Solvent Structure at a Hydrophobic Protein Surface
Proteins: Struct. Funct. Genet. **27** (1997) 395-404
- 97.07 S. Hayward, A. Kitao and H.J.C. Berendsen
 Model-Free Methods of Analyzing Domain Motions in Proteins From Simulation: A Comparison of Normal Mode Analysis and Molecular Dynamics Simulation of Lysozyme
Proteins: Struct. Funct. Genet. **27** (1997) 425-437
- 97.08 A.P. Nanzer, A.E. Torda, C. Bisang, C. Weber, J.A. Robinson and W.F. van Gunsteren
 Dynamical Studies of Peptide Motifs in the *Plasmodium falciparum* Circumsporozoite Surface Protein by Restrained and Unrestrained MD Simulations
J. Mol. Biol. **267** (1997) 1012-1025
- 97.09 I.G Tironi, B.A. Luty and W.F. van Gunsteren
 Space-time correlated reaction field: A stochastic dynamical approach to the dielectric continuum
J. Chem. Phys. **106** (1997) 6068-6075

- 97.10 U. Röthlisberger and M. Parrinello
Ab initio molecular dynamics simulation of liquid hydrogen fluoride
J. Chem. Phys. **106** (1997) 4658-4664
- 97.11 F. Müller-Plathe and W.F. van Gunsteren
Solvation of poly(vinyl alcohol) in water, ethanol and an equimolar water-ethanol mixture: structure and dynamics studied by molecular dynamics simulation
Polymer **38** (1997) 2259-2268
- 97.12 T.L. Huber
Searching and sampling methods for biomolecular modelling
thesis, ETH Zürich, May 1997
- 97.13 M. Sprik, U. Röthlisberger and M.L. Klein
Structure of Solid Poly(tetrafluoroethylene): A Computer Simulation Study of Chain Orientational, Translational, and Conformational Disorder
J. Phys. Chem. B **101** (1997) 2745-2749
- 97.14 D.M.F. van Aalten, B.L. de Groot, J.B.C. Findlay, H.J.C. Berendsen and A. Amadei
A Comparison of Techniques for Calculating Protein Essential Dynamics
J. Comp. Chem. **18** (1997) 169-181
- 97.15 D. van der Spoel and H.J.C. Berendsen
Molecular Dynamics Simulations of Leu-Enkephalin in Water and DMSO
Biophys. J. **72** (1997) 2032-2041
- 97.16 M.E.F. Apol
The Quasi-Gaussian Entropy Theory
thesis, University of Groningen, June 1997
- 97.17 F.A. Hamprecht, W.R.P. Scott and W.F. van Gunsteren
Generation of Pseudonative Protein Structures for Threading Proteins:
Struct. Funct. Genet. **28** (1997) 522-529
- 97.18 W.F. van Gunsteren and A.E. Mark
Computational Chemistry: Abschied vom Experiment?
ETH-Bulletin **266** (1997) 18-19
- 97.19 P.H. Hünenberger, J.K. Granwehr, J.-N. Aebscher, N. Ghoneim, E. Haselbach and W.F. van Gunsteren
Experimental and Theoretical Approach to Hydrogen-Bonded Diastereomeric Interactions in a Model Complex
J. Am. Chem. Soc. **119** (1997) 7533-7544
- 97.20 T. Huber, A.E. Torda and W.F. van Gunsteren
Structure Optimisation Combining Soft-Core Interaction Functions, the Diffusion Equation Method and Molecular Dynamics
J. Phys. Chem. **101** (1997) 5926-5930
- 97.21 X. Daura, W.F. van Gunsteren, D. Rigo, B. Jaun and D. Seebach
Studying the Stability of a Helical β -Heptapeptide by Molecular Dynamics Simulations
Chemistry - a European Journal **3** (1997) 1410-1417
- 97.22 C.D. Berweger, W.F. van Gunsteren and F. Müller-Plathe
Finite Element Interpolation for Combined Classical/Quantum Mechanical Molecular Dynamics Simulations
J. Comput. Chemistry **18** (1997) 1484-1495
- 97.23 B. Hess, H. Bekker, H.J.C. Berendsen and J.G.E.M. Fraaije
LINCS: A Linear Constraint Solver for Molecular Simulations
J. Comput. Chem. **18** (1997) 1463-1472

- 97.24 T. Nezel, F. Müller-Plathe, M.D. Müller and H.R. Buser
 Theoretical Considerations about chiral PCBs and their Methylthio and Methylsulfonyl Metabolites being possibly present as stable Enantiomers
Chemosphere **35** (1997) 1895-1906
- 97.25 P.H. Hünenberger and W.F. van Gunsteren
 Empirical classical interaction functions for molecular simulation
 In: "Computer Simulation of Biomolecular Systems, Theoretical and Experimental Applications", Vol. **3**, W.F. van Gunsteren, P.K. Weiner, A.J. Wilkinson eds., Kluwer Academic Publishers, Dordrecht, The Netherlands, (1997), pp. 3-82
- 97.26 S.R. Billeter and W.F. van Gunsteren
 A modular molecular dynamics/quantum dynamics program for non-adiabatic proton transfers in solution
Comp. Phys. Comm. **107** (1997) 61-91
- 97.27 B.L. de Groot, D.M.F. van Aalten, R.M. Scheek, A. Amadei, G. Vriend and H.J.C. Berendsen
 Prediction of Protein Conformational Freedom From Distance Constraints
Proteins: Struct. Funct. Genet. **29** (1997) 240-251
- 97.28 H.J.C. Berendsen and J. Mavri
 Simulating Proton Transfer Processes: Quantum Dynamics Embedded in a Classical Environment
 In: "Theoretical Treatmens of Hydrogen Bonding", D. Hadzi (ed.), Wiley (1997) pp. 119-141
- 97.29 K. Park and W.F. van Gunsteren
 Parameter Optimization for Calculation of Proton Chemical Shift in Protein
J. of Korean Mag. Res. Soc. **1** (1997) 71-78
- 97.30 K. Park and W.F. van Gunsteren
 Solution Structure of Bovine Pancreatic Trypsin Inhibitor using NMR Chemical Shift Restraints
J. of Korean Mag. Res. Soc. **1** (1997) 79-94
- 97.31 D.P. Tieleman, S.J. Marrink and H.J.C. Berendsen
 A computer perspective of membranes: molecular dynamics studies of lipid bilayer systems
Biochim. Biophys. Acta, Reviews on Membranes **1331** (1997) 235-270
- 97.32 D.M.F. Van Aalten, D.A. Conn, B.L. De Groot, H.J.C. Berendsen, J.B.C. Findlay and A. Amadei
 Protein dynamics derived from clusters of crystal structures
Biophys. J. **73** (1997) 2891-2896
- 97.33 M. Lauterbach, G. Wipff, A.E. Mark and W.F. van Gunsteren
 Liquid-Liquid ion extraction: Influence of the water content of the organic phase on the ion extraction selectivity. An MD and FEP study of calix[4]crown-6 alkali cation complexes in binary chloroform-water mixtures
Gazzetta Chimica Italiana, **127** (1997) 669-708
- 1998**
- 98.01 W.R.P. Scott
 Molecular Dynamics Simulation of Biomolecules. Software Engineering, Parallelisation and Methodology
 thesis, ETH Zürich, March 1998
- 98.02 X. Daura, A.E. Mark and W.F. van Gunsteren
 Parametrization of Aliphatic CH_n United Atoms of GROMOS96 Force Field
J. Comput. Chem. **19** (1998) 535-547
- 98.03 W.F. van Gunsteren and A.E. Mark
 Validation of molecular dynamics simulation
J. Chem. Phys. **108** (1998) 6109-6116
- 98.04 P.H. Hünenberger and W.F. van Gunsteren
 Alternative schemes for the inclusion of a reaction-field correction into molecular dynamics simulations: Influence on the simulated energetic, structural and dielectric properties of liquid water
J. Chem. Phys. **108** (1998) 6117-6134

- 98.05 U. Röthlisberger, M. Sprik and M.L. Klein
 Living polymers: *Ab initio* molecular dynamics study of the initiation step in the polymerization of isoprene induced by ethyl lithium
J. Chem. Soc., Faraday Trans. **94** (1998) 501-508
- 98.06 W.F. van Gunsteren, H. Liu and F. Müller-Plathe
 The elucidation of enzymatic reaction mechanisms by computer simulation:
 Human Immunodeficiency Virus protease catalysis
J. Mol. Structure (Theochem) **432** (1998) 9-14
- 98.07 C.D. Berweger, W.F. van Gunsteren and F. Müller-Plathe
 Molecular dynamics simulation with an *ab initio* potential energy function and finite element interpolation:
 The photoisomerization of *cis*-stilbene in solution
J. Chem. Phys. **108** (1998) 8773-8781
- 98.08 S.R. Billeter and W.F. van Gunsteren
 Protonizable Water Model for Quantum Dynamical Simulations
J. Phys. Chem. A **102** (1998) 4669-4678
- 98.09 D. van der Spoel, P.J. van Maaren and H.J.C. Berendsen
 A systematic study of water models for molecular simulation: Derivation of water models optimized for use with a reaction field
J. Chem. Phys. **108** (1998) 10220-10230
- 98.10 T. Huber and W.F. van Gunsteren
 SWARM-MD: Searching Conformational Space by Cooperative Molecular Dynamics
J. Phys. Chem. A **102** (1998) 5937-5943
- 98.11 X. Daura, B. Jaun, D. Seebach, W.F. van Gunsteren and A.E. Mark
 Reversible Peptide Folding in Solution by Molecular Dynamics Simulation
J. Mol. Biol. **280** (1998) 925-932
- 98.12 L.J. Smith, A.E. Mark, C.M. Dobson and W.F. van Gunsteren
 Molecular Dynamics Simulations of Peptide Fragments from Hen Lysozyme:
 Insight into Non-native Protein Conformations
J. Mol. Biol. **280** (1998) 703-719
- 98.13 A.M.J.J. Bonvin, M. Sunnerhagen, G. Otting and W.F. van Gunsteren
 Water Molecules in DNA Recognition II: A Molecular Dynamics View of the Structure and Hydration of the *trp* Operator
J. Mol. Biol. **282** (1998) 859-873
- 98.14 M. Sunnerhagen, V.P. Denisov, K. Venu, A.M.J.J. Bonvin, J. Carey, B. Halle and G. Otting
 Water Molecules in DNA Recognition I: Hydration Lifetimes of *trp* Operator DNA in Solution Measured by NMR Spectroscopy
J. Mol. Biol. **282** (1998) 847-858
- 98.15 D. Roccatano, A. Amadei, M.E.F. Apol, A. Di Nola and H.J.C. Berendsen
 Application of the quasi-Gaussian entropy theory to molecular dynamics simulations of Lennard-Jones fluids
J. Chem. Phys. **109** (1998) 6358-6363
- 98.16 S. Billeter
 Quantum dynamical simulation of non-adiabatic proton transfers in aqueous solution: methodology, molecular models and applications
 thesis, ETH Zürich, July 1998
- 98.17 W.R.P. Scott, A.E. Mark and W.F. van Gunsteren
 On using time-averaging restraints in molecular dynamics simulation
J. Biomol. NMR **12** (1998) 501-508
- 98.18 P. Tieleman
 Theoretical studies of membrane models: Molecular dynamics of water, lipids and membrane proteins
 thesis, University of Groningen, December 1998

- 98.19 A. Mark
 Free energy perturbation calculations
 In: "Encyclopaedia of Computational Chemistry", Vol. 2, P. von Ragué Schleyer, N.L. Allinger, T. Clark, J. Gasteiger, P.A. Kollman, H.F. Schaefer III, P.R. Schreiner (eds.), Wiley & Sons, Chichester, 1998, pp. 1070-1083
- 98.20 W.F. van Gunsteren, X. Daura and A.E. Mark
 GROMOS force field
 In: "Encyclopaedia of Computational Chemistry", Vol. 2, P. von Ragué Schleyer, N.L. Allinger, T. Clark, J. Gasteiger, P.A. Kollman, H.F. Schaefer III, P.R. Schreiner (eds.), Wiley & Sons, Chichester, 1998, pp. 1211-1216
- 98.21 L.D. Creveld, A. Amadei, R.C. van Schaik, H.A.M. Pepermans, J. de Vlieg and H.J.C. Berendsen
 Identification of Functional and Unfolding Motions of Cutinase as Obtained From Molecular Dynamics Computer Simulations
Proteins: Struct. Funct. Genet. **33** (1998) 253-264
- 98.22 B. van Vlimmeren
 Mesoscopic Dynamics
 thesis, Univ. of Groningen, The Netherlands, September 1998
- 98.23 A. Amadei
 Theoretical models for fluid thermodynamics based on the quasi-Gaussian entropy theory
 thesis, Univ. of Groningen, The Netherlands, November 1998
- 98.24 T. Linssen
 Molecular Dynamics Simulations of Haloalkane Dehalogenase
 thesis, Univ. of Groningen, The Netherlands, November 1998
- 1999**
- 99.01 P.H. Hünenberger and W.F. van Gunsteren
 Empirical Classical Force Fields for Molecular Systems
 In: "Potential Energy Surfaces", Proceedings of the Mariapfarr Workshop in Theoretical Chemistry, A.F. Sax ed., Springer-Verlag Berlin, 1999, pp. 178-214
- 99.02 A.E. Mark, H. Schäfer, H. Liu and W.F. van Gunsteren
 Estimating Relative Free Energies from a Single Simulation of the Initial State
 In: "Computational Molecular Dynamics: Challenges, Methods, Ideas", Proceedings of the 2nd Intl. Symp. on Algorithms for Macromol. Mod., P. Deuflhard, J. Hermans, B. Leimkuhler, A.E. Mark, S. Reich, R.D. Skeel (eds.), Springer-Verlag Berlin, 1999, pp. 149-162
- 99.03 X. Daura, K. Gademann, B. Jaun, D. Seebach, W.F. van Gunsteren and A.E. Mark
 Peptide Folding: When Simulation Meets Experiment
Angew. Chemie Intl. Ed. **38** (1999) 236-240
Angew. Chem. **111** (1999) 249-253
- 99.04 X. Daura, R. Suter and W.F. van Gunsteren
 Validation of molecular simulation by comparison with experiment: Rotational reorientation of tryptophan in water
J. Chem. Phys. **110** (1999) 3049-3055
- 99.05 X. Daura, W.F. van Gunsteren and A.E. Mark
 Folding-Unfolding Thermodynamics of a β -Heptapeptide From Equilibrium Simulations
Proteins: Struct. Funct. Genet. **34** (1999) 269-280
- 99.06 L.J. Smith, C.M. Dobson and W.F. van Gunsteren
 Side-chain Conformational Disorder in a Molten Globule: Molecular Dynamics Simulations of the A-state of Human α -lactalbumin
J. Mol. Biol. **286** (1999) 1567-1580
- 99.07 R. Walser, A.E. Mark and W.F. van Gunsteren
 On the validity of Stokes' law at the molecular level
Chem. Phys. Letters **303** (1999) 583-586

- 99.08 S. Portmann, J.M. Galbraith, H.F. Schaefer, G.E. Scuseria and H.P. Lüthi
 Some new structures of C₂₈
Chem. Phys. Letters **301** (1999) 98-104
- 99.09 W. Klopper and H.P. Lüthi
 The MP2 limit correction applied to coupled cluster calculations of the electronic dissociation energies of the hydrogen fluoride and water dimers
Mol. Phys. **96** (1999) 559-570
- 99.10 H.P. Lüthi and S. Portmann
 Bringing Theory to the Classroom: Summer School in Computational Quantum Chemistry (CQCS-98)
Chimia **53** (1999) 41-42
- 99.11 W.R.P. Scott, P.H. Hünenberger, I.G. Tironi, A.E. Mark, S.R. Billeter, J. Fennen, A.E. Torda,
 T. Huber, P. Krüger and W.F. van Gunsteren
 The GROMOS Biomolecular Simulation Program Package
J. Phys. Chem. A **103** (1999) 3596-3607
- 99.12 M.F. Lensink, J. Mavri and H.J.C. Berendsen
 Simulation of Slow Reaction with Quantum Character: Neutral Hydrolysis of Carboxylic Ester
J. Comput. Chem. **20** (1999) 886-895
- 99.13 L.J. Smith, C.M. Dobson and W.F. van Gunsteren
 Molecular Dynamics Simulations of Human α -lactalbumin. Changes to the Structural and Dynamical Properties of the Protein at Low pH
Proteins: Struct. Funct. Genet. **36** (1999) 77-86
- 99.14 W.F. van Gunsteren, A.M.J.J. Bonvin, X. Daura and L.J. Smith
 Aspects of Modeling Biomolecular Structure on the Basis of Spectroscopic or Diffraction Data
 In "Structure Computation and Dynamics in Protein NMR", Biol. Magnetic Resonance Vol. **17**, R.N. Krishna and L.J. Berliner eds., Plenum Publishers, New York, 1999, pp. 3-35
- 99.15 C.A. Schiffer and W.F. van Gunsteren
 Accessibility and Order of Water Sites in and Around Proteins: A Crystallographic Time-Averaging Study
Proteins: Struct. Funct. Genet. **36** (1999) 501-511
- 99.16 X. Daura, I. Antes, W.F. van Gunsteren, W. Thiel and A.E. Mark
 The Effect of Motional Averaging on the Calculation of NMR-Derived Structural Properties
Proteins: Struct. Funct. Genet. **36** (1999) 542-555
- 99.17 K.A. Feenstra, B. Hess and H.J.C. Berendsen
 Improving Efficiency of Large Time-Scale Molecular Dynamics Simulations of Hydrogen-Rich Systems
J. Comput. Chem. **20** (1999) 786-798
- 99.18 D.P. Tieleman, M.S.P. Sansom and H.J.C. Berendsen
 Alamethicin Helices in a Bilayer and in Solution: Molecular Dynamics Simulations
Biophys. J. **76** (1999) 40-49
- 99.19 B.L. de Groot, G. Vriend and H.J.C. Berendsen
 Conformational Changes in the Chaperonin GroEL: New Insights Into the Allosteric Mechanism
J. Mol. Biol. **286** (1999) 1241-1249
- 99.20 A. Amadei, B.L. de Groot, M.-A. Ceruso, M. Paci, A. Di Nola and H.J.C. Berendsen
 A Kinetic Model for the Internal Motions of Proteins: Diffusion Between Multiple Harmonic Wells
Proteins: Struct. Funct. Genet. **35** (1999) 283-292
- 99.21 H.J.C. Berendsen
 Molecular Dynamics Simulations: The Limits and Beyond
 In: "Computational Molecular Dynamics: Challenges, Methods, Ideas", Proceedings of the 2nd Intl. Symp. on Algorithms for Macromol. Mod., P. Deuflhard, J. Hermans, B. Leimkuhler, A.E. Mark, S. Reich, R.D. Skeel (eds.), Springer-Verlag Berlin, 1999, pp. 3-36

- 99.22 C.D. Berweger, W.F. van Gunsteren and F. Müller-Plathe
 The Photoisomerization of *cis*-Stilbene Does not Follow the Minimum Energy Path
Angew. Chemie Int'l. Edit. **38** (1999) 2609-2611
Angew. Chem. **111** (1999) 2771-2773
- 99.23 C.D. Berweger, W.F. van Gunsteren and F. Müller-Plathe
 Viscosity dependence and solvent effects in the photoisomerisation of *cis*-stilbene: Insight from a molecular dynamics study with an *ab initio* potential-energy function
J. Chem. Phys. **111** (1999) 8987-8999
- 99.24 H. Schäfer, W.F. van Gunsteren and A.E. Mark
 Estimating Relative Free Energies from a Single Ensemble: Hydration Free Energies
J. Comput. Chem. **20** (1999) 1604-1617
- 99.25 X. Daura, A.E. Mark and W.F. van Gunsteren
 Peptide folding simulations: no solvent required?
Comp. Phys. Comm. **123** (1999) 97-102
- 99.26 C.D. Berweger
 Molecular Dynamics Simulations with a Quantum-Chemical Core: Methodology and Applications in Photochemistry and Bioinorganic Chemistry
 thesis, ETH Zürich, December 1999
- 99.27 P.H. Hünenberger, V. Helms, N. Narayana, S.S. Taylor and J.A. McCammon
 Determinants of ligand binding to c-AMP dependent protein kinase
Biochemistry **38** (1999) 2358-2366
- 99.28 P.I.W. de Bakker, P.H. Hünenberger and J.A. McCammon
 Molecular dynamics simulations of the hyperthermophilic protein Sac7d from *Sulfolobus acidocaldarius*: Contribution of salt bridges to thermostability
J. Mol. Biol. **285** (1999) 1811-1830
- 99.29 P.H. Hünenberger and J.A. McCammon
 Ewald artifacts in computer simulations of ionic solvation and ion-ion interaction: A continuum electrostatics study
J. Chem. Phys. **110** (1999) 1856-1872
- 99.30 P.H. Hünenberger and J.A. McCammon
 Effect of artificial periodicity in simulation of biomolecules under Ewald boundary conditions: A continuum electrostatic study
Biophys. Chem. **78** (1999) 69-88
- 99.31 N.A. Baker, P.H. Hünenberger and J.A. McCammon
 Polarization around an ion in a dielectric continuum with truncated electrostatic interactions
J. Chem. Phys. **110** (1999) 10679-10692
Erratum: *J. Chem. Phys.* **113** (2000) 2510-2511
- 99.32 P.H. Hünenberger
 Lattice-sum methods for computing electrostatic interactions in molecular simulations
 In: "Simulation and theory of electrostatic interactions in solution: Computational chemistry, biophysics and aqueous solution", L.R. Pratt and G. Hummer eds., AIP, New York, 1999, pp. 17-83
- 99.33 P.F. Flükiger, S. Portmann and H.P. Lüthi
 Synchronous Communication of Molecular and Electronic Structure Information in a Distributed Computing Environment
 In: "Lecture Notes in Computer Science", 1615, High Performance Computing, Springer Verlag, 1999
- 99.34 S. Tsuzuki, W. Klopper and H.P. Lüthi
 High-level *ab initio* computations of structures and relative energies of two isomers of the CO₂ trimer
J. Chem. Phys. **111** (1999) 3846-3854

