Scientific publications, books

Edited:

- W.F. van Gunsteren, P.K. Weiner, eds.
  Computer Simulation of Biomolecular Systems, Theoretical and Experimental Applications,
  ISBN 90-72199-03-0

  Computer Simulation of Biomolecular Systems, Theoretical and Experimental Applications, Vol. 2,
  ISBN 90-72199-15-4

  Computer Simulation of Biomolecular Systems, Theoretical and Experimental Applications, Vol. 3,
  ISBN 90-72199-25-1

Authored:

  Biomolecular Simulation: The GROMOS96 Manual and User Guide
  Vdf Hochschulverlag AG an der ETH Zürich, Zürich, Switzerland, 1996, 1042 pages
  ISBN 3 7281 2422 2
Scientific publications, articles

1. W.F. van Gunsteren, E. Boeker and K. Allaart
   The FBCS model and the inverse gap equations applied to the tin isotopes
   Z. Phys. 267 (1974) 87-96

2. K. Allaart and W.F. van Gunsteren
   Projected quasiparticle calculations in large model spaces

3. W.F. van Gunsteren and K. Allaart
   Can the o+ states of even superfluid nuclei be described by anharmonic pairing vibrations?

4. W.F. van Gunsteren and K. Allaart
   Influence of an enlargement of the model space on number projected quasiparticle calculations
   Z. Phys. A276 (1976) 1-8

5. W.F. van Gunsteren, K. Allaart and E. Boeker
   A particle-quasiparticle description of 112,114,116Sb

6. W.F. van Gunsteren
   A hole-quasiparticle description of 114,116In

7. W.F. van Gunsteren, P. Hofstra and H. Muether
   Influence of the effective interaction on spectra of superfluid nuclei

8. W.F. van Gunsteren
   The nuclear quasiparticle model

9. W.F. van Gunsteren and D. Rabenstein
   Properties of the low-lying levels of 122Sb

10. W.F. van Gunsteren and H.J.C. Berendsen
    Algorithms for macromolecular dynamics and constraint dynamics
    Mol. Phys. 34 (1977) 1311-1327

11. W.F. van Gunsteren, K. Allaart and P. Hofstra
    Number-projected three-quasiparticle description of the odd Sn isotopes

12. W.F. van Gunsteren, H.J.C. Berendsen and J.A.C. Rullmann
    Inclusion of Reaction Fields in Molecular Dynamics: Application to Liquid Water

13. 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

14. W.F. van Gunsteren
    Constrained dynamics of flexible molecules

15. W.F. van Gunsteren and M. Karplus
    A Method for Constrained Energy Minimization of Macromolecules
W.F. van Gunsteren, H.J.C. Berendsen and J.A.C. Rullmann
Stochastic dynamics for molecules with constraints Brownian dynamics of n-alkanes

W.F. van Gunsteren and M. Karplus
Effect of constraints, solvent and crystal environment on protein dynamics
Nature 293 (1981) 677-678

H.J.C. Berendsen, J.P.M. Postma, W.F. van Gunsteren and J. Hermans

W.F. van Gunsteren and M. Karplus
Effect of Constraints on the Dynamics of Macromolecules

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

W.F. van Gunsteren and H.J.C. Berendsen
Algorithms for brownian dynamics

W.F. van Gunsteren and H.J.C. Berendsen
On the fluctuation-dissipation theorem for interacting brownian particles

W.F. van Gunsteren and H.J.C. Berendsen
Molecular dynamics: perspective for complex systems
Biochem. Soc. Trans. 10 (1982) 301-305

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

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

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",

W.F. van Gunsteren and J.H.C. Berendsen

H.J.C. Berendsen and W.F. van Gunsteren

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

H.J.C. Berendsen and W.F. van Gunsteren
31. 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

32. 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

33. 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.,

34. 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

35. W.F. van Gunsteren, R. Kaptein and E.R.P. Zuiderweg
   Use of Molecular Dynamics Computer Simulations When Determining Protein Structure by 2D NMR,
   1984, Orsay, 79-92 (CECAM, France)

   Molecular dynamics computer simulation of the hydration of two simple organic solutes Comparison with the
   simulation of an empty cavity

   A Protein Structure from Nuclear Magnetic Resonance Data lac Repressor Headpiece

38. 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

   A Molecular Dynamics Study of the C-terminal Fragment of the L7/12 Ribosomal Protein. Secondary
   Structure Motion in a 150 Picosecond Trajectory

   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

41. 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

42. 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

43. 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
44. 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

   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

46. J. Äqvist, 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

47. 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.