- 99.36 D.P. Tieleman, H.J.C. Berendsen and M.S.P. Sansom
 An Alamethicin Channel in a Lipid Bilayer: Molecular Dynamics Simulations
Biophys. J. **76** (1999) 1757-1769
- 99.37 D.P. Tieleman, H.J.C. Berendsen and M.S.P. Sansom
 Surface Binding of Alamethicin Stabilizes its Helical Structure: Molecular Dynamics Simulations
Biophys. J. **76** (1999) 3186-3191
- 99.38 P. Meulenhoff
 Interfacial Action of Phospholipase A₂: a molecular dynamics study
 thesis, Univ. of Groningen, The Netherlands, October 1999
- 99.39 B. de Groot
 Native State Protein Dynamics: A Theoretical Approach
 thesis, Univ. of Groningen, The Netherlands, January 1999
- 99.40 M. Mangoni, D. Roccatano and A. Di Nola
 Docking of Flexible Ligands to Flexible Receptors in Solution by Molecular Dynamics Simulation
Proteins: Struct. Funct. Genet. **35** (1999) 153-162
- 99.41 S. Hayward
 Structural Principles Governing Domain Motions in Proteins
Proteins: Struct. Funct. Genet. **36** (1999) 425-435
- 99.42 W.F. van Gunsteren and J. Hermans
 Herman Berendsen: Researcher, Teacher, Colleague, Skipper
Proteins Struct. Funct. Genet. **36** (1999) 381-382
- 2000**
- 00.01 D. Seebach, J.V. Schreiber, S. Abele, X. Daura and W.F. van Gunsteren
 Structure and Conformation of β -Oligopeptide Derivatives with Simple Proteinogenic Side-Chains: Circular Dichroism and Molecular Dynamics Investigations
Helv. Chim. Acta **83** (2000) 34-57
- 00.02 A.M.J.J. Bonvin and W.F. van Gunsteren
 β -Hairpin Stability and Folding: Molecular Dynamics Studies of the First β -hairpin of Tendamistat
J. Mol. Biol. **296** (2000) 255-268
- 00.03 M.J. Mayor-Lopez, J. Weber, H.P. Lüthi and K. Hegetschweiler
 SCO Trimers as High-energy Materials? A Density Functional Study
J. Mol. Model. **6** (2000) 55-64
- 00.04 C.W. Jefford, M. Grigorov, J. Weber, H.P. Lüthi and J.M.J. Tronchet
 Correlating the Molecular Electrostatic Potentials of Some Organic Peroxides with Their Antimalarial Activities
J. Chem. Inf. Comput. Sci. **40** (2000) 354-357
- 00.05 S.R. Billeter and W.F. van Gunsteren
 Computer Simulation of Proton Transfers of Small Acids in Water
J. Phys. Chem. A **104** (2000) 3276-3286
- 00.06 W. Weber, P.H. Hünenberger and J.A. McCammon
 Molecular Dynamics Simulations of a Polyalanine Octapeptide under Ewald Boundary Conditions: Influence of Artificial Periodicity on Peptide Conformation
J. Phys. Chem. B **104** (2000) 3668-3675
- 00.07 U. Stocker
 Computer Simulation of Biomolecules: Investigation of Molecular Environment and Simulation Parameters
 thesis no 13686, ETH Zürich, May 2000
- 00.08 W. Damm and W.F. van Gunsteren
 Reversible Peptide Folding: Dependence on the Molecular Force Field Used
J. Comput. Chem. **21** (2000) 774-787

- 00.09 R. Walser, A.E. Mark, W.F. van Gunsteren, M. Lauterbach and G. Wipff
 The effect of force-field parameters on properties of liquids: Parametrization of a simple three-site model for methanol
J. Chem. Phys. **112** (2000) 10450-10459
- 00.10 U. Stocker and W.F. van Gunsteren
 Molecular Dynamics Simulation of Hen Egg White Lysozyme: A Test of the GROMOS96 Force Field Against Nuclear Magnetic Resonance Data
Proteins: Struct. Funct. Genet. **40** (2000) 145-153
- 00.11 X. Daura, E. Haaksma and W.F. van Gunsteren
 Factor Xa: Simulation studies with an eye to inhibitor design
J. Computer-Aided Mol. Des. **14** (2000) 507-529
- 00.12 R. Walser, A.E. Mark and W.F. van Gunsteren
 On the Temperature and Pressure Dependence of a Range of Properties of a Type of Water Model Commonly Used in High-Temperature Protein Unfolding Simulations
Biophys. J. **78** (2000) 2752-2760
- 00.13 D.P. Tieleman, D. van der Spoel and H.J.C. Berendsen
 Molecular Dynamics Simulations of Dodecylphosphocholine Micelles at Three Different Aggregate Sizes: Micellar Structure and Chain Relaxation
J. Phys. Chem. B **104** (2000) 6380-6388
- 00.14 H.P. Lüthi
 Metacomputing, an emerging technology?
Comp. Phys. Commun. **128** (2000) 326-332
- 00.15 A.M.J.J. Bonvin, A.E. Mark and W.F. van Gunsteren
 The GROMOS96 benchmarks for molecular simulation
Comp. Phys. Commun. **128** (2000) 550-557
- 00.16 C. Peter, X. Daura and W.F. van Gunsteren
 Peptides of Aminoxy Acids: A Molecular Dynamics Simulation Study of Conformational Equilibria under Various Conditions
J. Am. Chem. Soc. **122** (2000) 7461-7466
- 00.17 S. Voordijk, T. Hansson, D. Hilvert and W.F. van Gunsteren
 Molecular Dynamics Simulations Highlight Mobile Regions in Proteins: A Novel Suggestion for Converting a Murine V_H Domain into a More Tractable Species
J. Mol. Biol. **300** (2000) 963-973
- 00.18 H. Schäfer
 Calculation of Free Energy and Entropy from Molecular Simulations: Methodology and Application
 thesis no 13826, ETH Zürich, September 2000
- 00.19 R. Walser
 Molecular Dynamics Simulations: Solvent Properties and Solvent Effects on Proteins
 thesis no 13845, ETH Zürich, September 2000
- 00.20 R.R. Tykwinski, A. Hilger, F. Diederich, H.P. Lüthi, P. Seiler, V. Gramlich, J.-P. Gisselbrecht, C. Boudon and M. Gross
 Donor-Acceptor-Functionalized Tetraethynylethenes with Nitrothienyl Substituents: Structure-Property Relationsships
Helv. Chim. Acta **83** (2000) 1484-1508
- 00.21 U. Stocker, K. Spiegel and W.F. van Gunsteren
 On the similarity of properties in solution or in the crystalline state:
 A molecular dynamics study of hen lysozyme
J. Biomol. NMR **18** (2000) 1-12
- 00.22 L.D. Schuler and W.F. van Gunsteren
 On the Choice of Dihedral Angle Potential Energy Functions for *n*-Alkanes
Molecular Simulation **25** (2000) 301-319

- 00.23 C.D. Berweger, W. Thiel and W.F. van Gunsteren
 Molecular-Dynamics Simulation of the β Domain of Metallothionein with a
 Semi-Empirical Treatment of the Metal Core
Proteins: Struct. Funct. Genet. **41** (2000) 299-315
- 00.24 J.W. Pitera and P.A. Kollman
 Exhaustive Mutagenesis In Silico: Multicoordinate Free Energy Calculations on Proteins and Peptides
Proteins: Struct. Funct. Genet. **41** (2000) 385-397
- 00.25 H. Schäfer, A.E. Mark and W.F. van Gunsteren
 Absolute entropies from molecular dynamics simulation trajectories
J. Chem. Phys. **113** (2000) 7809-7817
- 00.26 P.H. Hünenberger
 Optimal charge-shaping functions for the particle-particle-particle-mesh (P³M) method
 for computing electrostatic interactions in molecular simulations
J. Chem. Phys. **113** (2000) 10464-10476
- 00.27 L. Schuler
 Molecular Dynamics Simulation of Aggregates of Lipids: Development of Force-Field Parameters and
 Application to Membranes and Micelles
 thesis no 14009, ETH Zürich, December 2000
- 00.28 C. Oostenbrink, J.W. Pitera, M.M.H. van Lipzig, J.H.N. Meerman and W.F. van Gunsteren
 Simulations of the Estrogen Receptor Ligand Binding Domain: Affinity of Natural
 Ligands and Xenoestrogens
J. Med. Chem. **43** (2000) 4594-4605
- 00.29 S. Portmann, A. Inauen, H.P. Lüthi and S. Leutwyler
 Chiral discrimination in hydrogen-bonded complexes
J. Chem. Phys. **113** (2000) 9577-9585
- 00.30 W. Alda, D.A. Yuen, H.P. Lüthi and J. Rustad
 Exothermic and Endothermic Chemical Reactions Involving Very Many Particles Modelled with Molecular
 Dynamics
Physica D **146** (2000) 261-
- 00.31 M.J. Mayor-Lopez, H.P. Lüthi, H. Koch, P.-Y. Morgantini and J. Weber
 Coupled-cluster calculations on ferrocene and its protonated derivative: towards the final word on the
 mechanism of protonation of ferrocene?
J. Chem. Phys. **113** (2000) 8009-8014
- 00.32 S. Portmann and H.P. Lüthi
 MOLEKEL: An Interactive Molecular Graphics Tool
Chimia **54** (2000) 766-770
- 00.33 S.J. Marrink, D.P. Tieleman and A.E. Mark
 Molecular Dynamics Simulation of the Kinetics of Spontaneous Micelle Formation
J. Phys. Chem. B **104** (2000) 12165-12173
- 00.34 M. Fioroni, K. Burger, A.E. Mark and D. Roccatano
 A New 2,2,2-Trifluoroethanol Model for Molecular Dynamics Simulations
J. Phys. Chem. B **104** (2000) 12347-12354
- 00.35 H.J.C. Berendsen and S. Hayward
 Collective protein dynamics in relation to function
Curr. Opin. Struct. Biol. **10** (2000) 165-169
- 00.36 E.J.W. Wensink, A.C. Hoffmann, M.E.F. Apol and H.J.C. Berendsen
 Properties of Adsorbed Water Layers and the Effect of Adsorbed Layers on Intermolecular Forces by Liquid
 Bridging
Langmuir **16** (2000) 7392-7400

2001

- 01.01 W.F. van Gunsteren, R. Bürgi, C. Peter and X. Daura
The Key to Solving the Protein-Folding Problem Lies in an Accurate Description of the Denatured State
Angew. Chemie Intl. Ed. **40** (2001) 351-355
Angew. Chem. **113** (2001) 363-367
- 01.02 R. Walser and W.F. van Gunsteren
Viscosity Dependence of Protein Dynamics
Proteins: Struct. Funct. Genet. **42** (2001) 414-421
- 01.03 F.A. Hamprecht
Modern Methods for the Analysis of Multi-dimensional Data in the Natural Sciences
thesis no 14069, ETH Zürich, February 2001
- 01.04 F.A. Hamprecht, C. Peter, X. Daura, W. Thiel and W.F. van Gunsteren
A strategy for analysis of (molecular) equilibrium simulations: Configuration space density estimation, clustering, and visualization
J. Chem. Phys. **114** (2001) 2079-2089
- 01.05 R. Bürgi, X. Daura, A. Mark, M. Bellanda, S. Mammi, E. Peggion and W.F. van Gunsteren
Folding study of an Aib-rich peptide in DMSO by molecular dynamics simulations
J. Peptide Res. **57** (2001) 107-118
- 01.06 M. Bellanda, E. Peggion, R. Bürgi, W.F. van Gunsteren and S. Mammi
Conformational study of an Aib-rich peptide in DMSO by NMR
J. Peptide Res. **57** (2001) 97-106
- 01.07 S.R. Billeter, C.F.W. Hanser, T.Z. Mordasini, M. Scholten, W. Thiel and W.F. van Gunsteren
Molecular dynamics study of oxygenation reactions catalysed by the enzyme
p-hydroxybenzoate hydroxylase
Phys. Chem. Chem. Phys. **3** (2001) 688-695
- 01.08 V. Kräutler, W.F. van Gunsteren and P.H. Hünenberger
A Fast SHAKE Algorithm to Solve Distance Constraint Equations for Small Molecules
in Molecular Dynamics Simulations
J. Comput. Chem. **22** (2001) 501-508
- 01.09 S. Tsuzuki and H.P. Lüthi
Interaction energies of van der Waals and hydrogen bonded systems calculated using density functional theory: Assessing the PW91 model
J. Chem. Phys. **114** (2001) 3949-3957
- 01.10 X. Daura, K. Gademann, H. Schäfer, B. Jaun, D. Seebach and W.F. van Gunsteren
The β -Peptide Hairpin in Solution: Conformational Study of a β -Hexapeptide in Methanol by NMR Spectroscopy and MD Simulation
J. Am. Chem. Soc. **123** (2001) 2393-2404
- 01.11 H. Schäfer, X. Daura, A.E. Mark and W.F. van Gunsteren
Entropy Calculations on a Reversibly Folding Peptide: Changes in Solute Free Energy Cannot Explain Folding Behaviour
Proteins: Struct. Func. Genet. **43** (2001) 45-56
- 01.12 J.W. Pitera and W.F. van Gunsteren
The Importance of Solute-Solvent van der Waals Interactions with Interior Atoms of Biopolymers
J. Am. Chem. Soc. **123** (2001) 3163-3164
- 01.13 R. Walser, B. Hess, A.E. Mark and W.F. van Gunsteren
Further investigation on the validity of Stokes-Einstein behaviour at the molecular level
Chem. Phys. Letters **334** (2001) 337-342
- 01.14 R. Bürgi, J. Pitera and W.F. van Gunsteren
Assessing the effect of conformational averaging on the measured values of observables
J. Biomol. NMR **19** (2001) 305-320

- 01.15 R.A. King, H.P. Lüthi, H.F. Schaefer III, F. Glarner and U. Burger
 The Photohydration of N-Alkylpyridinium Salts: Theory and Experiment
Chem. Eur. J. **7** (2001) 1734-1742
- 01.16 R. Walser, P.H. Hünenberger and W.F. van Gunsteren
 Comparison of Different Schemes to Treat Long-Range Electrostatic Interactions in
 Molecular Dynamics Simulations of a Protein Crystal
Proteins: Struct. Funct. Genet. **44** (2001) 509-519
- 01.17 C.F. Wong, P.H. Hünenberger, P. Akamine, N. Narayana, T. Diller, J.A. McCammon, S. Taylor and N.-H. Xuong
 Computational Analysis of PKA-Balanol Interactions
J. Med. Chem. **44** (2001) 1530-1539
- 01.18 U. Börjesson and P.H. Hünenberger
 Explicit-solvent molecular dynamics simulation at constant pH: Methodology and
 application to small amines
J. Chem. Phys. **114** (2001) 9706-9719
- 01.19 R. Zangi, H. Kovacs, W.F. van Gunsteren, J. Johansson and A.E. Mark
 Free Energy Barrier Estimation of Unfolding the α -Helical Surfactant-Associated Polypeptide C
Proteins: Struct. Funct. Genet. **43** (2001) 395-402
- 01.20 B.L. de Groot, X. Daura, A.E. Mark and H. Grubmüller
 Essential dynamics of reversible peptide folding: Memory-free conformational dynamics governed by
 internal hydrogen bonds
J. Mol. Biol. **309** (2001) 299-313
- 01.21 D.P. Tieleman, H.J.C. Berendsen and M.S.P. Sansom
 Voltage-Dependent Insertion of Alamethicin at Phospholipid/Water and Octane/Water Interfaces
Biophys. J. **80** (2001) 331-346
- 01.22 R.P. Bürgi
 Towards Understanding Polypeptide Structure and Titration: Theoretical Studies
 and Computer Simulations
 thesis no 14244, ETH Zürich, June 2001
- 01.23 W.F. van Gunsteren, D. Bakowies, W. Damm, T. Hansson, U. Stocker and X. Daura
 Practical Aspects of Simulation Studies of Biomolecular Systems
 in: *Dynamics, Structure and Function of Biological Macromolecules*, O. Jardetzky and M.D. Finucane, eds.,
 NATO ASI Series **A315**, IOS Press, Amsterdam, 2001, pp. 1-26
- 01.24 J.W. Pitera, M. Falta and W.F. van Gunsteren
 Dielectric Properties of Proteins from Simulation: The effects of Solvent, Ligands, pH, and Temperature
Biophys. J. **80** (2001) 2546-2555
- 01.25 S.J. Marrink and A.E. Mark
 Effect of Undulations on Surface Tension in Simulated Bilayers
J. Phys. Chem. B **105** (2001) 6122-6127
- 01.26 L.D. Schuler, X. Daura and W.F. van Gunsteren
 An Improved GROMOS96 Force Field for Aliphatic Hydrocarbons in the Condensed Phase
J. Comput. Chem. **22** (2001) 1205-1218
- 01.27 U. Stocker and W.F. van Gunsteren
 Molecular-dynamics simulation of protein crystals: convergence of molecular properties of ubiquitin
 in: *Crystallography of Biological Macromolecules*, M.G. Rossmann and E. Arnold, eds., *Intl. Tables for
 Crystallography*, Volume F, Kluwer Academic Publishers, Dordrecht, NL, 2001, pp. 481-495
- 01.28 T.N. Heinz, W.F. van Gunsteren and P.H. Hünenberger
 Comparison of four methods to compute the dielectric permittivity of liquids
 from molecular dynamics simulations
J. Chem. Phys. **115** (2001) 1125-1136

- 01.29 L. Gobbi, N. Elmaci, H.P. Lüthi and F. Diederich
N,N-Dialkylaniline-Substituted Tetraethynylethenes: a New Class of Chromophores Possessing an Emitting Charge-Transfer State. Experimental and Computational Studies
ChemPhysChem **2** (2001) 432-433
- 01.30 W. Czechtizky, X. Daura, A. Vasella and W.F. van Gunsteren
Oligonucleotide Analogues with a Nucleobase-Including Backbone.
Part 7: Molecular Dynamics Simulation of a DNA Duplex Containing a 2'-Deoxyadenosine 8-(Hydroxymethyl)-Derived Nucleotide
Helv. Chim. Acta **84** (2001) 2132-2145
- 01.31 C. Peter, X. Daura and W.F. van Gunsteren
Calculation of NMR-relaxation parameters for flexible molecules from molecular dynamics simulations
J. Biomol. NMR **20** (2001) 297-310
- 01.32 L.D. Schuler, P. Walde, P.L. Luisi and W.F. van Gunsteren
*Molecular dynamics simulation of *n*-dodecyl phosphate aggregate structures*
Eur. Biophys. J. **30** (2001) 330-343
- 01.33 D. Roccatano, A.E. Mark and S. Hayward
Investigation of the Mechanism of Domain Closure in Citrate Synthase by Molecular Dynamics Simulation
J. Mol. Biol. **310** (2001) 1039-1053
- 01.34 W.F. van Gunsteren, D. Bakowies, R. Bürgi, I. Chandrasekhar, M. Christen, X. Daura, P. Gee, A. Glättli, T. Hansson, C. Oostenbrink, C. Peter, J. Pitera, L. Schuler, T. Soares and H.B. Yu
Molecular Dynamics Simulation of Biomolecular Systems
CHIMIA **55** (2001) 856-860
- 01.35 P.H. Hünenberger, U. Börjesson and R.D. Lins
Electrostatic Interactions in Biomolecular Systems
CHIMIA **55** (2001) 861-866
- 01.36 F.A. Hamprecht, D. Jost, M. Rüttimann, F. Calamai and J.J. Kowalski
Preliminary results on the prediction of countershock success with fibrillation power
Resuscitation **50** (2001) 297-299
- 01.37 F.A. Hamprecht, U. Achleitner, A.C. Krismer, K.H. Lindner, V. Wenzel, H.-U. Strohmenger, W. Thiel, W.F. van Gunsteren and A. Amann
Fibrillation power, an alternative method of ECG spectral analysis for prediction of countershock success in a porcine model of ventricular fibrillation
Resuscitation **50** (2001) 287-296
- 01.38 L.D. Creveld, W. Meijberg, H.J.C. Berendsen and H.A.M. Pepermans
*DSC studies of *Fusarium solani pisi* cutinase: consequences for stability in the presence of surfactants*
Biophys. Chem. **92** (2001) 65-75
- 01.39 H.J.C. Berendsen
Slow Events in Complex Systems: Potentials of Mean Force and the Smoluchowski limit in biological systems
Simu Newsletter **3** (2001) 33-50
- 01.40 M. Fiorini, K. Burger, A.E. Mark and D. Roccatano
Model of 1,1,1,3,3-Hexafluoro-propan-2-ol for Molecular Dynamics Simulations
J. Phys. Chem. B **105** (2001) 10967-10975
- 01.41 R. Bürgi, F. Läng and W.F. van Gunsteren
A Comparison of Seven Fast but Approximate Methods to Compute the Free Energy of Deprotonation for Amino Acids in Aqueous Solution
Molecular Simulation **27** (2001) 215-236
- 01.42 J.W. Pitera and W.F. van Gunsteren
One-Step Perturbation Methods for Solvation Free Energies of Polar Solutes
J. Phys. Chem. B **105** (2001) 11264-11274

- 01.43 W.F. van Gunsteren, R. Bürgi, C. Peter and X. Daura
 Reply to the Comment on the Communication by van Gunsteren *et al.*,
Angew. Chem. Int. Ed. **40** (2001) 4616-4618
Angew. Chem. **113** (2001) 4752-4754
- 01.44 I. Chandrasekhar and W.F. van Gunsteren
 Sensitivity of Molecular Dynamics Simulations of Lipids to the Size of the Ester Carbon
Current Science **81** (2001) 1325-1327
- 01.45 C.T. Choma, D.P. Tieleman, D. Cregut, L. Serrano and H.J.C. Berendsen
 Towards the design and computational characterization of a membrane protein
J. Mol. Graph. Mod. **20** (2001) 219-234
- 01.46 H.J.C. Berendsen
 Reality Simulation - Observe While it Happens
Science **294** (2001) 2304-2305
- 01.47 S.J. Marrink, E. Lindahl, O. Edholm and A.E. Mark
 Simulation of the Spontaneous Aggregation of Phospholipids into Bilayers
J. Am. Chem. Soc. **123** (2001) 8638-8639
- 2002**
- 02.01 B. Hess
 Stochastic Concepts in Molecular Simulation
 thesis, Univ. of Groningen, The Netherlands, January 2002
- 02.02 H. Schäfer, L.J. Smith, A.E. Mark and W.F. van Gunsteren
 Entropy Calculations of the Molten Globule State of a Protein: Side-Chain
 Entropies of α -Lactalbumin
Proteins: Struct. Funct. Genet. **46** (2002) 215-224
- 02.03 J.W. Pitera and W.F. van Gunsteren
 A Comparison of Non-bonded Scaling Approaches for Free Energy Calculations
Molecular Simulation **28** (2002) 45-65
- 02.04 G. Colombo, D. Roccatano and A.E. Mark
 Folding and Stability of the Three-Stranded β -Sheet Peptide Betanova:
 Insights from Molecular Dynamics Simulations
Proteins: Struct. Funct. Genet. **46** (2002) 380-392
- 02.05 A. Villa and A.E. Mark
 Calculation of the Free Energy of Solvation for Neutral Analogues of Amino Acid Side Chains
J. Comput. Chem. **23** (2002) 548-553
- 02.06 P.J. Gee, F.A. Hamprecht, L.D. Schuler, W.F. van Gunsteren, E. Duchardt, H. Schwalbe, M. Albert and D. Seebach
 A Molecular-Dynamics Simulation Study of the Conformational Preferences of Oligo-(3-hydroxy-alkanoic acids) in Chloroform Solution
Helv. Chim. Acta **85** (2002) 618-632
- 02.07 F.A. Hamprecht, W. Thiel and W.F. van Gunsteren
 Chemical Library Subset Selection Algorithms: A Unified derivation Using Spatial Statistics
J. Chem. Inf. Comput. Sci. **42** (2002) 414-428
- 02.08 T. Hansson, C. Oostenbrink and W.F. van Gunsteren
 Molecular dynamics simulations
Curr. Opinion Struct. Biol. **12** (2002) 190-196
- 02.09 C. Peter, W.F. van Gunsteren and P.H. Hünenberger
 Solving the Poisson equation for solute-solvent systems using fast Fourier transforms
J. Chem. Phys. **116** (2002) 7434-7451

- 02.10 P.H. Hünenberger
Calculation of the group-based pressure in molecular simulations: I. A general formulation including Ewald and particle-particle-particle-mesh electrostatics
J. Chem. Phys. **116** (2002) 6880-6897
- 02.11 B. Oliva and P.H. Hünenberger
Calculation of the group-based pressure in molecular simulations: II. Numerical tests and application to liquid water
J. Chem. Phys. **116** (2002) 6898-6909
- 02.12 I. Chandrasekhar and W.F. van Gunsteren
A comparison of the potential energy parameters of aliphatic alkanes:
molecular dynamics simulations of triacylglycerols in the alpha phase.
Eur. Biophys. J. **31** (2002) 89-101
- 02.13 D. Bakowies and W.F. van Gunsteren
Simulations of *Apo*- and *Holo*-Fatty Acid Binding Protein: Structure and Dynamics of Protein, Ligand and Internal Water
J. Mol. Biol. **315** (2002) 713-736
- 02.14 C. Jamorski, J.B. Foresman, C. Thilgen and H.P. Lüthi
Assessment of time-dependent density-functional theory (TDDFT) for the calculation of critical features in the absorption spectra of a series of aromatic donor-acceptor systems.
J. Chem. Phys. **116** (2002) 8761-8771
- 02.16 S.J. Marrink and A.E. Mark
Molecular Dynamics Simulations of Mixed Micelles Modeling Human Bile
Biochemistry **41** (2002) 5375-5382
- 02.17 M.G. Pikkemaat, A.B.M. Linssen, H.J.C. Berendsen and D.B. Janssen
Molecular dynamics simulations as a tool for improving protein stability
Protein Engineering **15** (2002) 185-192
- 02.18 A. Glättli, X. Daura and W.F. van Gunsteren
Derivation of an improved simple point charge model for liquid water: SPC/A and SPC/L
J. Chem. Phys. **116** (2002) 9811-9828
- 02.19 D. Bakowies and W.F. van Gunsteren
Water in Protein Cavities: A Procedure to Identify Internal Water and Exchange Pathways and Application to Fatty Acid-Binding Protein
Proteins: Struct. Funct. Genet. **47** (2002) 534-545
- 02.20 R. Bürgi, P.A. Kollman and W.F. van Gunsteren
Simulating Proteins at Constant pH: An Approach Combining Molecular Dynamics and Monte Carlo Simulation
Proteins: Struct. Funct. Genet. **47** (2002) 469-480
- 02.21 G. Groenhof, M.F. Lensink, H.J.C. Berendsen, J.G. Snijders and A.E. Mark
Signal Transduction in the Photoactive Yellow Protein. I: Photon Absorption and the Isomerization of the Chromophore
Proteins: Struct. Funct. Genet. **48** (2002) 202-211
- 02.22 G. Groenhof, M.F. Lensink, H.J.C. Berendsen and A.E. Mark
Signal Transduction in the Photoactive Yellow Protein. II: Proton Transfer Initiates Conformational Changes
Proteins : Struct. Funct. Genet. **48** (2002) 212-219
- 02.23 R. Zangi, M.L. de Vocht, G.T. Robillard and A.E. Mark
Molecular Dynamics Study of the Folding of Hydrophobin SC3 at a Hydrophilic/Hydrophobic Interface
Biophys. J. **83** (2002) 112-124

- 02.24 J.A. Flohil, G. Vriend and H.J.C. Berendsen
Completion and Refinement of 3-D Homology Models with Restricted Molecular Dynamics: Application to Targets 47, 58, and 111 in the CASP Modeling Competition and Posterior Analysis
Proteins: Struct. Funct. Genet. **48** (2002) 593-604
- 02.25 L.J. Smith, X. Daura and W.F. van Gunsteren
Assessing Equilibration and Convergence in Biomolecular Simulations
Proteins: Struct. Funct. Genet. **48** (2002) 487-496
- 02.26 F. van Lune, L. Manning, K. Dijkstra, H.J.C. Berendsen and R.M. Scheek
Order-parameter tensor description of HPr in a medium of oriented bicelles
J. Biomol. NMR **23** (2002) 169-179
- 02.27 A.N. Morozov
Orientational Transitions in Block-Copolymer Melts under Shear Flow
thesis, Univ. of Groningen, The Netherlands, February 2002
- 02.28 K.A. Feenstra
Long Term Dynamics of Proteins and Peptides
thesis, Univ. of Groningen, The Netherlands, July 2002
- 02.29 B. Hess, H. Saint-Martin and H.J.C. Berendsen
Flexible constraints: An adiabatic treatment of quantum degrees of freedom, with application to the flexible and polarizable MCDHO model for water
J. Chem. Phys. **116** (2002) 9602-9610
- 02.30 R. Walser, P.H. Hünenberger and W.F. van Gunsteren
Molecular Dynamics Simulations of a Double Unit Cell in a Protein Crystal: Volume Relaxation at Constant Pressure and Correlation of Motions between the Two Unit Cells
Proteins: Struct. Funct. Genet. **48** (2002) 327-340
- 02.31 K.A. Feenstra, C. Peter, R.M. Scheek, W.F. van Gunsteren and A.E. Mark
A comparison of methods for calculating NMR cross-relaxation rates (NOESY and ROESY intensities) in small peptides
J. Biomol. NMR **23** (2002) 181-194
- 02.32 C. Jamorski Jödicke and H.P. Lüthi
Time-dependent density-functional theory investigation of the formation of the charge transfer excited state for a series of aromatic donor-acceptor systems. Part I
J. Chem. Phys. **117** (2002) 4146-4156
- 02.33 W.F. van Gunsteren
Computersimulatie van complexe (bio)moleculaire systemen: Mogelijkheden, onmogelijkheden en perspectieven
NWO/Huygens-lezing, Den Haag, NL, 14.11.2001, NWO, Den Haag, 2002
(*only available in Dutch*)
- 02.34 M.F. Lensink
Non-adiabatic Proton Transfer in Biomolecular Systems
thesis, Univ. of Groningen, The Netherlands, March 2002
- 02.35 E. AB
Structural Studies on IIB^{Chb}
thesis, Univ. of Groningen, The Netherlands, June 2002
- 02.36 P.A.W. van den Berg, K.A. Feenstra, A.E. Mark, H.J.C. Berendsen and A.J.W.G. Visser
Dynamic Conformations of Flavin Adenine Dinucleotide: Simulated Molecular Dynamics of the Flavin Cofactor Related to the Time-Resolved Fluorescence Characteristics
J. Phys. Chem. B **106** (2002) 8858-8869
- 02.37 C. Jamorski Jödicke and H.P. Lüthi
Time-dependent density-functional theory investigation of the formation of the charge transfer excited state for a series of aromatic donor-acceptor systems - Part II
J. Chem. Phys. **117** (2002) 4157-4167

- 02.38 W.F. van Gunsteren, X. Daura and A.E. Mark
 Computation of Free Energy
Helv. Chim. Acta **85** (2002) 3113-3129
- 02.39 D. Kony, W. Damm, S. Stoll and W.F. van Gunsteren
 An Improved OPLS-AA Force Field for Carbohydrates
J. Comput. Chem. **23** (2002) 1416-1429
- 02.40 A. Glättli, X. Daura, D. Seebach and W.F. van Gunsteren
 Can One Derive the Conformational Preference of a β -Peptide from Its CD Spectrum?
J. Am. Chem. Soc. **124** (2002) 12972-12978
- 02.41 D. Roccatano, G. Colombo, M. Fioroni and A.E. Mark
 Mechanism by which 2,2,2-trifluoroethanol/water mixtures stabilize secondary structure formation in peptides: A molecular dynamics study
Proc. Natl. Acad. Sci. **99** (2002) 12179-12184
- 02.42 X. Daura, A. Glättli, P. Gee, C. Peter and W.F. van Gunsteren
 The Unfolded State of Peptides
Adv. Prot. Chem. **62** (2002) 341-360
- 02.43 R. Baron, D. Bakowies, W.F. van Gunsteren and X. Daura
 β -Peptides with Different Secondary-Structure Preferences: How Different Are Their Conformational Spaces?
Helv. Chim. Acta **85** (2002) 3872-3882
- 02.44 I. Antes, W. Thiel and W.F. van Gunsteren
 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
Eur. Biophys. J. **31** (2002) 504-520
- 02.45 P. Soto and A.E. Mark
 The Effect of the Neglect of Electronic Polarization in Peptide Folding Simulations
J. Phys. Chem. B **106** (2002) 12830-12833
- 02.46 D. Seebach, T. Sifferlen, D. Bierbaum, M. Rueping, B. Jaun, B. Schweizer, J. Schaefer, A.K. Mehta, R.D. O'Connor, B.H. Meier, M. Ernst and A. Glättli
 Isotopically Labelled and Unlabelled β -Peptides with Geminal Dimethyl-Substitution in 2-Position of Each Residue - Synthesis and NMR-Investigation in Solution and in the Solid State
Helv. Chim. Acta **85** (2002) 2877-2917
- 02.47 S.S. Park, K.H. Lee, Y. Suh, C. Lee and H.P. Lüthi
 Geometries and Relative Stabilities of AIN Four-Membered-Ring Compound Isomers: *Ab initio* Study
Bull. Korean Chem. Soc. **23**, 2002, 241-244
- 02.48 M.E.F. Apol, H.J.C. Berendsen, A.E. Mark and A.C. Hoffmann
 Interparticle Forces for DEM by MD Simulations
Proceed. 4th World Congr. on Particle Tech., Sydney (2002)
- 2003**
- 03.01 U. Stocker, D. Juchli and W.F. van Gunsteren
 Increasing the Time Step and Efficiency of Molecular Dynamics Simulations: Optimal Solutions for Equilibrium Simulations or Structure Refinement of Large Biomolecules
Molecular Simulation **29** (2003) 123-138
- 03.02 H. Yu, T. Hansson and W.F. van Gunsteren
 Development of a simple, self-consistent polarizable model for liquid water
J. Chem. Phys. **118** (2003) 221-234
- 03.03 C. Jamorski Jödicke an H.P. Lüthi
 Time-Dependent Density Functional Theory (TDDFT) Study of the Excited Charge-Transfer State Formation of a Series of Aromatic Donor--Acceptor Systems
J. Am. Chem. Soc. **125** (2003) 252-264

- 03.04 I. Chandrasekhar, M. Kastenholz, R.D. Lins, C. Oostenbrink, L.D. Schuler, D.P. Tieleman and W.F. van Gunsteren
A consistent potential energy parameter set for lipids: Dipalmitoylphosphatidylcholine as a benchmark of the GROMOS96 45A3 force field
Eur. Biophys. J. **32** (2003) 67-77
- 03.05 C. Jamorski Jödicke and H.P. Lüthi
A time-dependent density-functional theory investigation of the fluorescence behavior of related cyano and di-cyano isomers of 4-(*N,N*-dimethylamino)benzonitrile
Chem. Phys. Letters **368** (2003) 561-567
- 03.06 G. Colombo, S.J. Marrink and A.E. Mark
Simulation of MsCl Gating in a Bilayer under Stress
Biophys. J. **84** (2003) 2331-2337
- 03.07 C. Peter
A Critical Analysis of Various Aspects of Biomolecular Simulation: from Electrostatic Forces, NMR Spectra, and Entropy to Peptide Folding
thesis no 15160, ETH Zürich, June 2003
- 03.08 A. Glättli, X. Daura and W.F. van Gunsteren
A Novel Approach for Designing Simple Point Charge Models for Liquid Water with Three Interaction Sites
J. Comput. Chem. **24** (2003) 1087-1096
- 03.09 D. Bakowies
Trendberichte Theoretische Chemie 2003: Kraftfelder für biomolekulare Simulationen
Nachr. Chem. **51** (2003) 325-327
- 03.10 D. Bakowies
Trendberichte Theoretische Chemie 2003: Biomolekulare Reality-Simulationen
Nachr. Chem. **51** (2003) 788-793
- 03.11 R. Zangi and A.E. Mark
Monolayer Ice
Physical Review Letters **91** (2003) 025502
- 03.12 R. Zangi and A.E. Mark
Bilayer ice and alternate liquid phases of confined water
J. Chem. Phys. **119** (2003) 1694-1700
- 03.13 M. Fioroni, K. Burger, A.E. Mark and D. Roccatano
The Influence of Trifluoromethyl Groups on the Miscibility of Fluorinated Alcohols with Water: A Molecular Dynamics Simulation Study of 1,1,1-Trifluoropropan-2-ol in Aqueous Solution
J. Phys. Chem. B **107** (2003) 4855-4861
- 03.14 D.P. Tieleman, H. Leontiadou, A.E. Mark and S.-J. Marrink
Simulation of Pore Formation in Lipid Bilayers by Mechanical Stress and Electric Fields
J. Am. Chem. Soc. **125** (2003) 6382-6283
- 03.15 M. Bergdorf, C. Peter and P.H. Hünenberger
Influence of cutoff truncation and artificial periodicity of electrostatic interactions in molecular simulations of solvated ions: a continuum electrostatics study
J. Chem. Phys. **119** (2003) 9129-9144
- 03.16 R. Gargallo, P.H. Hünenberger, F.X. Avilés and B. Oliva
Molecular Dynamics simulation of highly-charged proteins: Comparison of the particle-particle particle-mesh and reaction field methods for the calculation of electrostatic interactions
Prot. Sci. **12** (2003) 2161-2172
- 03.17 C. Oostenbrink and W.F. van Gunsteren
Single-step perturbations to calculate free energy differences from unphysical reference states: limits on size, flexibility and character
J. Comput. Chem. **24** (2003) 1730-1739

- 03.18 U. Börjesson and P.H. Hünenberger
 Effect of mutations involving charged residues on the stability of *Staphylococcal* nuclease: A continuum electrostatics study
Protein Engineering **16** (2003) 831-840
- 03.19 C. Peter, W.F. van Gunsteren and P.H. Hünenberger
 A fast-Fourier-transform method to solve continuum-electrostatics problems with truncated electrostatic interactions: algorithm and application to ionic solvation and ion-ion interaction
J. Chem. Phys. **119** (2003) 12205-12223
- 03.20 X. Daura, D. Bakowies, D. Seebach, J. Fleischhauer, W.F. van Gunsteren and P. Krüger
 Circular dichroism spectra of β -peptides: Sensitivity to molecular structure and effects of motional averaging
Eur. Biophys. J. **32** (2003) 661-670
- 03.21 C. Peter, M. Rüping, H.J. Wörner, B. Jaun, D. Seebach and W.F. van Gunsteren
 Molecular dynamics simulations of small peptides: Can one derive conformational preferences from ROESY spectra ?
Chem. Eur. J. **9** (2003) 5838-5849
- 03.22 K.H. Lee, C.Lee, S.S. Park, Y. Kim, H.P. Lüthi, S.Lee, Y.S. Lee
 Structures and energetics of borafullerene dimer conformers
Synthetic Mat **135** (2003) 723-724
- 03.23 R. Talhout, A. Villa, A.E. Mark and J.B.F.N. Engberts
 Understanding Binding Affinity: A Combined Isothermal Titration Calorimetry/Molecular Dynamics Study of the Binding of a Series of Hydrophobically Modified Benzamidinium Chloride Inhibitors to Trypsin
J. Am. Chem. Soc. **125** (2003) 10570-10579
- 03.24 C. Jamorski Jödicke and H.P. Lüthi
 Rational classification of a series of aromatic donor-acceptor systems within the twisting intramolecular charge transfer model, a time-dependent density-functional theory investigation
J. Chem. Phys. **119** (2003) 12852-12865
- 03.25 H. Fan and A.E. Mark
 Relative Stability of Protein Structures Determined by X-ray Crystallography or NMR Spectroscopy: Simulation Study
Proteins: Struct. Funct. Genet. **53** (2003) 111-120
- 03.26 S.J. Marrink and A.E. Mark
 Molecular Dynamics Simulation of the Formation, Structure, and Dynamics of Small Phospholipid Vesicles
J. Am. Chem. Soc. **125** (2003) 15233-15242
- 03.27 S.-J. Marrink and A.E. Mark
 The Mechanism of Vesicle Fusion as Revealed by Molecular Dynamics Simulations
J. Am. Chem. Soc. **125** (2003) 11144-11145
- 03.28 A. Villa, R. Zangi, G. Pieffet and A.E. Mark
 Sampling and convergence in free energy calculations of protein-ligand interactions: The binding of triphenoxyppyridine derivatives to Factor Xa and Trypsin
J. Computer-Aided Mol. Des. **17** (2003) 673-686
- 2004**
- 04.01 H. Yu, X. Daura and W.F. van Gunsteren
 Molecular dynamics simulations of peptides containing an unnatural amino Acid: Dimerization, folding and protein binding
Proteins: Struct. Funct. Bioinf. **54** (2004) 116-127
- 04.02 M.A. Kastenholz and P.H. Hünenberger
 Influence of artificial periodicity and ionic strength in molecular dynamics simulations of charged biomolecules employing lattice-sum-methods
J. Phys. Chem. B **108** (2004), 774-778

- 04.03 C. Oostenbrink and W.F. van Gunsteren
 Free energies of binding of polychlorinated biphenyls to the estrogen receptor from a single simulation
Proteins: Struct. Funct. Bioinf. **54** (2004) 237-246
- 04.04 N.F.A. van der Vegt and W.F. van Gunsteren
 Entropic contributions in co-solvent binding to hydrophobic solutes in water
J. Phys. Chem. B **108** (2004) 1056-1064
- 04.05 L.J. Smith, H.J.C. Berendsen and W.F. van Gunsteren
 Computer simulation of urea-water mixtures: A test of force field parameters for use in biomolecular simulation
J. Phys. Chem. B **108** (2004) 1065-1071
- 04.06 D.P. Geerke, C. Oostenbrink, N.F.A. van der Vegt and W.F. van Gunsteren
 An effective force field for molecular dynamics simulations of dimethyl sulfoxide and dimethyl sulfoxide-water mixtures
J. Phys. Chem. B **108** (2004) 1436 - 1445
- 04.07 D. Trzesniak, N.F.A. van der Vegt, W.F. van Gunsteren
 Computer simulation studies on the solvation of aliphatic hydrocarbons in 6.9 M aqueous urea solution
Phys. Chem. Chem. Phys. **6** (2004) 697-702
Erratum: Computer simulation studies on the solvation of aliphatic hydrocarbons in 6.9 M aqueous urea solution
Phys. Chem. Chem. Phys. **6** (2004) amendment published 3rd August
- 04.08 N.F.A. van der Vegt, D. Trzesniak, B. Kasumaj and W.F. van Gunsteren
 Energy-Entropy compensation in the transfer of nonpolar solutes from water to co-solvent/water mixtures
ChemPhysChem **5** (2004) 144-147 and *Erratum*
- 04.09 C. Peter, C. Oostenbrink, A. van Dorp, W.F. van Gunsteren
 Estimating entropies from molecular dynamics simulations
J. Chem. Phys. **120** (2004) 2652-2661
- 04.10 A. Glättli, C. Oostenbrink, X. Daura, D.P. Geerke, H. Yu, W.F. van Gunsteren
 On the transferability of the SPC/L water model to biomolecular simulation
Brazilian J. of Phys. **34** (2004) 116-125
- 04.11 A.H. de Vries, A.E. Mark and S.-J. Marrink
 The binary mixing behaviour of phospholipids in a bilayer: A molecular dynamics study
J. Phys. Chem. B **108** (2004) 2454-2463
- 04.12 H. Fan and A.E. Mark
 Refinement of homology-based protein structures by molecular dynamics simulation techniques
Protein Science **13** (2004) 211-220
- 04.13 H. Leontiadou, A.E. Mark and S.-J. Marrink
 Molecular dynamics simulations of hydrophilic pores in lipid bilayers
Biophysical Journal **86** (2004) 2156-2164
- 04.14 U. Börjesson
 Electrostatic interactions in computer simulations of biomolecular systems: influence of system size, solvation, and titration
 thesis no 15454, ETH Zürich, February 2004
- 04.15 R.D. Lins, C.S. Pereira and P.H. Hünenberger
 Trehalose-protein interaction in aqueous solution
Proteins: Struct. Funct. Bioinf. **55** (2004) 177-186
- 04.16 C.S. Pereira, R.D. Lins, I. Chandrasekhar, L.C.G. Freitas, P.H. Hünenberger
 Interaction of the disaccharide trehalose with a phospholipid bilayer: A molecular dynamics study
Biophys. J. **86** (2004) 2273-2285

- 04.17 S. Calero, S. Lago, W.F. van Gunsteren, X. Daura
 Modelling of the complex between a 15-residue peptide from mSos2 and the N-terminal SH3 domain of Grb2 by molecular dynamics simulation
Chem. Biodiv. **1** (2004) 505-519
- 04.18 A.H. de Vries, A.E. Mark and S.J. Marrink
 Molecular dynamics simulation of the spontaneous formation of a small DPPC vesicle in water in atomistic detail
J. Am. Chem. Soc. **126** (2004) 4488-4489 and suppl. mat.
- 04.19 H. Fan and A.E. Mark
 Mimicking the action of folding chaperones in molecular dynamics simulations: Application to the refinement of homology-based protein structures
Protein Science **13** (2004) 992-999
- 04.20 R. Zangi and A.E. Mark
 Electrofreezing of confined water
J. Chem. Phys. **120** (2004) 7123-7130
- 04.21 G. Groenhof, M. Bouxin-Cademartory, B. Hess, S.P. de Visser, H.J.C. Berendsen, M. Olivucci, A.E. Mark, M.A. Robb
 Photoactivation of the Photoactive Yellow Protein: Why photon absorption triggers a *trans*-to-*cis* isomerization of the chromophore in the protein
J. Am. Chem. Soc. **126** (2004) 4228-4233 and suppl. mat.
- 04.22 S.J. Marrink, A.H. de Vries and A.E. Mark
 Coarse grained model for semiquantitative lipid simulations
J. Phys. Chem. B **108** (2004) 750-760
- 04.23 D. Kony, W. Damm, S. Stoll and P.H. Hünenberger
 Explicit-solvent molecular-dynamics simulations of the $\beta(1 \rightarrow 3)$ - and $\beta(1 \rightarrow 6)$ -linked disaccharides β -laminarabiose and β -gentiobiose in water
J. Phys. Chem. B **108** (2004) 5815-5826
- 04.24 T. Heinz and P.H. Hünenberger
 A fast pairlist construction algorithm for molecular simulations under periodic boundary conditions
J. Comput. Chem. **25** (2004) 1474-1486
- 04.25 H. Yu, M. Amann, T. Hansson, J. Köhler, G. Wich, W.F. van Gunsteren
 Effect of methylation on the stability and solvation free energy of amylose and cellulose fragments: A molecular dynamics study
Carbohydrate Research **339** (2004) 1697-1709
- 04.26 H. Yu, M. Ramseier, R. Bürgi, W.F. van Gunsteren
 Comparison of properties of Aib-rich peptides in crystal and solution: A molecular dynamics study
ChemPhysChem **5** (2004) 633-641
- 04.27 I. Chandrasekhar, C. Oostenbrink and W.F. van Gunsteren
 Simulating the physiological phase of hydrated dipalmitoylphosphatidylcholine bilayers: The ester moiety
Soft Materials **2** (2004) 27-45
- 04.28 C. Oostenbrink, A. Villa, A.E. Mark and W.F. van Gunsteren
 A biomolecular force field based on the free enthalpy of hydration and solvation: the GROMOS force-field parameter sets 53A5 and 53A6
J. Comp. Chem. **25** (2004) 1656-1676
- 04.29 A. Glättli
 Computer simulation of biomolecular systems: From the formulation of models for water, to the interpretation of experiment, to the investigation of polypeptide folding and membrane protein dynamics
 thesis no 15609, ETH Zürich, June 2004