48. W.F. van Gunsteren, H.J.C. Berendsen and J.P. Hollenberg
   Prospects for complex molecular systems
   Supercomputer 7 (1985) 26-36

49. P. Kruger, W. Strassburger, A. Wollner and W.F. van Gunsteren
   A comparison of the structure and dynamics of avian pancreatic polypeptide hormone in solution and in the
   crystal

50. 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

   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.,

52. 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

53. 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

   A Molecular Dynamics Computer Simulation of an Eight-Base-Pair DNA Fragment in Aqueous Solution:
   Comparison with Experimental Two- Dimensional NMR Data

   Simulations of Proteins in Water

56. W.F. van Gunsteren
   Ontwerpen van medicijnen en gemodificeerde enzymen met behulp van computersimulatie (in Dutch)
   Biotechnologie in Nederland 1 (1986) 13-15
57. P. Sandblom, J. Äqvist, 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

58. 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

59. J. Äqvist, 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

60. 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

61. J. Lautz, H. Kessler, R. Boelens, R. Kaptein and W.F. van Gunsteren
Conformational analysis of a cyclic thymopoietin-analogue by 1H NMR spectroscopy and restrained molecular
dynamics simulations
Int. J. Peptide Protein Res. 30 (1987) 404-414

62. W.F. van Gunsteren
Molecular dynamics of proteins and nucleic acids

63. 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

64. 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

65. 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.,

66. 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,

67. J. Koehler, W. Saenger and W.F. van Gunsteren
A molecular dynamics simulation of crystalline α-cyclodextrin hexahydrate

68. J. Koehler, W. Saenger and W.F. van Gunsteren
Molecular dynamics simulation of crystalline β-cyclodextrin dodecahydrate at 293 K and 120 K

69. P. Kollman and W.F. van Gunsteren
Molecular Mechanics and Dynamics in Protein Design Methods in Enzymology Vol 154, Recombinant DNA,
70. J.E.H. Koehler, W. Saenger and W.F. van Gunsteren
The flip-flop hydrogen bonding phenomenon: Molecular dynamics simulation of crystalline β-cyclodextrin

71. W.F. van Gunsteren and H.J.C. Berendsen
A leap-frog algorithm for stochastic dynamics
Molecular Simulation 1 (1988) 173-185

72. Shi Yun-yu, Yun Ru-huai and W.F. van Gunsteren
Molecular Dynamics Simulation of Despentapeptide Insulin in a Crystalline Environment

Conformational Dynamics Detected by Nuclear Magnetic Resonance NOE Values and J-Coupling Constants

74. W.F. van Gunsteren
Classical molecular dynamics simulations: algorithms and applications, stochastic dynamics, and free energies,

75. 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

76. 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

77. R. Kaptein, R. Boelens, R.M. Scheek and W.F. van Gunsteren
Protein Structures from NMR
Biochemistry 27 (1988) 5389-5395

78. Shi Yun-yu, Wang Lu 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) 369-388

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 3 (1988) 209-218

80. W.F. van Gunsteren
The role of computer simulation techniques in protein engineering
Protein Engineering 2 (1988) 5-13

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

82. W. Soppe, C. van der Marel, W.F. van Gunsteren and H.W. den Hartog
New insights into the structure of B2O3 glass
J. of Non-Crystalline Solids 103 (1988) 201-209
83. A.E. Torda, B.C. Mabbutt, 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