- 04.30 R. Baron, D. Bakowies and W.F. van Gunsteren
Carbopeptoid folding: effects of stereochemistry, chain length and solvent
Angew. Chem. Int. Ed. **43** (2004) 4055-4059 and suppl. mat.
Angew. Chem. **116** (2004) 4147-4151
- 04.31 H. Yu
Biomolecular simulation: inclusion of polarizability, prediction of conformational stability, and analysis of peptide folding and association
thesis no 15670, ETH Zürich, August 2004
- 04.32 T. Soares, M. Christen, K. Hu and W.F. van Gunsteren
Alpha- and beta-polypeptides show a different stability of helical secondary structure
Tetrahedron **60** (2004) 7775-7780
- 04.33 U. Börjesson and P.H. Hünenberger
pH-Dependent stability of a decalysine α -helix studied by explicit-solvent molecular dynamics simulations at constant pH
J. Phys. Chem. B **108** (2004) 13551-13559
- 04.34 C.M. Santiveri, M.A. Jiménez, M. Rico, W.F. van Gunsteren and X. Daura
 β -Hairpin folding and stability: Molecular dynamics simulations of designed peptides in aqueous solution
J. Peptide Sci. **10** (2004) 546-565
- 04.35 A. Glättli and W.F. van Gunsteren
Are NMR-derived model structures for peptides representative for the ensemble of structures adopted in solution? Probing the fourth helical secondary structure of β -peptides by molecular dynamics simulation
Angew. Chem. Int. Ed. Engl. **43** (2004) 6312-6316 and suppl. mat.
Angew. Chem. **116** (2004) 6472-6476
- 04.36 A. Glättli, D. Seebach and W.F. van Gunsteren
Do valine side-chains have an influence on the folding behavior of α -substituted α -peptides?
Helv. Chim. Act. **87** (2004) 2487-2506
- 04.37 M.G. Giuffreda, M. Bruschi and H.P. Lüthi
Electron delocalization in linearly π -conjugated systems: A concept for quantitative analysis
Chem. Eur. J. **10** (2004) 5671-5680
- 04.38 M. van den Bosch, M. Swart, W.F. van Gunsteren and G.W. Canters
Simulation of the substrate cavity dynamics of quercetinase
J. Mol. Biol. **344** (2004) 725-738 and suppl. mat.
- 04.39 S.J. Marrink and A.E. Mark
Molecular view of hexagonal phase formation in phospholipid membranes.
Biophys. Journal **87** (2004) 3894-3900
- 04.40 H. Yu and W.F. van Gunsteren
Charge-on-spring polarizable water models revisited: From water clusters to liquid water to ice
J. Chem. Phys. **121** (2004) 9549-9564
- 04.41 R. Faller and S.J. Marrink
Simulation of domain formation in DLPC-DSPC mixed bilayers
Langmuir **20** (2004) 7686-7693
- 04.42 T.A. Soares, X. Daura, C. Oostenbrink, L.J. Smith, W.F. van Gunsteren
Validation of the GROMOS force-field parameter set 45A3 against nuclear magnetic resonance data of hen egg lysozyme
J. Biomol. NMR **30** (2004) 407-422
- 04.43 C. Oostenbrink
Free energies from biomolecular simulation: Force fields, methodology and applications
thesis no 15748, ETH Zürich, October 2004

- 04.44 R. Zangi
Water confined to a slab geometry: a review of recent computer simulations studies
J. of Physics **16** (2004) 5371-5388
- 2005**
- 05.01 C. Oostenbrink and W.F. van Gunsteren
Methane clustering in explicit water: Effect of urea on hydrophobic interactions
Phys. Chem. Chem. Phys. **7** (2005) 53-58
- 05.02 K. Pervushin, B. Vögeli, T.N. Heinz, P.H. Hünenberger
Measuring ^1H - ^1H and ^1H - ^{13}C RDCs in methyl groups: example of pulse sequences with numerically optimized coherence transfer schemes
J. of Magnetic Resonance **172** (2005) 36-47
- 05.03 L.J. Smith, R.M. Jones and W.F. van Gunsteren
Characterisation of the denaturation of human α -lactalbumin in urea by molecular dynamics simulations
Proteins: Struct. Funct. Bioinf. **58** (2005) 439-449
- 05.04 J. Dolenc, C. Oostenbrink, J. Koller and W.F. van Gunsteren
Molecular dynamics simulations and free energy calculations of netropsin and distamycin binding to an AAAAA DNA binding site
Nucleic Acids Research **33** (2005) 725-733
- 05.05 R. Baron, D. Bakowies and W.F. van Gunsteren
Principles of carbopeptoid folding: A molecular dynamics simulation study
J. Peptide Science **11** (2005) 74-84
- 05.06 P.H. Hünenberger
Thermostat algorithms for molecular dynamics simulations
Adv. Polym. Sci. **173** (2005) 105-149
- 05.07 T.A. Soares, P.H. Hünenberger, M.A. Kastenholz, V. Kräutler, T. Lenz, R.D. Lins, C. Oostenbrink and W.F. van Gunsteren
An improved nucleic-acid parameter set for the GROMOS force field
J. Comput. Chem. **26** (2005) 725-737
- 05.08 M. van den Bosch, M. Swart, J.G. Snijders, H.J.C. Berendsen, A.E. Mark, C. Oostenbrink, W.F. van Gunsteren and G.W. Canters
Calculation of the redox potential of the protein azurin and some mutants
ChemBioChem **6** (2005) 738 - 746
- 05.09 D. Kovalskyy, V. Dubyna, A.E. Mark and A. Kornelyuk
A molecular dynamics study of the structural stability of HIV-1 protease under physiological conditions: The role of Na^+ ions in stabilizing the active site.
Proteins: Struct. Funct. Bioinf. **58** (2005) 450-458
- 05.10 P. Soto, J. Cladera, A.E. Mark and X. Daura
Stability of SIV gp32 fusion peptide single layer protofibrils as monitored by molecular dynamics simulations
Angw. Chem. **117** (2005) 1089-1091
- 05.11 S. Donnini, A.E. Mark, A.H. Juffer and A. Villa
Incorporating the effect of ionic strength in free energy calculations using explicit ions
J. Comput. Chem. **26** (2005) 115-122
- 05.12 V. Knecht, M. Mueller, M. Bonn, S.J. Marrink and A.E. Mark
Simulation studies of pore and domain formation in a phospholipid monolayer
J. Chem. Phys. **122** (2005) 247040-247049
- 05.13 R. Zangi and J.B.F.N. Engberts
Physisorption of hydroxide ions from aqueous solution to a hydrophobic surface
J. Am. Chem. Soc. **7** (2005) 2272-2276

- 05.14 K. Pagel, K. Seeger, B. Seiwert, A. Villa, A.E. Mark, S. Berger and B. Koksch
Advanced approaches for the characterization of a *de novo* designed antiparallel coiled coil peptide
Organic & Biomolecular Chemistry, 3 (2005) 1189-1194
- 05.15 C. Oostenbrink and W.F. van Gunsteren
Free energies of ligand binding for structurally diverse compounds
Proc. Natl. Acad. Sci. **102** (2005) 6750-6754
- 05.16 C. Oostenbrink, T.A. Soares, N.F.A. van der Vegt and W.F. van Gunsteren
Validation of the 53A6 GROMOS force field
Eur. Biophys. J. **34** (2005) 273-284
- 05.17 A.H. de Vries, I. Chandrasekhar, W.F. van Gunsteren and P.H. Hünenberger
Molecular dynamics simulations of phospholipid bilayers: Influence of artificial periodicity, system size, and simulation time
J. Phys. Chem. B **109** (2005) 11643-11652
- 05.18 Y. Zhou, C. Oostenbrink, W.F. van Gunsteren, W.R. Hagen, S.R. de Leeuw and J.A. Jongejan
The relative stability of homochiral and heterochiral alanine dipeptides. Effects of perturbation pathways and force-field parameters on free energy calculations
Mol. Phys. **103** (2005) 1961-1969
- 05.19 H. Fan, A.E. Mark, J. Zhu, B. Honig
Comparative study of generalized Born models; Protein dynamics
Proc. Natl. Acad. Sci. **102** (2005) 6760-6764
- 05.20 P. Gee
Studies relating to the numerical simulation of molecular dynamics
Thesis Nr. 15938, ETH Zürich. 2005
- 05.21 S.D. Hsu, C. Peter, W.F. van Gunsteren and A.M.J.J. Bonvin
Entropy calculation of HIV-1 Env gp 120, its receptor CD4 and their complex: an analysis of entropy changes upon complexation
Biophys. J. **88** (2005) 15-24
- 05.22 C. Oostenbrink and W.F. van Gunsteren
Efficient calculation of stacking and pairing free energies in DNA from molecular dynamics simulations
Chem. Eur. J. **11** (2005) 4340-4348
- 05.23 B. Zagrovic, J. Lipfert, E.J. Sorin, I.S. Millett, W.F. van Gunsteren, S. Doniach and V.S. Pande
Unusual compactness of a polyproline type II structure
Proc. Natl. Acad. Sci. **102** (2005) 11698-11703
- 05.24 A. Aemiseger, V. Kräutler, W.F. van Gunsteren and D. Hilvert
A Photoinducible β -Hairpin
J. Am. Chem. Soc. **127** (2005) 2929-2936
- 05.25 V. Kräutler, A. Aemiseger, P.H. Hünenberger, D. Hilvert, T. Hansson and W.F. van Gunsteren
Use of molecular dynamics in the design and structure determination of a photoinducible β -Hairpin
J. Am. Chem. Soc. **127** (2005) 4935-4942
- 05.26 I. Chandrasekhar, D. Bakowies, A. Glättli, P.H. Hünenberger, C. Pereira and W.F. van Gunsteren
Molecular dynamics simulation of lipid bilayers with GROMOS96: Application of surface tension
Molecular Simulation **31** (2005) 543-548
- 05.27 R.D. Lins and P.H. Hünenberger
A new GROMOS force field for hexopyranose-based carbohydrates
J. Comput. Chem. **26** (2005) 1400-1412
- 05.28 J.H. Missimer, M.O. Steinmetz, W. Jahnke, F.K. Winkler, W.F. van Gunsteren and X. Daura
Molecular-dynamics simulations of C- and N-terminal peptide derivatives of GCN4-p1 in aqueous solution
Chem. & Biodiversity **2** (2005) 1086-1104

- 05.29 C. Oostenbrink, D. Juchli, W.F. van Gunsteren
Amine hydration: A united-atom force field solution
ChemPhysChem **6** (2005) 1800-1804
- 05.30 B. Zagrovic, G. Jayachandran, I.S. Millett, S. Doniach and V.S. Pande
How large is α -helix in solution? Studies of the radii of gyration of helical peptides by small-angle X-ray scattering and molecular dynamics
J. Mol. Biol. **353** (2005) 232-241
- 05.31 H. Yu and W.F. van Gunsteren
Accounting for polarization in molecular simulation
Comput. Phys. Commun. **172** (2005) 69-85
- 05.32 M. Christen, P.H. Hünenberger, D. Bakowies, R. Baron, R. Bürgi, D.P. Geerke, T.N. Heinz, M.A. Kastenholz, V. Kräutler, C. Oostenbrink, C. Peter, D. Trzesniak, W.F. van Gunsteren
The GROMOS software for biomolecular simulation: GROMOS05
J. Comput. Chem. **26** (2005) 1719-1751
- 05.33 A. Glättli, X. Daura, P. Bindschädler, B. Jaun, Y.R. Mahajan, R.I. Mathad, M. Rueping, D. Seebach and W.F. van Gunsteren.
On the influence of charged side-chains on the folding-unfolding equilibrium of beta-peptides - A molecular dynamics simulation study
Chem. Eur. J. **11** (2005) 7276-7293 and suppl. mat.
- 05.34 A. Glättli, I. Chandrasekhar and W.F. van Gunsteren
A molecular dynamics study of the bee venom melittin in aqueous solution, in methanol, and inserted in a phospholipid bilayer
Eur. Biophys. J. **35** (2006) 255-267
- 05.35 M. Christen and W.F. van Gunsteren
An approximate but fast method to impose flexible distance constraints in molecular dynamics simulations
J. Chem. Phys. **122** (2005) 144106 (DOI: 10.1063/1.1872792)
- 05.36 T.N. Heinz and P.H. Hünenberger
Combining the lattice-sum and reaction-field approaches for evaluating long-range electrostatic interactions in molecular simulations
J. Chem. Phys. **123** (2005) 034107 (DOI: 10.1063/1.1955525)
- 05.37 C. Oostenbrink and W.F. van Gunsteren
Calculating zeros: non-equilibrium free energy calculations
Chem. Phys. **323** (2006) 102-108
- 05.38 M. Bruschi, M.G. Giuffreda, H.P. Lüthi
Measuring electron delocalization in π -conjugated systems
CHIMIA **59** (2005) 539-544
- 05.39 M. Bruschi, M.G. Giuffreda, H.P. Lüthi
Through versus cross electron delocalization in polytriacetylene oligomers: A computational analysis
ChemPhysChem **6** (2005) 511-519
- 05.40 M.A. Kastenholz
Electrostatic interactions in computer simulations of (bio-)molecular system
Thesis Nr. 16342, ETH Zürich. 2005
- 05.41 M. Bruschi
Electron delocalization in linearly π -conjugated compounds; a new approach of analysis
Thesis Nr. 16343, ETH Zürich. 2005
- 05.42 D. Trzesniak, A. Glättli, B. Jaun and W.F. van Gunsteren
Interpreting NMR data for β -peptides using molecular dynamics simulations
J. Am. Chem. Soc. **127** (2005) 14320-14329

- 05.43 S.J. Marrink, H.J. Risselada and A.E. Mark
Simulation of the order-disorder transformation in lipid bilayers using a coarse grained model
Chem. Phys. Lip. **135** (2005) 223-244
- 05.44 A.H. de Vries, S. Yefimov, A.E. Mark and S.J. Marrink
Molecular structure of the lecithin ripple phase
Proc. Natl. Acad. Sci. **102** (2005) 5392-5396
- 05.45 A. Pineiro, A. Villa, T. Vagt, B. Koks, and A.E. Mark
A molecular dynamics study of the formation, stability, and oligomerization state of two designed coiled coils: possibilites and limitations
Biophys. J. **89** (2005) 3701-3713
- 05.46 S. Donnini, A.E. Mark, A. H. Juffer, A. Villa
Incorporating the Effect of Ionic Strength in Free Energy Calculations Using Explicit Ions
J. Comput. Chem. **26** (2005) 115.122
- 05.47 D. Kovalskyy, V. Dubyna, A.E. Mark, A. Kornelyuk
A Molecular Dynamics Study of the Structural Stability of HIV-1 Protease under Physiological Conditions:
The Role of Na⁺ Ions in Stabilizing the Active Site
Proteins: Struct. Funct. Bioinf. **58** (2005) 450-458
- 05.51 D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A.E. Mark, H.J.C. Berendsen
GROMACS: Fast, Flexible, and Free
J. Comput. Chem. **26** (2005) 1701-1718
- 05.52 H. Fan, A.E. Mark, J. Zhu, B. Honig
Comparative study of generalized Born models
Proc. Natl. Acad. Sci. **102** (2005) 6760-6764
- 05.53 M. Schenk, B. Smit, T.L.M. Maesen, T.J.H. Vlugt
Molecular simulations of the adsorption of cycloalkanes in MFI-Type silica
Phys. Chem. Chem. Phys. **7** (2005) 2622-2628
- 2006**
- 06.01 P.J. Gee and W.F. van Gunsteren
Numerical simulation of the effect of solvent viscosity on the motions of a beta-peptide heptamer
Chem. Eur. J. **12** (2006) 72-75
- 06.02 P.J. Gee and W.F. van Gunsteren
Acetonitrile revisited: a molecular dynamics study of the liquid phase
Mol. Phys. **104** (2006) 477-483
- 06.03 I. Chandrasekhar, W.F. van Gunsteren, G. Zandomeneghi, P.T.F. Williamson and B. Meier
Orientation and conformational preference of Leucine-Enkephalin at the surface of a hydrated dimyristoylphosphatidylcholine bilayer: NMR and MD simulation
J. Am. Chem. Soc. **128** (2006) 159-170 and suppl. material
- 06.04 P.J. Gee and W.F. van Gunsteren
Terminal-group effects on the folding behaviour of selected beta-peptides
Proteins: Struct. Funct. Bioinf. **63** (2006) 136-143
- 06.05 B. Zagrovic and W.F. van Gunsteren
Comparing atomistic simulation data with the NMR experiment: How much can NOE's actually tell us?
Proteins: Struct. Funct. Bioinf. **63** (2006) 210-218
- 06.06 D.P. Geerke and W.F. van Gunsteren
Force field evaluation for biomolecular simulation: Free enthalpies of solvation of polar and apolar compounds in various solvents
ChemPhysChem **7** (2006) 671-678

- 06.07 Y. Zhou, C. Oostenbrink, A. Jongejan, W.F. van Gunsteren, W.R. Hagen, S.W. de Leeuw, J.A. Jongejan
Computational study of ground state chiral induction in small peptides: Comparison of the relative stability of selected amino acid dimers and oligomers in homochiral and heterochiral combinations
J. Comput. Chem. **27** (2006) 857–867
- 06.08 P.J. Gee and W.F. van Gunsteren
Numerical simulation of the pressure-denaturation of a helical beta-peptide heptamer solvated in methanol
Helv. Chim. Acta **89** (2006) 475-482
- 06.09 M.A. Cuendet
Statistical mechanical derivation of the Jarzynski identity for non-Hamiltonian thermostated dynamics
Phys. Rev. Lett. **96** (2006) 120602 (DOI: 120602)
- 06.10 M.A. Kastenholz and P.H. Hünenberger
Computation of methodology-independent ionic solvation free energies from molecular simulations: I. The electrostatic potential in molecular liquids
J. Chem. Phys. **124** (2006) 124106 (DOI: 10.1063/1.2172593)
- 06.11 M.A. Kastenholz and P.H. Hünenberger
Development of a lattice-sum method emulating nonperiodic boundary conditions for the treatment of electrostatic interactions in molecular simulations: A continuum-electrostatics study
J. Chem. Phys. **124** (2006) 124108 (DOI: 10.1063/1.2177249)
- 06.12 R. Baron, A.H. de Vries, P.H. Hünenberger, W.F. van Gunsteren
Comparison of atomic-level and coarse-grained models for liquid hydrocarbons from molecular dynamics configurational entropy estimates
J. Phys. Chem. B **110** (2006) 8464-8473
- 06.13 C. S. Pereira, D. Kony, R. Baron, M. Müller, W.F. van Gunsteren, P.H. Hünenberger
Conformational and dynamical properties of disaccharides in water: a molecular dynamics study
Biophys. J. **90** (2006) 4337-4344
- 06.14 V. Kräutler and P.H. Hünenberger
A multiple-timestep algorithm compatible with a large number of distance classes and an arbitrary distance dependence of the timestep size for the fast evaluation of non-bonded interactions in molecular simulations
J. Comput. Chem. **27** (2006) 1163-1176
- 06.15 M.A. Kastenholz and P.H. Hünenberger
Computation of methodology-independent ionic solvation free energies from molecular simulations: II. The hydration free energy of the sodium cation
J. Chem. Phys. **124** (2006) 224501 (DOI: 10.1063/1.2201698)
- 06.16 W.F. van Gunsteren, D. Bakowies, R. Baron, I. Chandrasekhar, M. Christen, X. Daura, P. Gee, D.P. Geerke, A. Glättli, P.H. Hünenberger, M.A. Kastenholz, C. Oostenbrink, M. Schenk, D. Trzesniak, N.F.A. van der Vegt and H.B. Yu
Biomolecular modelling: goals, problems, perspectives
Angew. Chem. **118** (2006) 4168-4198
Angew. Chem. Int. Ed. **45** (2006) 4064-4092
- 06.17 J. Dolenc, R. Baron, C. Oostenbrink, J. Koller and W.F. van Gunsteren
Configurational entropy change of netropsin and distamycin upon DNA minor-groove binding
Biophysical J. **91** (2006) 1460-1470
- 06.18 R. Baron, A.H. de Vries, P.H. Hünenberger and W.F. van Gunsteren
Configurational entropies of lipids in pure and mixed bilayers from atomic level and coarse-grained molecular dynamics simulations
J. Phys. Chem. B **110** (2006) 15602-15614 and suppl. material
- 06.19 D. Seebach, D.F. Hook, A. Glättli
Helices and other secondary structures of β - and γ -peptides
Biopolymers (Peptide Science) **84** (2006) 23-37

- 06.20 N.F.A. van der Vegt, M.-E. Lee, D. Trzesniak, W.F. van Gunsteren
Enthalpy-entropy compensation in the effects of urea on hydrophobic interactions
J. Phys. Chem. B **110** (2006) 12852-12855
- 06.21 C.S. Pereira and P.H. Hünenberger
Interaction of the sugars trehalose, maltose and glucose with a phospholipid bilayer: a comparative molecular dynamics study
J. Phys. Chem. B **110** (2006) 15572-15581 and suppl. material
- 06.22 H. Yu, D.P. Geerke, H. Liu and W.F. van Gunsteren
Molecular dynamics simulations of liquid methanol and methanol-water mixtures with polarizable models
J. Comput. Chem. **27** (2006) 1494-1504
- 06.23 R. Baron
Biomolecular simulation: calculation of entropy and free energy, polypeptide and carbopeptoid folding, simplification of the force field for lipid simulations.
Thesis Nr. 16584, ETH Zürich, 2006
- 06.24 M. Christen
Algorithms and software for efficient biomolecular simulation
Thesis Nr. 16564, ETH Zürich, 2006
- 06.25 M. Christen, A.-P.E. Kunz, W.F. van Gunsteren
Sampling of rare events using hidden restraints
J. Phys. Chem. B **110** (2006) 8488-8498
Erratum: *J. Phys. Chem. B* **112** (2008) 11446, (DOI: 10.1021/jp806613d)
- 06.26 D. Trzesniak, R.D. Lins, W.F. van Gunsteren
A protein under pressure: Molecular dynamics simulation of the Arc repressor
Proteins: Struct. Funct. Bioinf. **65** (2006) 136-144
- 06.27 V. Kräutler
Classical Molecular Dynamics Simulation: Contributions to Methodology Development and Applications to Biomolecular Systems
Thesis Nr. 16662, ETH Zürich, 2006
- 06.28 M. Christen and W.F. van Gunsteren
Multigraining: an algorithm for simultaneous fine-grained and coarse-grained simulation of molecular systems
J. Chem. Phys. **124** (2006) 154106 (DOI: 10.1063/1.2187488)
- 06.29 M.A. Kastenholz, T.U. Schwartz, P.H. Hünenberger
The transition between the B and Z conformations of DNA investigated by targeted molecular dynamics simulations with explicit solvation
Biophys. J. **91** (2006) 2976-2990
- 06.30 M.A. Cuendet
The Jarzynski identity derived from general Hamiltonian or non-Hamiltonian dynamics reproducing NVT or NPT ensembles
J. Chem. Phys. **125** (2006) 144109 (DOI: 10.1063/1.2338535)
- 06.31 D. Trzesniak, W.F. van Gunsteren
Pathway dependence of the efficiency of calculating free energy and entropy of solute-solute association in water
Chem. Phys. **330** (2006) 410-416 (DOI:10.1016/j.chemphys.2006.09.012)
- 06.32 D. Trzesniak
Interplay between computer simulations and experimental data in physical chemistry and structural biology: testing, interpretation and prediction
Thesis Nr. 16661, ETH Zürich, 2006

- 06.33 D. Trzesniak, A.-P.E. Kunz, W.F. van Gunsteren
 A comparison of methods to compute a potential of mean force
ChemPhysChem **8** (2007) 162-169 (DOI: 10.1002/cphc.200600527)
- 06.34 D. Trzesniak, B. Jaun, R.I. Mathad, W.F. van Gunsteren
 Simulation of an all- β^3 -icosapeptide containing the twenty proteinogenic side chains: effect of temperature, pH, counterions, solvent and force field on helix stability
Biopolymers **83** (2006) 636-645 and supporting mat. on-line DOI: 10.1002/bip.20601
- 06.35 T. Heinz
 Computer simulation of molecular systems: new algorithms and selected applications
 Thesis Nr. 16608, ETH Zürich, 2006
- 06.36 M.A. Cuendet
 Aspects of thermostated and noautonomous molecular dynamics
 Thesis Nr. 16863, ETH Zürich, 2006
- 06.37 H. Yu, A. Kohl, H.K. Binz, A. Plückthun, M.G. Grütter and W.F. van Gunsteren
 Molecular Dynamics Study of the Stabilities of Consensus Designed Repeat Proteins
Proteins: Struct. Funct. Bioinf. **65** (2006) 285-295
- 06.38 D. Trzesniak, W.F. van Gunsteren
 Catalytic mechanism of Cyclophilin as observed in molecular dynamics simulations: pathway prediction and reconciliation of X-ray crystallographic and NMR solution data
Protein Science **11** (2006) 2544-2551 and supporting mat.
- 06.39 A. Villa, A.E. Mark, G.A.A. Saracino, U. Cosentino, D. Pitea, G. Moro, M. Salmona
 Conformational polymorphism of the PrP106-126 peptide in different environments: A molecular dynamics study
J. Phys. Chem. B **110** (2006) 1423-1428
- 06.40 T.A. Wassenaar, A.E. Mark
 The effect of Box shape on the dynamic properties of proteins simulated under periodic boundary conditions
J. Comput. Chem. **27** (2006) 316-325
- 06.41 V. Knecht, A.E. Mark, S.-J. Marrink
 Phase Behavior of a Phospholipid/Fatty Acid/Water Mixture Studied in Atomic Detail
J. Am. Chem. Soc. **128** (2006) 2030-2034
- 06.42 H. Fan, A.E. Mark
 Mimicking the action of GroEL in molecular dynamics simulations: Application to the refinement of protein structures
Prot. Sci. **15** (2006) 441-448
- 06.43 H. Fan, X. Wang, J. Zhu, G.T. Robillard, A.E. Mark
 Molecular Dynamics simulations of the Hydrophobin SC3 at a Hydrophobic/Hydrophilic Interface
Proteins: Struct. Funct. Bioinf. **64** (2006) 863-873
- 06.44 D.P. Tieleman, S.-J. Marrink
 Lipids Out of Equilibrium: Energetics of Desorption and Pore Mediated Flip-Flop
J. Am. Chem. Soc. **128** (2006) 12462-12467
- 06.45 H. Leontiadou, A.E. Mark, S.-J. Marrink
 Antimicrobial Peptides in Action
J. Am. Chem. Soc. **128** (2006) 12156-12161
- 06.46 T. Kampmann, D.S. Mueller, A.E. Mark, P. R. Young, B. Kobe
 The Role of Histidine Residues in Low-pH-Mediated Viral Membrane Fusion
Structure **14** (2006) 1481-1487

- 06.47 L. Smith, R.J. Davies and W.F. van Gunsteren
 Molecular dynamics simulations of *Hydrogenobacter thermophilus* cytochrome c₅₅₂; Comparisons of the wild type protein, a b-type variant and the Apo state
Proteins: Struct. Funct. Bioinf. **65** (2006) 702-711
- 06.48 R. Baron, W.F. van Gunsteren and P.H. Hünenberger
 Estimating the configurational entropy from molecular dynamics simulations: anharmonicity and correlation corrections to the quasi-harmonic approximation
Trends in Physical Chemistry **11** (2006) 87-122
- 2007**
- 07.01 B. Keller, M. Christen, C. Oostenbrink and W.F. van Gunsteren
 On using oscillating time-dependent restraints in MD simulation
J. Biomol. NMR **37** (2007) 1-14
- 07.02 C. Oostenbrink, M.M.H. van Lipzig and W.F. van Gunsteren
 Applications of molecular dynamics simulations in drug design
 In "Comprehensive Medicinal Chemistry II" Vol. 4, Computer-Assisted Drug Design, J.B. Taylor and D.J. Triggle Eds., Elsevier, Amsterdam, 2007, 651-668
- 07.03 R. Baron, D. Trzesniak, A.H. de Vries, A. Elsener, S.J. Marrink, W.F. van Gunsteren
 Comparison of thermodynamic properties of coarse-grained and atomic-level simulation models
ChemPhysChem **8** (2007) 452-461, incl. supp. mat
- 07.04 B. Zagrovic, W.F. van Gunsteren
 Computational analysis of the mechanism and thermodynamics of inhibition of phosphodiesterase 5A by synthetic ligands
J. Chem. Theory Comput. **3** (2007) 301-311, incl. supp. material
- 07.05 Z. Gattin, A. Glättli, B. Jaun, W.F. van Gunsteren
 Simulation of beta-depsipeptides: The effect of missing hydrogen-bond donors on their folding equilibria
Biopolymers **85** (2007) 318-332, incl. supp. mat.
- 07.06 D. Trzesniak, N.F.A. van der Vegt, W.F. van Gunsteren
 Analysis of neo-pentane-urea pair potentials of mean force in aqueous urea
Mol. Phys. **105** (2007) 33-39
- 07.07 M. E. Siwko, S.J. Marrink, A.H. de Vries, A. Kozubek, A.J.M. Schoot Uiterkamp, A.E. Mark
 Does isoprene protect plant membranes from thermal shock? A molecular dynamics study
Biochimica et Biophysica Acta **1768** (2007) 198-206
- 07.08 X. Periole, A.E. Mark
 Convergence and sampling efficiency in replica exchange simulations of peptide folding in explicit solvent
J. Chem. Phys. **126** (2007) 014903 (DOI 10.1063/1.2404954, Art. No. 014903)
- 07.09 N. Schmid, B. Zagrovic, W.F. van Gunsteren
 Mechanism and thermodynamics of binding of the polypyrimidine tract binding protein to RNA
Biochemistry **46** (2007) 6500-6512 (DOI: 10.1021/bi60626133)
- 07.10 C.D. Christ, W.F. van Gunsteren
 Enveloping Distribution Sampling: A method to calculate free energy differences from a single simulation
J. Chem. Phys. **126** (2007) 184110 (DOI: 10.1063/1.2730508)
- 07.11 D.B. Kony, P.H. Hünenberger, W.F. van Gunsteren
 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 **16** (2007) 1101-1118
- 07.12 W.F. van Gunsteren, Z. Gattin
 Simulation of folding equilibria
 In: "Foldamers: Structure, properties and applications" S. Hecht & I. Huc eds., Wiley, Weinheim, Germany, 2007, 173-192

- 07.13 M. Christen, C.D. Christ, W.F. van Gunsteren
 Free energy calculations using flexible-constrained, hard-constrained and non-constrained MD simulations
ChemPhysChem. **8** (2007) 1557-1564 (DOI: 10.1002/cphc.200700176)
- 07.14 J.H. Missimer, M.O. Steinmetz, R. Baron, F.K. Winkler, R.A. Kammerer, X. Daura, W.F. van Gunsteren
 Configurational entropy elucidates the role of salt-bridge networks in protein thermostability
Prot. Sci. **16** (2007) 1349-1359 incl. supporting material (DOI: 10.1110/ps.062542907)
- 07.15 M.I. El-Barghouthi, M. Schenk, M.B. Zughul, A.A. Badwan, W.F. van Gunsteren
 Comparison of estimates of free energy for binding of mono- and di-substituted benzenes with alpha-cyclodextrin obtained by single-step perturbation and thermodynamic integration
J. Incl. Phenom Macrocycl. Chem. **57** (2007) 375-377 (DOI: 10.1007/s10847-006-9257-0)
- 07.16 D.B. Kony, W. Damm, S. Stoll, W.F. van Gunsteren, P.H. Hünenberger
 Explicit-solvent molecular dynamics simulations of the polysaccharide schizophyllan in water
Biophys. J. **93** (2007) 442-455 (DOI: 10.1529/biophysj.106.086116)
- 07.17 E.S. Leite, S.R. Santana, P.H. Hünenberger, L.C.G. Feitas, R.L. Longo
 On the relative stabilities of the alkaly cations 222 cryptates in the gas phase and in water-methanol solution
J. Mol. Modl. **13** (2007) 1017-1025 (DOI: 10.1007/s00894-007-0213-8)
- 07.18 V. Kräutler, M. Müller, P.H. Hünenberger
 Conformation, dynamics, solvation and relative stabilities of selected beta-hexopyranoses in water: a molecular dynamics study with the GROMOS 45A4 force field.
Carbohydr. Res. **342** (2007) 2097-2124, incl. supp. Material
- 07.19 M. Christen, W.F. van Gunsteren
 On searching in, sampling of, and dynamically moving through conformational space of biomolecular systems: a review
J. Comput. Chem. **29** (2007) 157-166 (DOI: 10.1002/jcc.20725)
- 07.20 D. Bakowies
 Extrapolation of electron correlation energies to finite and complete basis set targets
J. Chem. Phys. **127** (2007) 084105, incl. supp. mat. (DOI: 10.1063/1.2749516)
- 07.21 D.P. Geerke, W.F. van Gunsteren
 The performance of non-polarizable and polarizable force-field parameter sets for ethylene glycol in molecular dynamics simulation of the pure liquid and its aqueous mixtures
Mol. Phys. **105** (2007) 1861-1881
- 07.22 W. F. van Gunsteren, D.P. Geerke, C. Oostenbrink, D. Trzesniak, N. F. A. van der Vegt
 Analysis of the driving forces for biomolecular solvation and association
 In: "Protein Folding and Drug Design", Proceedings of the Int. School of Physics "Enrico Fermi", course CLXV, R.A. Broglia, L. Serrano and G. Tiana, eds., IOS Press, Amsterdam – SIF, Bologna (2007), pp 177-191
- 07.23 D. Bakowies
 Accurate extrapolation of electron correlation energies from small basis sets
J. Chem. Phys. **127** (2007) 164109, incl. supp. mat.
- 07.24 N. Schmid, B. Zagrovic, W.F. van Gunsteren
 Folding-unfolding equilibrium of a methylene substituted beta-peptide
Helv. Chim. Acta **90** (2007) 1966-1979
- 07.25 D.P. Geerke, St. Thiel, W. Thiel, W.F. van Gunsteren
 QM-MM Interactions in Simulations of Liquid Water using Combined Semi-Empirical/Classical Hamiltonians
Phys. Chem. Chem. Phys. **10** (2008) 297-302 (DOI: 10.1039/b713197f)

- 07.26 D.P. Geerke, W.F. van Gunsteren
On the calculation of atomic forces in classical simulation using the charge-on-spring method to explicitly treat electronic polarisation
J. Chem. Theory Comput. **3** (2007) 2128-2137 (DOI: 10.1021/ct700164k)
- 07.27 M.A. Cuendet, W.F. van Gunsteren
On the calculation of velocity-dependent properties in molecular dynamics simulations using the leap-frog integration algorithm
J. Chem. Phys. **127** (2007) 184102 (DOI: 10.1063/1.2779878)
- 07.28 D.P. Geerke, St. Thiel, W. Thiel, W. F. van Gunsteren
Combined QM/MM molecular dynamics study on a condensed-phase S_N2 reaction at saturated nitrogen: the effect of explicitly including solvent polarization
J. Chem. Theory Comput. **3** (2007) 1499-1509 (DOI: 10.1021/ct7000123)
- 07.29 M. Christen, B. Keller and W.F. van Gunsteren
Biomolecular structure refinement based on adaptive restraints using local-elevation simulation
J. Biomol. NMR **39** (2007) 265-273 (DOI: 10.1007/s10858-007-9194-2)
- 07.30 D. Geerke
Classical Hamiltonians in molecular simulation: force-field development and explicit inclusion of electronic polarization and quantum effects
Thesis Nr. 17348, ETH Zurich, 2007
- 07.31 M. Winger, H. Yu, Ch. Redfield, W.F. van Gunsteren
Molecular dynamics simulation of human interleukin-4: comparison with NMR data and effect of pH, counterions and force field on tertiary structure stability
Molecular Simulation **33** (2007) 1143-1154
- 07.32 B. Zagrovic
Helical signature motif in the fiber diffraction patterns of random-walk chains
Mol. Phys. **105** (2007) 1299-1306
- 07.33 S. Takahashi, H. Satoh, Y. Hongo, H. Koshino
Structural Revision of Terpenoids with a (3Z)-2-Methyl-3-penten-2-ol Moiety by the Synthesis of (23E)- and (23Z)-Cycloart-23-ene-3 α ,25-diols"
J. Org. Chem. **72** (2007) 4578-4581
- 07.34 H. Satoh
Numerical Representation of Stereochemical Environments by Using FRAU
Croatica Chimica Acta **80** (2007) 217-225
- 07.35 S. Koichi, S. Iwata, T. Uno, H. Koshino, H. Satoh
Algorithm for Advanced Canonical Coding of Planar Chemical Structures that Considers Stereochemical and Symmetric Information
J. Chem. Inf. Model. **47** (2007) 1734-1746
- 07.36 A. Elsener, C.C.M. Samson, M.P. Brändle, P. Bühlmann, H.P. Lüthi
Statistical Analysis of Quantum Chemical Data Using Generalized XML/CML Archives for the Derivation of Molecular Design Rules
Chimia **61** (2007) 165–168
- 07.37 D.P. Geerke, W.F. van Gunsteren
Calculation of the free energy of polarization: quantifying the effect of explicitly treating electronic polarization on the transferability of force-field parameters
J. Phys. Chem. B **111** (2007) 6425-6436
- 07.38 M. Terzer, M. Jovanovic, A. Choutko, O. Nikolayeva, A. Korn, D. Brockhoff, F. Zürcher, M. Friedmann, R. Schütz, E. Zitzler, J. Stelling, S. Panke
Design of a biological half ladder
IET Synth.Biol **1** (2007) 53-58

2008

- 08.01 M.O. Steinmetz, Z. Gattin, R. Verel, B. Ciani, T. Stromer, J.M. Green, P. Tittmann, C. Schultze-Brise, H. Gross, W.F. van Gunsteren, B.H. Meier, L.C. Serpell, S.A. Müller, R. Kammerer
Atomic model of *de novo* designed cc β -Met amyloid-like fibrils
J. Mol. Biol. **376** (2008) 898-912
- 08.02 Z. Gattin, W.F. van Gunsteren
A molecular dynamics study of the ASC and NALP1 Pyrin domains at low pH
ChemBioChem **9** (2008) 923-933, DOI: 10.1002/cbic.200700434
- 08.03 R. Boned, W.F. van Gunsteren, X. Daura
Estimating the temperature dependence of peptide-folding entropies and free enthalpies from total energies in molecular dynamics simulations
Chem. Eur. J. **14** (2008) 5039-5046, DOI: 10.1002/chem.200701380
- 08.04 W.F. van Gunsteren, J. Dolenc
Biomolecular simulation: historical picture and future perspectives
Biochem. Soc. Trans. **36** (2008) 11-15, DOI: 10.1042/BST0360011
- 08.05 W.F. van Gunsteren, J. Dolenc, A.E. Mark
Molecular simulation as an aid to experimentalists
Curr. Opin. Struct. Biology **18** (2008) 149-153, DOI: 10.1016/j.sbi.2007.12.007
- 08.06 B. Zagrovic, Z. Gattin, J. Kai-Chi Lau, M. Huber, W.F. van Gunsteren
Structure and dynamics of two β -peptides in solution from molecular dynamics simulations validated against experiment
Eur. Biophys. J. **6** (2008) 903-912, DOI: 10.1007/s00249-008-0307-y
- 08.07 P.A. Limacher, H.P. Lüthi
2,3-Diphenylbutadiene and donor-acceptor functionalized derivatives: Exploring the competition between conjugation paths in branched pi-systems
J. Phys. Chem. A **112** (2008) 2913-2919
- 08.08 C.D. Christ, W.F. van Gunsteren
Multiple free energies from a single simulation: Extending enveloping distribution sampling to non-overlapping phase-space distributions
J. Chem. Phys. **128** (2008) 174112, DOI: 10.1063/1.293050
Erratum: *J. Chem. Phys.* **134** (2011) 229901, DOI: 10.1063/1.3596725
- 08.09 J. Dolenc, R. Baron, J.H. Missimer, M.O. Steinmetz, W.F. van Gunsteren
Exploring the conserved water sites and hydration of a coiled-coil trimerization motif: a MD simulation study
ChemBioChem **9** (2008) 1749-1756, DOI: 10.1002/cbic.200800096
- 08.10 V. Kräutler, P.H. Hünenberger
Explicit-solvent molecular dynamics simulations of a DNA tetradecanucleotide duplex: lattice-sum versus reaction-field electrostatics
Molecular Simulation **34** (2008) 491-499
- 08.11 T. Todorova, P.H. Hünenberger, J. Hutter
Car-Parrinello molecular dynamics simulation of CaCl₂ aqueous solutions
J. Chem. Theory Comput. **4** (2008) 779-789
- 08.12 L. Peric, C.S. Pereira, S. Pérez, P.H. Hünenberger
Conformation, dynamics and ion-binding properties of single-chain polyuronates: a molecular dynamics study
Molecular Simulation **34** (2008) 421-446, incl.suppl.mat.
- 08.13 C.S. Pereira, P.H. Hünenberger
The influence of polyhydroxylated compounds on a hydrated phospholipid bilayer: a molecular dynamics study
Molecular Simulation **34** (2008) 403-420

- 08.14 W.F. van Gunsteren, D.P. Geerke
 Computer simulation of biomolecular systems: where do we stand?
 In: "From Computational Biophysics to Systems Biology (CBSB08)", Proceedings John von Neumann Institute for Computing (NIC), Vol. 40, U.H.E. Hansmann, J.H. Meinke, S. Mohanty, W. Nadler, O. Zimmermann, eds., (2008), Jülich, Germany, pp. 49-55
- 08.15 A. Choutko, A. Glättli, W.F. van Gunsteren
 Simulation of the outer membrane protein X in a lipid bilayer and in a micelle
 In: "From Computational Biophysics to Systems Biology (CBSB08)", Proceedings John von Neumann Institute for Computing (NIC), Vol. 40, U.H.E. Hansmann, J.H. Meinke, S. Mohanty, W. Nadler, O. Zimmermann, eds., (2008), Jülich, Germany, pp. 181-184
- 08.16 D.P. Geerke, S. Luber, K.H. Marti, W.F. van Gunsteren
 On the direct calculation of the free energy of quantisation for molecular systems in the condensed phase
J. Comput. Chem. **30** (2008) 514-523, DOI: 10.1002/jcc.21070
- 08.17 F. Schwab, W.F. van Gunsteren, B. Zagrovic
 Computational study of the mechanism and the relative free energies of binding of anticholesteremic inhibitors to squalene-hopene cyclase
Biochemistry **47** (2008) 2945-2951, incl. supp. mat.
- 08.18 C.S. Pereira, P.H. Hünenberger
 The effect of trehalose on a phospholipid membrane under mechanical stress
Biophys. J. **95** (2008) 3525-3534
- 08.19 M. Winger, W.F. van Gunsteren
 Use of molecular dynamics simulation for optimising protein stability: Consensus designed ankyrin repeat proteins
Helv. Chim. Acta **91** (2008) 1605-1613
- 08.20 N. Schmid, Ch. Bolliger, L.J. Smith, W.F. van Gunsteren
 Disulfide bond shuffling in bovine alpha-lactalbumin: MD simulation confirms experiment
Biochemistry **47** (2008) 12104-12107, DOI: 10.1021/bi8013455
- 08.21 Z. Gattin
 Computer simulations of peptides and proteins: a comparison of effects of solute and solvent variation upon simulated and measured observables
Diss. ETH No. 17954
- 08.22 M. Winger
 Classical molecular dynamics simulations at different levels of resolution: force field development and applications
Diss. ETH No. 18076
- 2009**
- 09.01 C.D. Christ, W.F. van Gunsteren
 Simple, efficient, and reliable computation of multiple free energy differences from a single simulation: a reference Hamiltonian parameter update scheme for enveloping distribution sampling (EDS)
J. Chem. Theory Comput. **5** (2009) 276-286, DOI: 10.1021/ct800424v
- 09.02 M. Winger, D. Trzesniak, R. Baron, W.F. van Gunsteren
 On using a too large integration time step in molecular dynamics simulations of coarse-grained molecular models
Phys. Chem. Chem. Phys. **11** (2009) 1934-1941, DOI: 10.1039/b818713d
- 09.03 H. Satoh, J. Hutter, H.P. Lüthi, S. Manabe, K. Ishii, Y. Ito
 Low barrier pathway for *endo*-cleavage induced anomeration of pyranosides with *N*-benzyl-2,3-*trans* Oxazolidinone groups
Eur. J. Org. Chem. **2009** (2009) 1127-1131, DOI: 10.1002/ejoc.200801140
- 09.04 M. Bruschi, P.A. Limacher, J. Hutter, H.P. Lüthi
 A scheme for the evaluation of electron delocalization and conjugation efficiency in linearly π -conjugated systems
J. Chem. Theory. Comput. **5** (2009) 506-514