84. W.F. van Gunsteren

85. M. Fujinaga, P. Gros and W.F. van Gunsteren
Testing the Method of Crystallographic Refinement Using Molecular Dynamics

86. 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

87. W.F. van Gunsteren
Computer simulation by molecular dynamics as a tool for modelling of molecular systems
Molecular Simulation 3 (1989) 187-200

Dynamical Structure of Carboxypeptidase A
J. Mol. Biol. 207 (1989) 201-216

89. A.E. Torda, R.M. Scheek and W.F. van Gunsteren
Time-dependent distance restraints in molecular dynamics simulations


91. 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

92. 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 6 (1989) 104-127

93. R.M. Scheek, W.F. van Gunsteren and R. Kaptein


95. W.F. van Gunsteren
96. 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

   On the Dependence of Molecular Conformation on the Type of Solvent Environment: A Molecular Dynamics
   Study of Cyclosporin A
   Biopolymers 29 (1990) 1669-1687

98. 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

99. W.F. van Gunsteren and H.J.C. Berendsen
   Computer Simulation of Molecular Dynamics: Methodology, Applications and
   Perspectives in Chemistry

100. 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
    Copenhagen, (1990), pp. 362-368

101. 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

102. A.E. Torda and W.F. van Gunsteren
    The Refinement of NMR structures by Molecular Dynamics Simulation

103. A.E. Mark, W.F. van Gunsteren and H.J.C. Berendsen
    Calculation of Relative Free Energy via Indirect Pathways

104. A.E. Mark, H.J.C. Berendsen, A.P. Heiner and W.F. van Gunsteren
    Calculation of Relative Free Energy by Molecular Dynamics, Proc. of the 7th Intl. Symp. on Metabolism and
    Enzymology of Nucleic Acids including Gene and Protein Engineering, Smolenic Castle, November 26-30

105. W.F. van Gunsteren
    Computer Simulation of Biomolecular Systems: Overview of time-saving techniques, in: "Advances in
    Conference Proceedings, Vol. 239, pp. 131-146

    On deriving spatial structure from NMR or X-ray diffraction data, in: "Protein Conformation", Ciba

107. 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

108. J. de Vlieg and W.F. van Gunsteren
    Combined Procedures of Distance Geometry and Molecular Dynamics for Determining Protein Structure from

109. 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
110. A.E. Torda, R.M. Scheek and W.F. van Gunsteren

111. W.F. van Gunsteren and A.E. Mark
On the interpretation of biochemical data by molecular dynamics computer simulation

112. 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

113. W.F. van Gunsteren
Molecular Dynamics Simulation in Practice
in: Les Cahiers IMABIO, no. 4, CNRS, April 1992, pp. 27-29

114. F. Müller-Plathe and W.F. van Gunsteren
Molecular Simulation of Polymer-Penetrant Systems
Polymer Preprints, ACS, 1992, 633-634

115. W.F. van Gunsteren, R.M. Brunne and A.E. Mark and S.P. van Helden

116. 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

117. W.F. van Gunsteren and A.E. Mark
Prediction of the Activity and Stability Effects of Site-directed Mutagenesis on a Protein Core

118. 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

119. F. Müller-Plathe, S.C. Rogers and W.F. van Gunsteren
Computational Evidence for Anomalous Diffusion of Small Molecules in Amorphous Polymers

120. 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

121. A.P. Heiner, H.J.C. Berendsen and W.F. van Gunsteren
MD Simulation of Subtilisin BPN' in a Crystal Environment
Proteins 14 (1992) 451-464

122. A.E. Torda and W.F. van Gunsteren
Molecular Modeling Using Nuclear Magnetic Resonance Data
123. A. Gunzinger, U. Müller, W. Scott, B. Bäumle, P. Kohler and W.F. van Gunsteren
   Architecture and Realization of a Multi Signalprocessor System

124. F. Müller-Plathe, W. Scott and W.F. van Gunsteren
   Molecular Dynamics on Supercomputers: Implementations and Applications
   SPEEDUP Journal 6 (1992) 33-38