- 09.05 D. Bakowies
Ab initio thermochemistry using optimal-balance models with isodesmic corrections: the ATOMIC protocol
J. Chem. Phys. **130** (2009) 144113, DOI:10.1063/1.3089241
- 09.06 M.M. Reif, V. Kräutler, M.A. Kastenholz, X. Daura, P.H. Hünenberger
Molecular dynamics simulations of a reversibly-folding beta-heptapeptide in methanol: Influence of the treatment of long-range electrostatic interactions.
J. Phys. Chem. B **113** (2009) 3112-3128, DOI:10.1021/jp807421a
- 09.07 Z. Gattin, J. Schwartz, R.I. Mathad, B. Jaun, W.F. van Gunsteren
Interpreting experimental data by using molecular simulation instead of model building
Chem. Eur. J. **15** (2009) 6389-6398, DOI: 10.1002/chem.200802523, incl. suppl. mat.
- 09.08 Z. Gattin, W.F. van Gunsteren
Influence of backbone fluorine substitution upon the folding equilibrium of a beta-heptapeptide
J. Phys. Chem. B **113** (2009) 8695-8703, DOI: 10.1021/jp811106e
- 09.09 A. Lange, Z. Gattin, H. Van Melckbeke, Ch. Wasmer, A. Soragni, W.F. van Gunsteren, B.H. Meier
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 **10** (2009) 1657-1665, DOI: 10.1002/cbic.200900019, incl. suppl. mat.
- 09.10 M. Winger, M. Christen, W.F. van Gunsteren
On the conformational properties of amylose and cellulose oligomers in solution
Int. J. Carbohydr. Chem **2009** (2009) 307695, DOI:10.1155/2009/307695
- 09.11 M. Winger, A.H. de Vries, W.F. van Gunsteren
Force-field dependence of the conformational properties of α , ω -dimethoxypolyethylene glycol
Mol. Phys. **107** (2009) 1313-1321
- 09.12 D. Wang, B. Jaun, W.F. van Gunsteren
Folding and unfolding of two mixed alpha/beta peptides
ChemBioChem **10** (2009) 2032-2041, DOI: 10.1002/cbic.200900125
- 09.13 C.L. Müller, I.F. Sbalzarini, W.F. van Gunsteren, B. Zagrovic, P. Hünenberger
In the eye of the beholder: inhomogeneous distribution of high-resolution shapes within the random-walk ensemble
J. Chem. Phys. **130** (2009) 214904, DOI: 10.1063/1.3140090
- 09.14 A.P. Kunz, W.F. van Gunsteren
Development of a non-linear classical polarisation model for liquid water and aqueous solutions: COS/D
J. Phys. Chem. A **113** (2009) 11570-11579, DOI:10.1021/jp903164s
- 09.15 C.D. Christ, W.F. van Gunsteren
Comparison of three enveloping distribution sampling Hamiltonians for the estimation of multiple free energy differences from a single simulation
J. Comput. Chem. **30** (2009) 1664-1679, DOI: 10.1002/jcc.21325
- 09.16 Z. Gattin, S.Riniker, P.J. Hore, K.H. Mok, W.F. van Gunsteren
Temperature and urea induced denaturation of the TRP-cage mini protein TC5b: a simulation study consistent with experimental observations
Prot. Sci. **18** (2009) 2090-2099, DOI: 10.1002/pro.223
- 09.17 J.R. Allison, W.F. van Gunsteren
A method to explore protein side chain conformational variability using experimental data
ChemPhysChem **10** (2009) 3213-3228, DOI: 10.1002/cphc.200900400
- 09.18 D. Bakowies
Ab initio thermochemistry with high-level computed isodesmic corrections: Validation of the ATOMIC protocol for a large set of compounds with first-row atoms (H, C, N, O, F)
J. Phys. Chem. A **113** (2009) 11517-11534

- 09.19 H.S. Hansen, P.H. Hünenberger
Using the local elevation method to construct optimized umbrella sampling potentials: calculation of the relative free energies and interconversion barriers of glucopyranose ring conformers in water
J. Comput. Chem. **31** (2010) 1-23, DOI 10.1002/jcc.21253
- 09.20 C.A. Lopez, A. Rzepiela, A.H. de Vries, P.H. Hünenberger, S.J. Marrink
The Martini coarse grained force field: extension to carbohydrates
J. Chem. Theory Comput. **5** (2009) 3195-3210, incl. suppl. mat.
- 09.21 R. Baron, P.H. Hünenberger, J.A. McCammon
Absolute single-molecule entropies from quasi-harmonic analysis of microsecond molecular dynamics: correction terms and convergence properties
J. Chem. Theory Comput. **5** (2009) 3150-3160, incl. suppl. mat.
- 09.22 K.H. Hughes, C.D. Christ, I. Burghardt
Effective-mode representation of non-Markovian dynamics: A hierarchical approximation of the spectral density. I. Application to single surface dynamics
J. Chem. Phys. **131** (2009) 024109, DOI:10.1063/1.3159671
- 09.23 B. Vögeli, T.F. Segawa, D. Leitz, A. Sobol, A. Choutko, D. Trzesniak, W.F. van Gunsteren, R. Riek
Exact distances and internal dynamics of ubiquitin from NOE buildups
J. Am. Chem. Soc. **131** (2009) 17215-17225, DOI: 10.1021/ja905366h
- 09.24 D. Poger, W.F. van Gunsteren, A.E. Mark
A new force field for simulating phosphatidylcholine bilayers
J. Comput. Chem. **31** (2010) 1117-1125, DOI 10.1002/jcc.21396
- 09.25 P.A. Limacher, K.V. Mikkelsen, H.P. Lüthi
On the accurate calculation of polarizabilities and second hyperpolarizabilities of polyacetylene oligomer chains using the CAM-B3LYP density functional
J. Chem. Phys. **130** (2009) 194114, DOI: 10.1063/1.3139023
- 09.26 S. Borini, P.A. Limacher, H.P. Lüthi
A systematic analysis of the structure and (hyper)polarizability of donor-acceptor substituted polyacetylenes using a Coulomb-attenuating density functional
J. Chem. Phys. **131** (2009), 124105, DOI: 10.1063/1.3216825
- 09.27 K.H. Hughes, C.D. Christ, I. Burghardt
Effective-mode representation of non-Markovian dynamics: A hierarchical approximation of the spectral density. II. Application to environment-induced nonadiabatic dynamics
J. Chem. Phys. **131** (2009) 124108, DOI:10.1063/1.3226343
- 09.28 C.D. Christ, A.E. Mark, W.F. van Gunsteren
Basic ingredients of free energy calculations: a review
J. Comput. Chem. **31** (2010) 1569-1582, DOI: 10.1002/jcc.21450
- 09.29 X. Periole, M. Cavalli, S.J. Marrink, M. Ceruso
Combining an elastic network with a coarse-grained molecular force field: structure, dynamics and intermolecular recognition
J. Chem. Theory Comput. **5** (2009) 2531-2543
- 09.30 D. Sengupta, A. Rampioni, S. J. Marrink
Simulations of the C-subunit of ATP-synthase reveal helix rearrangements
Mol. Membr. Biol. **26** (2009) 422-434
- 09.31 H.J. Risselada, S.J. Marrink
The freezing process of small lipid vesicles at molecular resolution
Soft Matter **5** (2009) 4531-4541
- 09.32 H. Lee, A.H. de Vries, S.J. Marrink, R.W. Pastor
A coarse-grained model for polyethylene oxide: conformation and hydrodynamics
J. Phys. Chem. B **113** (2009) 13186-13194

- 09.33 M.J. Hinner, S.J. Marrink, A.H. de Vries.
Location, tilt, and binding: a molecular dynamics study of voltage sensitve dyes in biomembranes
J. Phys. Chem. B **113** (2009) 15807-15819
- 09.34 C.D. Christ
Calculation of multiple free energy differences from a single simulation
Thesis Nr. 18377, ETH Zürich, 2009
- 09.35 B. Keller
Algorithms for the analysis of biomolecular simulations: ensemble averages, marginal distributions, clustering and markov models
Thesis Nr. 18642, ETH Zürich, 2009
- 09.36 L. Peric-Hassler
Computer simulation of carbohydrates
Thesis Nr. 18557, ETH Zürich, 2009
- 09.37 M.M. Reif
Single-ion solvation properties using atomistic simulation
Thesis Nr. 18813, ETH Zürich, 2009
- 2010**
- 10.01 K. Meier, W.F. van Gunsteren
A cyclic β -helical / β -hairpin D, L- α -peptide: study of its folding properties and structure refinement using molecular dynamics
J. Phys. Chem. A **114** (2010) 1852-1859, DOI: 10.1021/jp906218f
- 10.02 W.F. van Gunsteren, M. Winger
Reply to the comment on using a too large integration time step in molecular dynamics simulations of coarse-grained molecular models
Phys. Chem. Chem. Phys. **12** (2010) 2257-2258, DOI: 10.1039/b922516c
- 10.03 B. Keller, Z. Gattin, W.F. van Gunsteren
What stabilizes the 3_{14} -helix in β^3 -peptides? A conformational analysis using molecular simulation
Proteins: Struct. Funct. Bioinf. **78** (2010) 1677-1690, DOI: 10.1002/prot.22685
- 10.04 B. Keller, X. Daura, W.F. van Gunsteren
Comparing geometric and kinetic cluster algorithms for molecular simulation data
J. Chem. Phys. **132** (2010) 074110, DOI: 10.1063/1.3301140
- 10.05 Z. Gattin, J. Zaugg, W.F. van Gunsteren
Structure Determination of a Flexible Cyclic Peptide Based on NMR and MD Simulation 3J -Coupling
ChemPhysChem **11** (2010) 830-835, DOI: 10.1002/cphc.200900501
- 10.06 N. Schmid, M. Bötschi, W.F. van Gunsteren
A GPU solvent-solvent interaction calculation accelerator for biomolecular simulations using the GROMOS software
J. Comput. Chem. **31** (2010) 1636-1643, DOI 10.1002/jcc21447
- 10.07 S. Borini, P.A. Limacher, H.P. Lüthi
Structural Features Analysis and Nonlinearity of End-Cap-Substituted Polyacetylenes
J. Phys. Chem. A **114** (2010) 2221-2229, DOI: 10.1021/jp908439x
- 10.08 Z. Lin, H. Liu, W.F. van Gunsteren
Using one-step perturbation to predict the effect of changing force-field parameters on the simulated folding equilibrium of a β -peptide in solution
J. Comput. Chem. **31** (2010) 2419-2427, DOI: 10.1002/jcc.21534, incl. suppl. mat.
- 10.09 Z. Lin, J.Kornfeld, M. Mächler, W.F. van Gunsteren
Prediction of folding equilibria of differently substituted peptides using one-step perturbation
J. Am. Chem. Soc. **132** (2010) 7276-7278, DOI: 10.1021/ja100879k, incl. suppl. mat.

- 10.10 H. Satoh, H. Hansen, S. Manabe, P.H Hünenberger, W.F. van Gunsteren
 Theoretical Investigation of Solvent Effects on Glycosylation Reactions: Stereoselectivity Controlled by Preferential Conformations of the Intermediate Oxocarbonium - Counterion Complex
J. Chem. Theory Comput. **6** (2010) 1783-1797, DOI: 10.1021/ct1001347, incl. suppl. mat.
- 10.11 D. Wang, M. Friedmann, Z. Gattin, B. Jaun, W.F. van Gunsteren
 The propensity of aminoisobutyric acid (Aib) to induce helical secondary structure in an α -heptapeptide: a computational study
Helv. Chim. Acta **93** (2010) 1513-1531, DOI: 10.1002/hlca.200900420
- 10.12 D. Wang, T. Merz, W.F. van Gunsteren
 The thermal isomerization of the GFP chromophore: a computational study
Phys. Chem. Chem. Phys. **36** (2010) 11051-11061, DOI: 10.1039/C0CP00181C
- 10.13 A.P. Eichenberger, Z. Gattin, G. Yalak, W.F. van Gunsteren
 Molecular dynamics simulation of ester-linked hen egg white lysozyme reveals the effect of missing backbone hydrogen-bond donors on the protein structure
Helv. Chim. Acta **93** (2010) 1857-1869, DOI: 10.1002/hlca.201000077
- 10.14 J. Dolenc, J.H. Missimer, M.O. Steinmetz, W.F. van Gunsteren
 Methods of NMR structure refinement: molecular dynamics simulations improve the agreement with measured NMR data of a C-terminal peptide of GCN4-p1
J. Biomol. NMR **47** (2010) 221-235, DOI: 10.1007/s10858-010-9425-9
- 10.15 J.R. Allison, G.P. Moll, W.F. van Gunsteren
 Investigation of stability and disulfide bond shuffling of lipid transfer proteins by molecular dynamics simulation
Biochemistry **49** (2010) 6916-6927, DOI: 10.1021/bi100383m, incl. suppl. mat
- 10.16 L. Peric-Hassler, H.S. Hansen, R. Baron, P.H. Hünenberger
 Conformational properties of glucose-based disaccharides investigated using molecular dynamics simulations with local elevation umbrella sampling
Carbohydrate Res. **345** (2010) 1781-1801, DOI: 10.1016/j.carres.2010.05.026, incl. suppl. mat
- 10.17 J. Dolenc, S. Gerster, W.F. van Gunsteren
 Molecular dynamics simulations shed light on the enthalpic and entropic driving forces that govern the sequence specific recognition between netropsin and DNA
J. Phys. Chem. B **114** (2010) 11164-11172, DOI: 10.1021/jp100483f, incl. suppl. mat
- 10.18 B.A.C. Horta, A.H. de Vries, P.H. Hünenberger
 Simulating the transition between gel and liquid-crystal phases of lipid bilayers: dependence of the transition temperature on the hydration level
J. Am. Chem. Soc. **6** (2010) 2488-2500, DOI: 10.1021/ct100200w
- 10.19 V. Kräutler, S. Hiller, P.H. Hünenberger
 Residual structure in a peptide fragment of the outer membrane protein X under denaturing conditions: a molecular dynamics study
Eur. Biophys. J. **39** (2010) 1421-1432, DOI: 10.1007/s00249-010-0596-9
- 10.20 Z. Lin, A.P. Kunz, W.F. van Gunsteren
 A one-site polarizable model for liquid chloroform: COS/C
Mol. Phys. **108** (2010) 1749-1757, DOI: 10.1080/00268976.2010.489527
- 10.21 D.P. Geerke, W.F. van Gunsteren, P.H. Hünenberger
 Molecular dynamics simulations of the interaction between polyhydroxylated compounds and Lennard-Jones walls: preferential affinity/exclusion effects and their relevance for bioprotection
Molecular Simulation **36** (2010) 708-728, DOI: 10.1080/08927021003752804
- 10.22 D. Flemming Hansen, Ph. Neudecker, P. Vallurupalli, F.A.A. Mulder, L.E. Kay
 Determination of Leu side-chain conformations in excited protein states by NMR relaxation dispersion
J. Am. Chem. Soc. **132** (2010) 42-43, DOI: 10.1021/ja909294n

- 10.23 R. Otten, B. Chu, K. D. Krewulak, H.J. Vogel, F.A.A. Mulder
 Comprehensive and cost-effective NMR spectroscopy of methyl groups in large proteins
J. Am. Chem. Soc. **132** (2010) 2952-2960, DOI: 10.1021/ja907706a
- 10.24 M. Fuhrmans, B.P. Sanders, S.J. Marrink, A.H. de Vries
 Effects of bundling on the properties of the SPC water model
Theor. Chem. Acc. **125** (2010) 335-344, DOI: 10.1007/s00214-009-0590-4
- 10.25 S. Baoukina, S.J. Marrink, D.P. Tieleman
 Lateral pressure profiles in lipid monolayers
Farad. Discuss. **144** (2010) 393-409, DOI: 10.1039/b905647e
- 10.26 T. Apajalahti, P. Niemela, P.N. Govindan, M. Miettinen, E. Salonen, S.J. Marrink, I. Vattulainen
 Concerted diffusion of lipids in raft-like membranes
Farad. Discuss. **144** (2010) 411-430, DOI: 10.1039/b901487j
- 10.27 A. Rzepiela, D. Sengupta, N. Goga, S.J. Marrink
 Membrane poration by antimicrobial peptides combining atomistic and coarse grained descriptions
Farad. Discuss. **144** (2010) 431-443, DOI: 10.1039/b901615e
- 10.28 A.J. Rzepiela, L.V. Schäfer, N.Goga, H.J.Risselada, A.H. de Vries, S.J. Marrink
 Reconstruction of atomistic details from coarse grained structures
J. Comput. Chem. **31** (2010) 1333-1343, DOI: 10.1002/jcc.21415
- 10.29 K. Wood, D.J. Tobias, B. Kessler, F. Gabel, D. Oesterhelt, F.A.A. Mulder
 G. Zaccai, M. Weik
 The low-temperature inflection observed in neutron scattering measurements of proteins is due to methyl rotation: direct evidence using isotope labeling and molecular dynamics simulations
J. Am. Chem. Soc. **132** (2010) 4990-4991, DOI: 10.1021/ja910502g
- 10.30 J.A. Lycklama a Nijeholt, M. Bulacu, S.J. Marrink, A.J.M. Driessens
 Immobilization of the plug domain inside the SecY channel allows unrestricted protein translocation
J. Biol. Chem. **285** (2010) 23747-23754, DOI: 10.1074/jbc.M110.124636
- 10.31 S. Yesylevskyy, L.V. Schafer, D. Sengupta, S.J. Marrink
 Polarizable water model for the coarse-grained Martini force field
Comp. Biol. **6** (2010) e1000810, DOI: 10.1371/journal.pcbi.1000810
- 10.32 Y.G. Smirnova, S.J. Marrink, R. Lipowsky, V. Knecht
 Solvent-exposed tails as pre-stalk transition states for membrane fusion
J. Am. Chem. Soc. **132** (2010) 6710-6718, DOI: 10.1021/ja910050x
- 10.33 F.A.A. Mulder, M. Lundqvist, R. Scheek
 Nuclear Magnetic Resonance spectroscopy applied to (intrinsically) disordered proteins
 in "Instrumental Analysis of Intrinsically Disordered Proteins: Assessing Structure and Conformation"
 V. Uversky and S. Longhi (Eds.) John Wiley and Sons Ltd, New Jersey (2010)
- 10.34 H. Hansen, X. Daura, P.H. Hünenberger
 Enhanced conformational sampling in molecular dynamics simulations of solvated peptides: Fragment-based local elevation umbrella sampling
J. Chem. Theory Comput. **6** (2010) 2598-2621, DOI: 10.1021/ct1003059
- 10.35 H. Hansen, P.H. Hünenberger
 Ball-and-stick local elevation umbrella sampling: molecular simulations involving enhanced sampling within conformational or alchemical subspaces of low internal dimensionalities, minimal irrelevant volumes and problem-adapted geometries
J. Chem. Theory Comput. **6** (2010) 2622-2646, DOI: 10.1021/ct1003065
- 10.36 L. Peric-Hassler, P.H. Hünenberger
 Interaction of alginate single-chain polygluronate segments with mono- and divalent metal cations: A comparative molecular dynamics study
Molecular Simulation **36** (2010) 778-795, DOI: 10.1080/08927021003752853

- 10.37 S. Bachmann, B. Jaun, W.F. van Gunsteren, D. Wang
 The effect of fluoro substitution upon the β -hairpin fold of a β -tetrapeptide in methanol
Helv. Chim. Acta **93** (2010) 1870-1881, DOI: 10.1002/hlca.201000179
- 10.38 A. Choutko, A. Glättli, C. Fernández, C. Hilty, K. Wüthrich, W.F. van Gunsteren
 Membrane protein dynamics in different environments: simulation study of the outer membrane protein X
 in a lipid bilayer and in a micelle
Eur. Biophys. J. **40** (2011) 39-58, DOI: 10.1007/s00249-010-0626-7
- 10.39 B. Horta, L. Peric-Hassler, P.H. Hünenberger
 Interaction of the disaccharides trehalose and gentiobiose with lipid bilayers:
 A comparative molecular dynamics study
J. Mol. Graph. Model. **29** (2010) 331-346, DOI: 10.1016/j.jmgm.2010.09.013
- 10.40 Z. Lin, W.F. van Gunsteren
 Using one step perturbation to predict the folding equilibrium of differently stereochemically substituted
 β -peptides
Phys. Chem. Chem. Phys. **12** (2010) 15442-15447, DOI: 10.1039/c0cp00833h
- 10.41 J.H. Missimer, J. Dolenc, M.O. Steinmetz, W.F. van Gunsteren
 Exploring the trigger sequence of the GCN4 coiled-coil: biased molecular dynamics resolves apparent
 inconsistencies in NMR measurements
Prot. Sci. **19** (2010) 2462-2474, DOI: 10.1002/pro.528, incl. suppl. mat.
- 10.42 H.S. Hansen
 Enhanced conformational sampling in molecular dynamics simulations
 Thesis Nr. 19141, ETH Zürich, 2010
- 10.43 S. Riniker, X. Daura, W.F. van Gunsteren
 α -Cyclodextrin host-guest binding: A computational study analyzing the different driving forces
Helv. Chim. Acta **93** (2010) 2318-2325, DOI: 10.1002/hlca.201000251, incl. suppl. mat.
- 10.44 J. R. Allison, M. Müller, W.F. van Gunsteren
 A comparison of the different helices adopted by α - and β - peptides suggests different reasons for their
 stability
Prot. Sci. **19** (2010) 2186-2195, DOI: 10.1002/pro.504
- 10.45 L. Korosec, P.A. Limacher, H.P. Lüthi, M.P. Brändle
 Chemical information media in the chemistry lecture hall: A comparative
 assessment of two online encyclopedias
Chimia **64** (2010) 309-314, DOI: 10.2533/chimia2010.309
- 10.46 P.A. Limacher
 Electron delocalization in through and cross conjugated oligomers and its influence on the molecular
 properties
 Thesis Nr. 19211, ETH Zürich, 2010
- 10.47 A.P.E. Kunz
 Refinement of molecular simulation methodology: development of polarisable solvents and techniques to
 enhance configurational sampling
 Thesis Nr. 19479, ETH Zürich, 2010
- 2011**
- 11.01 Z. Lin, N. Schmid, W.F. van Gunsteren
 The effect of using a polarizable solvent model upon the folding equilibrium of different β -peptides
Mol. Phys. **109** (2011) 493-506, DOI: 10.1080/00268976.2010.532163, incl. suppl. mat.
- 11.02 A.P.E. Kunz, A.P. Eichenberger, W.F. van Gunsteren
 A simple, efficient polarisable molecular model for liquid carbon tetrachloride
Mol. Phys. **109** (2011) 365-372, DOI: 10.1080/00268976.2010.533208

- 11.03 S. Riniker, W.F. van Gunsteren
A simple, efficient polarisable coarse-grained water model for molecular dynamics simulations
J. Chem. Phys. **134** (2011) 084110, DOI: 10.1063/1.3553378
Erratum: J. Chem. Phys. **146** (2017) 129901, DOI: 10.1063/1.4979127
- 11.04 Z. Lin, F.H. Hodel, W.F. van Gunsteren
Influence of variation of a side chain on the folding equilibrium of a β -peptide
Helv. Chim. Acta **94** (2011) 597-610, DOI: 10.1002/hlca.201100003, incl. suppl. mat.
- 11.05 H. Hansen, P.H. Hünenberger
A reoptimized GROMOS force field for hexopyranose-based carbohydrates accounting for the relative free energies of ring conformers, anomers, epimers, hydroxymethyl rotamers and glycosidic linkage conformers
J. Comput. Chem. **32** (2011) 998-1032, DOI: 10.1002/jcc.21675
- 11.06 B. Keller, P.H. Hünenberger, W.F. van Gunsteren
An analysis of the validity of Markov state models for emulating the dynamics of classical molecular systems and ensembles
J. Chem. Theory Comput. **7** (2011) 1032-1044, DOI: 10.1021/ct200069c
- 11.07 J.R. Allison, K. Boguslawski, F. Fraternali, W.F. van Gunsteren
A refined, efficient mean solvation force model that includes the interior volume contribution
J. Phys. Chem. B **115** (2011) 4547-4557, DOI: 10.1021/jp2017117, incl. suppl. mat.
- 11.08 B. Horta, P.F.J. Fuchs, W.F. van Gunsteren, P.H. Hünenberger
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.
J. Chem. Theory Comput. **7** (2011) 1016-1031, DOI: 10.1021/ct1006407
- 11.09 A.P.E. Kunz, W.F. van Gunsteren
Enhancing the configurational sampling of ions in aqueous solution using adiabatic decoupling with translational temperature scaling
J. Phys. Chem. B **115** (2011) 2931-2936, DOI: 10.1021/jp110778k
- 11.10 M. Reif, P.H. Hünenberger
Computation of methodology-independent single-ion solvation properties from molecular simulations III. Correction terms for the solvation free energies, enthalpies, entropies heat capacities, volumes, compressibilities and expansibilities of solvated ions
J. Chem. Phys. **134** (2011) 144103, DOI: 10.1063/1.3567020, incl. suppl. mat.
- 11.11 M. Reif, P.H. Hünenberger
Computation of methodology-independent single-ion solvation properties from molecular simulations IV. Optimized Lennard-Jones interaction parameter sets for the alkali and halide ions in water
J. Chem. Phys. **134** (2011) 144104, DOI: 10.1063/1.3567022, incl. suppl. mat.
- 11.12 D. Steiner, C. Oostenbrink, F. Diederich, M. Zürcher, W.F. van Gunsteren
Calculation of binding free energies of inhibitors to Plasmeprin II
J. Comput. Chem. **32** (2011) 1801-1812, DOI: 10.1002/jcc.21761, incl. suppl. mat.
- 11.13 S. Riniker, A.P.E. Kunz, W.F. van Gunsteren
On the calculation of the dielectric permittivity and relaxation time of molecular models in the liquid phase
J. Chem. Theory Comput. **7** (2011) 1469-1475, DOI: org/10.1021/ct100610v
- 11.14 W. Huang, Z. Lin, W.F. van Gunsteren
Validation of the GROMOS 54A7 force field with respect to β -peptide folding
J. Chem. Theory Comput. **7** (2011) 1237-1243, DOI: org/10.1021/ct100747y
- 11.15 Z. Lin, W.F. van Gunsteren, H. Liu
Conformational state-specific free energy differences by one-step perturbation: protein secondary structure preferences of the GROMOS 43A1 and 53A6 force fields
J. Comput. Chem. **32** (2011) 2290-2297, DOI: 10.1002/jcc.21818, incl. suppl. mat.

- 11.16 B.A.C. Horta, P.H. Hünenberger
 Enantiomeric segregation in the gel phase of lipid bilayers
J. Am. Chem. Soc. **133** (2011) 8464-8466, DOI: dx.doi.org/10.1021/ja202479u
- 11.17 P.A. Limacher, H.P. Lüthi
 Cross-conjugation
J.W. & S. Ltd. **1** (2011) 477-486, DOI: 10.1002/wcms.16
- 11.18 H. Satoh, S. Manabe, Y. Ito, H.P. Lüthi, T. Laino, J. Hutter
 Endocyclic cleavage in glycosides with 2,3-*trans* cyclic protecting groups
J. Am. Chem. Soc. **133** (2011) 5610-5619, DOI: dx.doi.org/10.1021/ja201024a
- 11.19 N. Schmid, A.P. Eichenberger, A. Choutko, S. Riniker, M. Winger, A.E. Mark, W.F. van Gunsteren
 Definition and testing of the GROMOS force-field versions 54A7 and 54B7
Eur. Biophys. J. **40** (2011) 843-856, DOI: 10.1007/s00249-011-0700-9, incl. suppl. mat.
- 11.20 S. Riniker, C.D. Christ, N. Hansen, A.E. Mark, P.C. Nair, W.F. van Gunsteren
 Comparison of enveloping distribution sampling and thermodynamic integration to calculate binding free energies of phenylethanolamine N-methyltransferase inhibitors
J. Chem. Phys. **135** (2011) 024105, DOI: 10.1063/1.3604534, incl. suppl. mat.
- 11.21 A. Kuzmanic, D. Kruschel, W.F. van Gunsteren, B. Zagrovic
 Dynamics may significantly influence the estimation of interatomic distances in biomolecular X-ray structures
J. Mol. Biol. **411** (2011) 286-297, DOI: 10.1016/j.jmb.2011.05.033, incl. suppl. mat.
- 11.22 N. Schmid
 Development and application of efficient, object-oriented software for simulation and structure refinement of biomolecules
 Thesis Nr. 19630, ETH Zürich, 2011
- 11.23 A.P.E. Kunz, H. Liu, W.F. van Gunsteren
 Enhanced sampling of particular degrees of freedom in molecular systems based on adiabatic decoupling and temperature or force scaling
J. Chem. Phys. **135** (2011) 104106, DOI: 10.1063/1.3629450, incl. suppl. mat.
- 11.24 J. Dolenc, S. Riniker, R. Gaspari, X. Daura, W.F. van Gunsteren
 Free energy calculations offer insights into the influence of receptor flexibility on ligand-receptor binding affinities
J. Computer-Aided Mol. Des. **25** (2011) 709-716, DOI: 10.1007/s10822-011-9453-x, incl. suppl. mat.
- 11.25 N. Schmid, J.R. Allison, J. Dolenc, A.P. Eichenberger, A.P.E. Kunz, W.F. van Gunsteren
 Biomolecular structure refinement using the GROMOS simulation software
J. Biomolecular NMR. **51** (2011) 265-281, DOI: 10.1007/s10858-011-9534-0
- 11.26 A.P.E. Kunz, W.F. van Gunsteren
 A method for conformational sampling of loops in protein based on adiabatic decoupling and temperature or force scaling
ChemPhysChem **12** (2011) 2609-2614, DOI: 10.1002/cphc.201100305
- 11.27 A.P. Eichenberger, J.R. Allison, J. Dolenc, D.P. Geerke, B.A.C. Horta, K. Meier, C. Oostenbrink, N. Schmid, D. Steiner, D. Wang, W.F. van Gunsteren
 GROMOS++ software for the analysis of biomolecular simulation trajectories
J. Chem. Theory. Comp. **7** (2011) 3379-3390, DOI: 10.1021/ct2003622
- 11.28 Z. Lin, W.F. van Gunsteren
 Exploring the effect of side-chain substitutions upon the secondary structure preferences of β -peptides
J. Phys. Chem. B **115** (2011) 12984-12992, DOI: 10.1021/jp2053508
- 11.29 N. Hansen, P. Kraus, H. Sassmannshausen, T. Timmerscheidt, W.F. van Gunsteren
 An effective force field for molecular dynamics simulations of dimethyl sulfone
Mol. Phys. **109** (2011) 2593-2605, DOI: 10.1080/00268976.2011.624128

- 11.30 S. Riniker, C.D. Christ, H.S. Hansen, P.H. Hünenberger, C. Oostenbrink, D. Steiner, W.F. van Gunsteren
 Calculation of relative free energies for ligand-protein binding, solvation and conformational transitions using the GROMOS software
J. Phys. Chem. B **115** (2011) 13570-13577, DOI: 10.1021/jp204303a
- 11.31 A. Choutko, W.F. van Gunsteren, P.H. Hünenberger
 Preferential affinity of the components of liquid mixtures at a rigid non-polar surface:
 Enthalpic and entropic driving forces
ChemPhysChem **12** (2011) 3214-3223, DOI: 10.1002/cphc201100541
- 11.32 Z. Lin, H. Liu, S. Riniker, W.F. van Gunsteren
 On the use of enveloping distribution sampling (EDS) to compute free enthalpy differences between different conformational states of molecules: application to β_{10} -, α , and λ helices
J. Chem. Theory. Comp. **7** (2011) 3884-3897, DOI: 10.1021/ct200623b, incl. suppl. mat.
- 11.33 J.R. Allison, M. Bergeler, N. Hansen, W.F. van Gunsteren
 Current computer modeling cannot explain why two highly similar sequences fold into different structures
Biochemistry **50** (2011) 10965-10973 DOI: 10.1021/bi2015663, incl. suppl. mat.
- 11.34 D. Steiner
 Molecular simulation of proteins : how to account for conformational variability when calculating relative free energies and 3J -couplings?
 Thesis Nr. 20182, ETH Zürich, 2011
- 2012**
- 12.01 D.A. Niggli, M.O. Ebert, Z. Lin, D. Seebach, W.F. van Gunsteren
 Helical content of a β^3 -octapeptide in methanol:
 Molecular dynamics simulations explain a seeming discrepancy between conclusions derived from CD and NMR data
Chem. Eur. J. **18** (2012), 586-593, DOI: 10.1002/chem.201102667, incl. suppl. mat.
- 12.02 A.P. Eichenberger, L.J. Smith, W.F. van Gunsteren
 Ester-linked hen egg white lysozyme shows a compact fold in a molecular dynamics simulation - possible causes and sensitivity of experimentally observable quantities to structural changes maintaining this compact fold
FEBS Journal **279** (2012), 299-315, DOI: 10.1111/j.1742-4658.2011.08424.x, incl. suppl. mat.
- 12.03 K. Meier, W. Thiel, W.F. van Gunsteren
 On the effect of a variation of the force field, spatial boundary condition and size of the QM region in QM/MM MD simulations
J. Comput. Chem. **33** (2012), 363-378, DOI: 10.1002/jcc.21962
- 12.04 A.P.E. Kunz, J.R. Allison, D.P. Geerke, B.A.C. Horta, P.H. Hünenberger, S. Riniker, N. Schmid, W.F. van Gunsteren
 New functionalities in the GROMOS biomolecular simulation software
J. Comput. Chem. **33** (2012), 340-353, DOI: 10.1002/jcc.21954
- 12.05 N. Schmid, C.D. Christ, M. Christen, A.P. Eichenberger, W.F. van Gunsteren
 Architecture, implementation and parallelization of the GROMOS software for biomolecular simulation
Comp. Phys. Comm. **183** (2012), 890-903, DOI: 10.1016/j.cpc.2011.12.014
- 12.06 N. Hansen, J. Dolenc, M. Knecht, S. Riniker, W.F. van Gunsteren
 Assessment of enveloping distribution sampling to calculate relative free enthalpies of binding for eight netropsin-DNA duplex complexes in aqueous solution
J. Comput. Chem. **33** (2012) 640-651, DOI: 10.1002/jcc.22879, incl. suppl. mat
- 12.07 J.R. Allison, S. Riniker, W.F. van Gunsteren
 Coarse-grained models for the solvents dimethyl sulfoxide, chloroform and methanol
J. Chem. Phys. **136** (2012) 054505, DOI: 10.1063/1.3681140, incl. suppl. mat.

- 12.08 S. Riniker, B.A.C. Horta, B. Thijssen, S. Gupta, W.F. van Gunsteren, P.H. Hünenberger
Temperature dependence of the dielectric permittivity of acetic acid, propionic acid and their methyl esters: A molecular dynamics simulation study
ChemPhysChem **13** (2012) 1182-1190, DOI:10.1002/cphc.201100949
- 12.09 K. Meier
Molecular dynamics simulation based on quantum and classical statistical mechanics: methodological investigations, implementation and perspectives
Thesis Nr. 20352, ETH Zürich, 2012
- 12.10 A.P.E. Kunz, Z. Lin, W.F. van Gunsteren
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
Mol. Phys. **110** (2012) 407-417, DOI:10.1080/00268976.2011.650716
- 12.11 A. Choutko
Simulation of molecular processes and its diverse use in interpreting experimental data: from atomic liquids to biomolecular complexes
Thesis Nr. 20381, ETH Zürich, 2012
- 12.12 D. Steiner, C. Oostenbrink, W.F. van Gunsteren
Calculation of the relative free energy of oxidation of azurin at pH 5 and pH 9
J. Comput. Chem. **33** (2012) 1467-1477, DOI: 10.1002/jcc.22972, incl. suppl. mat.
- 12.13 S. Riniker
Methodology development for classical molecular dynamics simulations
Thesis Nr. 20461, ETH Zürich, 2012
- 12.14 D. Steiner, W.F. van Gunsteren
An improved structural characterisation of reduced french bean plastocyanin based on NMR data and local-elevation molecular dynamics simulation
Eur. Biophys. J. **41** (2012) 579-595, DOI: 10.1007/s00249-012-0824-6, incl. suppl. mat.
- 12.15 D. Steiner, J.R. Allison, A.P. Eichenberger, W.F. van Gunsteren
On the calculation of $^3J_{\alpha\beta}$ -coupling constants for side chains in proteins
J. Biomol. NMR **53** (2012) 223-246, DOI: 10.1007/s10858-012-9634-5, incl. suppl. mat.
- 12.16 S. Riniker, W.F. van Gunsteren
Mixing coarse-grained and fine-grained water in molecular dynamics simulations of a single system
J. Chem. Phys. **137** (2012) 044120, DOI: 10.1063/1.4739068
- 12.17 S. Riniker, A.P. Eichenberger, W.F. van Gunsteren
Structural effects of an atomic-level layer of water molecules around proteins solvated in supra-molecular coarse-grained water
J. Phys. Chem. B **116** (2012) 8873-8879, DOI: 10.1021/jp304188z, incl. suppl. mat.
- 12.18 Z. Lin, T.A. Timmerscheidt, W.F. van Gunsteren
Using enveloping distribution sampling (EDS) to compute the free enthalpy difference between right- and left-handed helices of a β -peptide in solution
J. Chem. Phys. **137** (2012) 064108, DOI: 10.1063/1.4742751, incl. suppl. mat.
- 12.19 S. Riniker, A.P. Eichenberger, W.F. van Gunsteren
Solvating atomic level fine-grained proteins in supra-molecular level coarse-grained water for molecular dynamics simulations
Eur. Biophys. J. **41** (2012) 647-661, DOI: 10.1007/s00249-012-0837-1
- 12.20 B.A.C. Horta, Z. Lin, W. Huang, S. Riniker, W.F. van Gunsteren, P.H. Hünenberger
Reoptimized interaction parameters for the peptide-backbone model compound N-methylacetamide in the GROMOS force field: influence on the folding properties of two beta-peptides in methanol
J. Comput. Chem. **33** (2011) 1907-1917, DOI: 10.1002/jcc.23021

- 12.21 S. Riniker, J.R. Allison, W.F. van Gunsteren
On developing coarse-grained models for biomolecular simulation: a review:
Phys. Chem. Chem. Phys. **14** (2012) 12423-12430, DOI:10.1039/C2CP40934H
- 12.22 W. Huang, A.P. Eichenberger, W.F. van Gunsteren
Molecular dynamics simulation of thionated hen egg white lysozyme
Prot. Sci. **21** (2012) 1153-1161, DOI:10.1002/pro.2102, incl. suppl. mat.
- 12.23 K. Meier, N. Schmid, W.F. van Gunsteren
Interfacing the GROMOS (bio) molecular simulation software to quantum-chemical program packages
J. Comput. Chem. **33** (2012) 2108-2117, DOI: 10.1002/jcc.23047
- 12.24 T.S. Hofer, W.F. van Gunsteren
Exploring the properties of small molecule protein binding via molecular simulation: the TRSH – p53 core domain complex
Mol. BioSyst. **8** (2012) 2891-2900, DOI: 10.1039/c2mb25166c, incl. suppl. mat.
- 12.25 B. Dahlgren, M.M. Reif, P.H. Hünenberger, N. Hansen
Calculation of derivate thermodynamic hydration and aqueous partial molar properties of ions based on atomistic simulations
J. Chem. Theory Comput. **8** (2012) 3542-3564, DOI: 10.1021/ct300260q, incl. suppl. mat.
- 12.26 M.M. Reif, P.H. Hünenberger, C. Oostenbrink
New interaction parameters for charged amino acid side chains in the GROMOS force field
J. Chem. Theory Comput. **8** (2012) 3705-3723, DOI: 10.1021/ct300156h, incl. suppl. mat.
- 12.27 P.F.J. Fuchs, H.S. Hansen, P.H. Hünenberger, B.A.C. Horta
A GROMOS parameter set for vicinal diether functions: properties of polyethyleneoxide and polyethyleneglycol
J. Chem. Theory Comput. **8** (2012) 3943-3963, DOI: 10.1021/ct300245h
- 12.28 P.H. Hünenberger, A.E. Mark, H.J.C. Berendsen
Wilfred van Gunsteren: 35 years of biomolecular simulation
J. Chem. Theory Comput. **8** (2012) 3425-3429, DOI: 10.1021/ct300692s
- 12.29 A. Choutko, W.F. van Gunsteren
Molecular dynamics simulation of the last step of a catalytic cycle: product release from the active site of the enzyme chorismate mutase of mycobacterium tuberculosis
Prot. Sci. **21** (2012) 1672-1681, DOI:10.1002/pro.2143, incl. suppl. mat.
- 12.30 J.R. Allison, S. Hertig, J.H. Missimer, L. J. Smith, M. O. Steinmetz, J. Dolenc
Probing the structure and dynamics of proteins by combining molecular dynamics simulations and experimental NMR data
J. Chem. Theory Comput. **8** (2012) 3430-3444, DOI: 10.1021/ct300393b, incl. suppl. mat.
- 12.31 J.H. Missimer, M.O. Steinmetz, W.F. van Gunsteren, J. Dolenc
Influence of 63Ser phosphorylation and dephosphorylation on the structure of the stathmin helical nucleation sequence: A molecular dynamics study
Biochemistry **51** (2012) 8455-8463, DOI: 10.1021/bi300885y, incl. suppl. mat.
- 12.32 A.P. Eichenberger
Molecular dynamics simulation of alkanes and proteins: methodology, prediction of properties and comparison to experimental data
Thesis Nr.20781, ETH Zürich, 2012
- 12.33 W.F. van Gunsteren, J. Dolenc
Thirty-five years of biomolecular simulation: development of methodology, force fields, and software
Molecular Simulation **38** (2012) 1271-1281, DOI: 10.1080/08927022.2012.701744
- 12.34 J. Kleinjung, W.R.P. Scott, J.R. Allison, W.F. van Gunsteren, F. Fraternali
Implicit solvation parameters derived from explicit water forces in large-scale molecular dynamics simulations
J. Chem. Theory Comput. **8** (2012) 2391-2403, DOI: 10.1021/ct200390j, incl. suppl. mat.

- 12.35 S. Riniker, L.J. Barandun, F. Diederich, O. Krämer, A. Steffen, W.F. van Gunsteren
 Free enthalpies of replacing water molecules in protein binding pockets
J. Computer-Aided Mol. Des. **26** (2012) 1293-1309, incl. suppl. mat.
- 12.36 D. Wang, F. Freitag, Z. Gattin, H. Haberkern, B. Jaun, M. Siwko, R. Vyas, W.F. van Gunsteren, J. Dolenc
 Validation of the GROMOS 54A7 force field regarding mixed α/β peptide molecules
Helv. Chim. Acta **95** (2012) 2562-2577, DOI: 10.1002/hlca.201200534, incl. suppl. mat.
- 12.37 D. Wang, W.F. van Gunsteren, Z. Chai
 Recent advances in computational actinide chemistry
Chem. Soc. Rev. **41** (2012) 5836-5865, DOI: 10.1039/c2cs15354h
Progress in Chemistry **7** (2011) 1566-1581 (Chinese version)
- 2013**
- 13.01 W.F. van Gunsteren
 The seven sins in academic behavior in the natural sciences
Angew. Chem. Int. Ed. **52** (2013) 118-122, DOI: 10.1002/anie.201204076
Angew. Chem. **125** (2013) 128-132, DOI: 10.1002/ange.201204076
- 13.02 L.J. Smith, W.F. van Gunsteren, J.R. Allison
 Multiple binding modes for palmitate to barley lipid transfer protein facilitated by the presence of proline 12
Prot. Sci. **22** (2013) 56-64, DOI: 10.1002/pro.2184, incl. suppl. mat.
- 13.03 M.M. Müller, J.R. Allison, N. Hongdilokkul, L. Gaillon, P. Kast, W.F. van Gunsteren, P. Marlière, D. Hilvert
 Directed evolution of a model primordial enzyme provides insights into the development of the genetic code
PLoS Genet **9** (2013) e1003187, DOI:10.1371/journal.pgen.1003187, incl. suppl. mat.
- 13.04 A. Choutko, W.F. van Gunsteren
 Conformational preferences of a β -octapeptide as function of solvent and force-field parameters
Helv. Chim. Acta **96** (2013) 189-200, DOI: 10.1002/hlca.201200173, incl. suppl. mat.
- 13.05 Z. Lin, W.F. van Gunsteren
 On the choice of a reference state for one-step perturbation calculations between polar and non-polar molecules in a polar environment
J. Comput. Chem. **34** (2013) 387-393, DOI: 10.1002/jcc.23146, incl. suppl. mat.
- 13.06 K. Meier, A. Choutko, J. Dolenc, A.P. Eichenberger, S. Riniker, W.F. van Gunsteren
 Multi-resolution simulation of biomolecular systems: a review of methodological issues
Angew. Chem. Int. Ed. **52** (2013) 2820-2834, DOI: 10.1002/anie.201205408
Angew. Chem. **125** (2013) 2-19, DOI: 10.1002/ange.201205408
- 13.07 Z. Lin, S. Riniker, W.F. van Gunsteren
 Free enthalpy differences between α -, π -, and 3_{10} -helices of an atomic level fine-grained alanine decapeptide solvated in supra-molecular coarse-grained water
J. Chem. Theory Comput. **9** (2013) 1328-1333, DOI: 10.1021/ct3010497
- 13.08 N. Hansen, P.H. Hünenberger, W.F. van Gunsteren
 Efficient combination of environment change and alchemical perturbation within the enveloping distribution sampling (EDS) scheme: twin system EDS and application to the determination of octanol-water partition coefficients
J. Chem. Theory Comput. **9** (2013) 1334-1346, DOI: 10.1021/ct300933y, incl. suppl. mat.
- 13.09 Z. Lin, W.F. van Gunsteren
 Combination of enveloping distribution sampling (EDS) of a soft-core reference-state Hamiltonian with one-step perturbation to predict the effect of side chain substitution on the relative stability of right- and left-helical folds of β -peptides
J. Chem. Theory Comput. **9** (2013) 126-134, DOI: 10.1021/ct300929q
- 13.10 K. Meier, W.F. van Gunsteren
 On the use of advanced modelling techniques to investigate the conformational discrepancy between two X-ray structures of the AppA BLUF domain
Molecular Simulation **39** (2013) 472-486, DOI: 10.1080/08927022.2012.743659

- 13.11 A.P. Eichenberger, W.F. van Gunsteren, L.J. Smith
Structure of hen egg-white lysozyme solvated in TFE/water: a molecular dynamics simulation study based on NMR data
J. Biomol. NMR **55** (2013) 339-353, DOI: 10.1007/s10858-013-9717-y, incl. suppl. mat.
- 13.12 A. Choutko, A.P. Eichenberger, W.F. van Gunsteren, J. Dolenc
Exploration of swapping enzymatic function between two proteins: a simulation study of chorismate mutase and isochorismate pyruvate lyase
Prot. Sci. **22** (2013) 809-822, DOI: 10.1002/pro.2264, incl. suppl. mat.
- 13.13 M. Laner, B.A.C. Horta, P.H. Hünenberger
Phase-transition properties of glycerol-monopalmitate lipid bilayers investigated by molecular dynamics simulation: influence of the system size and force-field parameters
Mol. Simul. **39** (2013) 563-583, DOI: 10.1080/08927022.2012.755526, incl. suppl. mat.
- 13.14 D. Wang, M.L. Amundadottir, W.F. van Gunsteren, P.H. Hünenberger
Intramolecular hydrogen-bonding in aqueous carbohydrates as a cause or consequence of conformational preferences: a molecular dynamics study of cellobiose stereoisomers
Eur. Biophys. J. **42** (2013) 521-537, DOI: 10.1007/s00249-013-0901-5
- 13.15 Z. Lin, W.F. van Gunsteren
Influence of variation of a side chain on the folding equilibrium of a β -peptide: limitations of one-step perturbation
J. Comput. Chem. **34** (2013) 1899-1906, DOI: 10.1002/jcc.23331
- 13.16 N. Hansen, J.R. Allison, F. Hodel, W.F. van Gunsteren
Relative free enthalpies for point mutations in two proteins with highly similar sequence but different folds
Biochemistry **52** (2013) 4962–4970, DOI: 10.1021/bi400272q
- 13.17 Z. Lin, W.F. van Gunsteren
The effect of branched side chains on the relative stability of α - and π - helices: a combination of the enveloping distribution sampling and one-step perturbation methods
Mol. Phys. **111** (2013) 2126-2130, DOI: 10.1080/00268976.2013.793828, incl. suppl. mat.
- 13.18 S.J. Bachmann, J. Dolenc, W.F. van Gunsteren
On the use of one-step perturbation to investigate the dependence of different properties of liquid water upon a variation of model parameters from a single simulation
Mol. Phys. **111** (2013) 2334-2344
- 13.19 L. Smith, Y. Roby, J.R. Allison, W.F. van Gunsteren
MD simulations of barley and maize lipid transfer proteins show different ligand binding preferences in agreement with experimental data
Biochemistry **52** (2013) 5029-5038, DOI: 10.1021/bi4006573
- 13.20 D. Wang, A. Böckmann, J. Dolenc, B. Meier, W.F. van Gunsteren
On the behavior of water at subfreezing temperatures in a protein crystal: evidence of higher mobility than in bulk water
J. Phys. Chem. B. **117** (2013) 11433–11447, DOI: 10.1021/jp400655v, incl. suppl. mat.
- 13.21 M. Pechlaner, R.K.O. Sigel, W.F. van Gunsteren, J. Dolenc
Structure and conformational dynamics of the domain 5 RNA hairpin of a bacterial group II intron revealed by solution NMR and molecular dynamics simulations
Biochemistry **52** (2013) 7099–7113, DOI: 10.1021/bi400784r, incl. suppl. mat.
- 13.22 Z. Lin, W.F. van Gunsteren
Enhanced conformational sampling using enveloping distribution sampling
J. Chem. Phys. **139** (2013) 144105, DOI: 10.1063/1.4824391
- 13.23 G.J. Rocklin, D.L. Mobley, K.A. Dill, P.H. Hünenberger
Calculating the binding free energies of charged species based on explicit-solvent simulations employing lattice-sum methods: An accurate correction scheme for electrostatic finite-size effects
J. Chem. Phys. **139** (2013) 184103, DOI: 10.1063/1.4826261

- 13.24 Z. Lin, W.F. van Gunsteren
 Refinement of the application of the GROMOS 54A7 force field to β -peptides
J. Comput. Chem. **34** (2013) 2796-2805, DOI: 10.1002/jcc.23459, incl. suppl. mat.
- 13.25 O.M. Szklarczyk
 Models and algorithms for multi-resolution simulation of complex systems
 Thesis Nr.21582, ETH Zürich, 2013
- 13.26 O.M. Szklarczyk, N. González-Segredo, P. Kukura, A. Oppenheim, D. Choquet, V. Sandoghdar, A. Helenius, I.F. Sbalzarini, H. Ewers
 Receptor concentration and diffusivity control multivalent binding of SV40 to membrane bilayers
PLoS Comput. Biol. **9** (2013): e1003310, DOI:10.1371/journal.pcbi.1003310, incl. suppl. mat.
- 13.27 S.J. Bachmann
 Development of models for biomolecular simulation: Polarisability and Solvation
 Thesis Nr. 21651, ETH Zürich, 2013
- 2014**
- 14.01 Z. Lin, C. Necula, W.F. van Gunsteren
 Using enveloping distribution sampling to compute the folding free enthalpy of a β -peptide with a very unstable folded conformation in solution: The advantage of focused sampling using EDS
Chem. Phys. **428** (2014) 156-163, DOI: 10.1016/j.chemphys.2013.11.016, incl. suppl. mat.
- 14.02 S.J. Bachmann, Z. Lin, T. Stafforst, W.F. van Gunsteren, J. Dolenc
 On the sensitivity of peptide nucleic acid duplex formation and crystal dissolution to a variation of force-field parameters
J. Chem. Theory Comput. **10** (2013) 391-400, DOI: 10.1021/ct400652w
- 14.03 Z. Lin, C. Oostenbrink, W.F. van Gunsteren
 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
Eur. Biophys. J. **43** (2014) 113-119, DOI 10.1007/s00249-014-0943-3
- 14.04 O.M. Szklarczyk, S.J. Bachmann, W.F. van Gunsteren
 A polarisable empirical force field for molecular dynamics simulation of liquid hydrocarbons
J. Comput. Chem. **35** (2014) 789–801, DOI: 10.1002/jcc.23551
- 14.05 W. Huang, S. Riniker, W.F. van Gunsteren
 Rapid sampling of folding equilibria of β -peptides in methanol using a supramolecular solvent model
J. Chem. Theory Comput. **10** (2014) 2213–2223, DOI 10.1021/ct500048c, incl. suppl. mat.
- 14.06 W. Huang, Z. Lin, W.F. van Gunsteren
 The use of enveloping distribution sampling to evaluate important characteristics of biomolecular force fields
J. Phys. Chem. B **118** (2014) 6424–6430, DOI: 10.1021/jp411005x, incl. suppl. mat.
- 14.07 S.J. Bachmann, W.F. van Gunsteren
 Polarisable model for DMSO and DMSO-water mixtures
J. Phys. Chem. B **118** (2014) 10175-10186, DOI: 10.1021/jp5035695
- 14.08 M. Laner, B.A.C. Horta, P.H. Hünenberger
 Effect of the cosolutes trehalose and methanol on the equilibrium and phase-transition properties of glycerol-monopalmitate lipid bilayers investigated using molecular dynamics simulations
Eur. Biophys. J. **43** (2014) 517-544, DOI 10.1007/s00249-014-0982-9, incl. suppl. mat.
- 14.09 N.S. Bieler, R. Häuselmann, P.H. Hünenberger
 Local elevation umbrella sampling applied to the calculation of alchemical free-energy changes *via* λ -dynamics: the λ -LEUS scheme
J. Chem. Theory Comput. **10** (2014) 3006-3022, DOI: 10.1021/ct500268g
- 14.10 N. Hansen, W.F. van Gunsteren
 Practical aspects of free-energy calculations: A review
J. Chem. Theory Comput. **10** (2014) 2632–2647, DOI: 10.1021/ct500161f

- 14.11 S.J. Bachmann, W.F. van Gunsteren
 On the compatibility of polarisable and non-polarisable models for liquid water
Mol. Phys. **112** (2014) 2761–2780, DOI: 10.1080/00268976.2014.910317
- 14.12 N. Hansen, F. Heller, N. Schmid, W.F. van Gunsteren
 Time-averaged order parameter restraints in molecular dynamics simulations
J. Biomol. NMR **60** (2014) 169–187, DOI: 10.1007/s10858-014-9866-7
- 14.13 N.S. Bieler, P.H. Hünenberger
 Estimating the initial biasing potential for λ -local-elevation umbrella-sampling (λ -LEUS) simulations via slow growth
J. Chem. Phys. **141** (2014) 201101, DOI: 10.1063/1.4902361
- 14.14 S.J. Bachmann, W.F. van Gunsteren
 An improved polarisable water model for use in biomolecular simulation
J. Chem. Phys. **141** (2014) 22D515, DOI: 10.1063/1.4897976
- 14.15 M.H. Graf, Z. Lin, U. Bren, D. Haltrich, W.F. van Gunsteren, C. Oostenbrink
 Pyranose Dehydrogenase Ligand Promiscuity: A Generalized Approach to Simulate Monosaccharide Solvation, Binding, and Product Formation
PLoS Comput. Biol. **10** (2014) e1003995, DOI:10.1371/journal.pcbi.1003995
- 14.16 W. Huang, N. Hansen, W.F. van Gunsteren
 On the use of a supramolecular coarse-grained model for the solvent in simulations of the folding equilibrium of an octa- β -peptide in MeOH and H₂O
Helv. Chim. Acta **97** (2014) 1591-1605
- 2015**
- 15.01 M. Laner, B.A.C. Horta, P.H. Hünenberger
 Long-timescale motions in glycerol-monopalmitate lipid bilayers investigated using molecular dynamics simulation.
J. Mol. Graph. Model. **55** (2015) 48-64, incl. suppl. mat.
- 15.02 M. Laner, P.H. Hünenberger
 Effect of methanol on the phase-transition properties of glycerol-monopalmitate lipid bilayers investigated using molecular dynamics simulations: in quest of the biphasic effect
J. Mol. Graph. Model. **55** (2015) 85-104, incl. suppl. mat.
- 15.03 A.P. Eichenberger, W.F. van Gunsteren, S. Riniker, L. von Ziegler, N. Hansen
 The key to predicting the stability of protein mutants lies in an accurate description and proper configurational sampling of the folded and denatured states
Biochim. Biophys. Acta, General Subjects **1850** (2015) 983-995, DOI: 10.1016/j.bbagen.2014.09.014, incl. suppl. mat.
- 15.04 W. Huang, W.F. van Gunsteren
 Challenge of representing entropy at different levels of resolution in molecular simulation
J. Phys. Chem. B **119** (2015) 753-763, DOI: 10.1021/jp505045m, incl. suppl. mat.
- 15.05 Z. Lin, S.J. Bachmann, W.F. van Gunsteren
 GROMOS polarisable charge-on-spring models for liquid urea: COS/U and COS/U2
J. Chem. Phys. **142** (2015) 094117, DOI: 10.1063/1.4913955
- 15.06 L.J. Smith, W.F. van Gunsteren, N. Hansen
 Characterisation of the flexible lip regions in bacteriophage lambda lysozyme using MD simulations
Eur. Biophys. J. **44** (2015) 235-237, incl. suppl. mat.
- 15.07 O. Szklarczyk, E. Arvaniti, W.F. van Gunsteren
 Polarisable coarse-grained models for molecular dynamics simulation of liquid cyclohexane
J. Comput. Chem. **36** (2015) 1311-1321

- 15.08 Z. Lin, W.F. van Gunsteren
On the effects of polarisable solvent models upon the relative stability of an α -helical and a β -hairpin structure of an alanine deca-peptide
J. Chem. Theory Comput. **11** (2015) 1983–1986
- 15.09 M. Laner, P.H. Hünenberger
Phase-transition properties of glycerol-dipalmitate lipid bilayers investigated using molecular dynamics simulation
J. Mol. Graph. Model. **59** (2015) 136–147
- 15.10 N.S. Bieler, P.H. Hünenberger
On the ambiguity of conformational states: A B&S-LEUS simulation study of the helical conformations of decaalanine in water
J. Chem. Phys. **142** (2015) 165102, incl. suppl. mat.
- 15.11 N.S. Bieler, J.P. Tschopp, P.H. Hünenberger
Multistate λ -local-elevation umbrella-sampling (MS- λ -LEUS): Method and application to the complexation of cations by crown ethers
J. Chem. Theory Comput. **11** (2015) 2575–2588, incl. suppl. mat.
- 15.12 Z. Lin, W.F. van Gunsteren
On the use of a weak-coupling thermostat in replica-exchange molecular dynamics simulations
J. Chem. Phys. **143** (2015) 034110, DOI: 10.1063/1.4926937
- 15.13 N.S. Bieler, P.H. Hünenberger
Orthogonal sampling in free-energy calculations of residue mutations in a tripeptide: TI versus λ -LEUS
J. Comput. Chem. **36** (2015) 1686–1697
- 15.14 A.P. Eichenberger, W. Huang, S. Riniker, W.F. van Gunsteren
Supra-atomic coarse-grained GROMOS force field for aliphatic hydrocarbons in the liquid phase
J. Chem. Theory Comput. **11** (2015) 2925–2937, DOI: 10.1021/acs.jctc.5b00295, incl. suppl. mat.
- 15.15 S.J. Bachmann, W.F. van Gunsteren
Structural and energetic effects of the use of polarisable water to solvate proteins
Mol. Phys. **113** (2015) 2815–2828, DOI: 10.1080/00268976.2015.1042085, incl. suppl. mat.
- 15.16 W.F. van Gunsteren
On the pitfalls of peer review
F1000Research **4** (2015) 1244, DOI: 10.12688/f1000research.7342.1
- 15.17 O.M. Szklarczyk, N.S. Bieler, P.H. Hünenberger, and W.F. van Gunsteren,
Flexible Boundaries for Multi-Resolution Solvation: an Algorithm for Spatial Multi-scaling in Molecular Dynamics Simulations
J. Chem. Theory Comput. **11** (2015) 5447–5463, DOI: 10.1021/acs.jctc.5b00406, incl. suppl. mat.

2016

- 16.01 Z. Lin, W.F. van Gunsteren
A comparison of pathway independent and pathway dependent methods in the calculation of conformational free enthalpy differences
Protein Science **25** (2016) 184–191, DOI: 10.1002/pro.2695
- 16.02 W. Plazinski, A. Lonardi, P.H. Hünenberger,
Revision of the GROMOS 56A6CARBO Force Field: Improving the Description of Ring-Conformational Equilibria in Hexopyranose-Based Carbohydrates Chains
J. Comput. Chem. **37** (2016) 354–365, incl. suppl. mat.
- 16.03 J. Dolenc, B.H. Meier, V.H. Rusu, W.F. van Gunsteren
Investigation of the structural preference and flexibility of the loop residues in amyloid fibrils of the HET-s prion
Phys.Chem.Chem.Phys. **18** (2016) 5860–5866, DOI: 10.1039/c6cp00057f, incl. suppl. mat.

- 16.04 V.H. Rusu, S.J. Bachmann, W.F. van Gunsteren
GROMOS polarisable model for acetone
Mol. Phys. **114** (2016) 845-854, DOI: 10.1080/00268976.2015.1126366
- 16.05 W.F. van Gunsteren
Going for a PhD: Joys and Pitfalls
Helv. Chim. Acta **99** (2016) 1-5
- 16.06 L. J. Smith, G. Rought Whitta, J. Dolenc, D. Wang, W. F. van Gunsteren
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
Bioorg. Med. Chem. **24** (2016) 4936-4948, DOI: 10.1016/j.bmc.2016.08.001, incl. suppl. mat.
- 16.07 L.J. Smith, W.F. van Gunsteren, N. Hansen
On the Use of Time-Averaging Restraints when Deriving Biomolecular Structure from ³J-coupling Values Obtained from NMR Experiments
J. Biomol. NMR **66** (2016) 69-83, DOI: 10.1007/s10858-016-0058-5, incl. suppl. mat.
- 16.08 W.F. van Gunsteren, J.R. Allison, X. Daura, J. Dolenc, N. Hansen, A.E. Mark, C. Oostenbrink, V.H. Rusu, L.J. Smith
Deriving structural information from experimentally measured data on biomolecules: a review
Angew. Chem. Int. Ed. **55** (2016) 15990-16010, DOI: 10.1002/anie.201601828
Angew. Chem. **128** (2016) 16222-16244, DOI: 10.1002/ange.201601828
- 16.09 W.F. van Gunsteren
Publication of Research Results: Use and Abuse
Infozine, Special Issue **1** (2016) 27-28, DOI: 10.3929/ethz-a-010745085
- 2017**
- 17.01 L.J. Smith, R. Athill, W.F. van Gunsteren, N. Hansen
Interpretation of seemingly contradictory data: low NMR S² order parameters observed in helices and high NMR S² order parameters in disordered loops of the protein hGH at low pH
Chem. Eur. J. **23** (2017) 9585-9591, DOI: 10.1002/chem.201700896, incl. suppl. mat.
- 17.02 L.J. Smith, W.F. van Gunsteren, N. Hansen
Using Complementary NMR Data Sets to Detect Inconsistencies and Model Flaws in the Structure Determination of Human Interleukin-4
J. Phys. Chem. B **121** (2017) 7055-7063, DOI: 10.1021/acs.jpcb.7b03647, incl. suppl. mat.
- 2018**
- 18.01 W.F. van Gunsteren, X. Daura, N. Hansen, A.E. Mark, C. Oostenbrink, S. Riniker, L.J. Smith
Validation of Molecular Simulation: An Overview of Issues
Angew. Chem. Int. Ed. **57** (2018) 884-902, DOI: 10.1002/anie.201702945
Angew. Chem. **130** (2018) 894-915, DOI: 10.1002/ange.201702945
- 18.02 W.F. van Gunsteren
Surfing versus Drilling in Fundamental Research
Infozine, Special Issue **2** (2018) 18-19, DOI: 10.3929/ethz-b-000294373
- 2019**
- 19.01 W.F. van Gunsteren
The Roots of Bio-Molecular Simulation: The eight-week CECAM workshop “Models for Protein Dynamics” of 1976
Helv. Chim. Acta **102** (2019) e1800239, DOI: 10.1002/hlca.201800239
- 19.02 J. Dolenc, W.F. van Gunsteren, A.E. Prota, M.O. Steinmetz, J.H. Missimer
Conformational properties of the chemotherapeutic drug analogue Epothilone A: How to model a flexible protein ligand using scarcely available experimental data
J. Chem. Inf. Model. **59** (2019) 2218-2230, DOI: 10.1021/acs.jcim.9b00171, incl. suppl. mat.

2020

- 20.01 M. Pechlaner, W.F. van Gunsteren
Algorithms to apply dihedral-angle constraints in molecular or stochastic dynamics simulations
J. Chem. Phys. **152** (2020) 024109, DOI: 10.1063/1.5124923

- 20.02 B. Lier, C. Öhlknecht, A. de Ruiter, J. Gebhardt, W.F. van Gunsteren, C. Oostenbrink, N. Hansen
A Suite of Advanced Tutorials for the GROMOS Biomolecular Simulation Software
Living J. Comp. Mol. Sci. **2** (2020) 18552, DOI: org/10.33011/livecoms.2.1.18552

2021

- 21.01 M. Pechlaner, A.P. Dorta, Z. Lin, V.H. Rusu, W.F. van Gunsteren
A method to apply bond-angle constraints in molecular dynamics simulation
J. Comput. Chem. **42** (2021) 418-434, DOI: 10.1002/jcc.26466
- 21.02 W.F. van Gunsteren, X. Daura, P.F.J. Fuchs, N. Hansen, B.A.C. Horta, P.H. Hünenberger, A.E. Mark, M. Pechlaner, S. Riniker, C. Oostenbrink
On the Effect of the Various Assumptions and Approximations used in Molecular Simulation on the Properties of Bio-Molecular Systems: Overview and Perspective on Issues
ChemPhysChem **22** (2021) 264–282, DOI: 10.1002/cphc.202000968
- 21.03 L.J. Smith, W.F. van Gunsteren, N. Hansen
On the Use of Side-Chain NMR Relaxation Data to Derive Structural and Dynamical Information on Proteins: A Case Study Using Hen Lysozyme
ChemBioChem **22** (2021) 1049-1064, DOI: 10.1002/cbic.202000674
- 21.04 L.J. Smith, W.F. van Gunsteren, N. Hansen
On the Use of 3J -coupling NMR Data to Derive Structural Information on Proteins
J. Biomol. NMR **75** (2021) 39-70, DOI: 10.1007/s10858-020-00355-5
- 21.05 M. Pechlaner, C. Oostenbrink, W.F. van Gunsteren
On the Use of Multiple-Time-Step Algorithms to Save Computing Effort in Molecular Dynamics Simulations of Proteins
J. Comput. Chem. **42** (2021) 1263-1282, DOI: 10.1002/jcc.26541
- 21.06 M. Pechlaner, W.F. van Gunsteren
On the Use of Intra-Molecular Distance and Angle Constraints to Lengthen the Time Step in Molecular and Stochastic Dynamics Simulations of Proteins
Proteins: Struct. Funct. Bioinf. **90** (2021) 543–559, DOI: 10.1002/prot.26251

2021

- 22.01 M. Pechlaner, W.F. van Gunsteren, N. Hansen, L.J. Smith
Molecular Dynamics Simulation or Structure Refinement of Proteins: Are Solvent Molecules Required? A Case Study Using Hen Lysozyme
Eur. Biophys. J. **51** (2022) 265–282, DOI: 10.1007/s00249-022-01593-1
- 22.02 W.F. van Gunsteren, M. Pechlaner, L.J. Smith, B. Stankiewicz, N. Hansen
A Method to Derive Structural Information on Molecules from Residual Dipolar Coupling NMR Data
J. Phys. Chem. B **126** (2022) 3867-3888, DOI: 10.1021/acs.jpcb.2c02410

In press, submitted or in preparation

- A723 M. Pechlaner, O.M. Szklarczyk, W.F. van Gunsteren
A Leap-Frog Algorithm for Stochastic Dynamics Simulation of Rigid Molecules using Quaternions
J. Chem. Phys. (2021) in preparation
- A724 M. Pechlaner, W.F. van Gunsteren, L.J. Smith, B. Stankiewicz, L.N. Wirz, N. Hansen
Molecular Structure Refinement Based on Residual Dipolar Couplings: Limitations of the Use of the Alignment-Tensor Approach
J. Biomol. NMR (2022) to be submitted

- A726 L.J. Smith, W.F. van Gunsteren, V.A. Higman, M. Pechlaner, C. Redfield, B. Stankiewicz, N. Hansen
Structure Refinement of Hen Egg White Lysozyme Based on Residual Dipolar Couplings Avoiding the
Limitations of the Alignment-Tensor Approach
ChemBioChem (2022) in preparation
- A727 M. Pechlaner, W.F. van Gunsteren, L.J. Smith, N. Hansen
Molecular Structure Refinement Based on Residual Dipolar Couplings Using Rotational Sampling and
Solvent Configurational Sampling
ChemPhysChem (2021) in preparation
- A728 M. Pechlaner, W.F. van Gunsteren, L.J. Smith, N. Hansen
Molecular Structure Refinement Based on Residual Dipolar Couplings Using Magnetic-Field Rotational
Sampling
J. Chem. Phys. (2022) to be submitted
- A729 M. Pechlaner, W.F. van Gunsteren, L.J. Smith, N. Hansen
Molecular Structure Refinement of a Beta-Heptapeptide Based on Residual Dipolar Couplings: Is the
Obtained Conformational Ensemble Compatible with NOE distance and 3J -coupling Data?
Chemistry Eur. J. (2022) in preparation