125. A. Gunzinger, U.A. Müller, W. Scott, B. Bäumle, P. Kohler, H.R. von der Mühll,
   F. Müller-Plathe, W.F. van Gunsteren, W. Guggenbühl
   Achieving Super Computer Performance with a DSP Array Processor

126. 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
   (1992), pp. 170-175

127. 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

128. P.M. King, R.M. Spycher and W.F. van Gunsteren
   Structure elucidation from rotation spectra: a penalty function approach

129. 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

130. W.F. van Gunsteren
   Molecular dynamics studies of proteins
   Current Opinion in Structural Biology 3 (1993) 277-281

   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

   and W.F. van Gunsteren
   Can the stability of protein mutants be predicted by free energy calculations ?
   Protein Engineering 6 (1993) 289-295

133. R.M. Brunne and W.F. van Gunsteren
   Dynamical properties of bovine pancreatic trypsin inhibitor from a
   molecular dynamics simulation at 5000 atm

134. 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

135. F. Müller-Plathe, S.C. Rogers and W.F. van Gunsteren
   Gas sorption and transport in polyisobutylene: Equilibrium and
   nonequilibrium molecular dynamics simulations
136. 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

137. 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

138. 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

139. 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

140. 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

141. C.K. Kuhn and W.F. van Gunsteren
Dynamics of solitons in polyacetylene in the step-potential model

142. F. Müller-Plathe, L. Laaksonen and W.F. van Gunsteren
Cooperative effects in the transport of small molecules through an
amorphous polymer matrix

143. 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.
(1993), pp. 3-36

144. 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.
(1993), pp. 315-348

145. 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.
(1993), pp. 182-212

146. P.E. Smith and W.F. van Gunsteren
The viscosity of SPC and SPC/E water at 277 and 300K

147. 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
148. 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

149. 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

150. 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

151. 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

152. 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

153. P.E. Smith and W.F. van Gunsteren
Translational and Rotational Diffusion of Proteins

Molecular Dynamics Simulations of Oxidized and Reduced Clostridium beijerinckii Flavodoxin
Biophysical Journal 66 (1994) 634-645

155. 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

156. 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

157. 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

158. 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

159. 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
The High-resolution Structure of the Histidine-containing Phosphocarrier Protein HPt from Escherichia coli
Determined by Restrained Molecular Dynamics from Nuclear Magnetic Resonance Nuclear Overhauser Effect Data
J. Mol. Biol. 237 (1994) 544-559

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

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

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

A.A. Gusev, F. Müller-Plathe, W.F. van Gunsteren and U.W. Suter
Dynamics of Small Molecules in Bulk Polymers

T.C. Beutler and W.F. van Gunsteren
Molecular dynamics free energy calculation in four dimensions

W. Scott, F. Müller-Plathe and W.F. van Gunsteren
Molecular dynamics study of the mixing and demixing of a binary Lennard-Jones fluid
Molecular Physics 82 (1994) 1049-1062

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

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

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

A.E. Torda and W.F. van Gunsteren
Algorithms For Clustering Molecular Dynamics Configurations

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

F. Müller-Plathe, W. Scott and W.F. van Gunsteren
PARALLACS: A benchmark for parallel molecular dynamics
Computer Physics Communications 84 (1994) 102-114
173. I.G. Tironi and W.F. van Gunsteren
   A molecular dynamics simulation study of chloroform
   Molecular Physics 83 (1994) 381-403

174. T. Huber, A.E. Torda and W.F. van Gunsteren
   Local elevation: A method for improving the searching properties of molecular dynamics simulation

175. P.E. Smith and W.F. van Gunsteren
   When are Free Energy Components Meaningful?
   J. Phys. Chem. 98 (1994) 13735-13740

176. 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

177. 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

178. W.F. van Gunsteren, P.M. King and A.E. Mark
   Fundamentals of drug design from a biophysical viewpoint

   Newtonian Dynamics in Unusual Places: Parameterising a Low Resolution Force Field

180. C.A. Schiffer, P. Gros and W.F. van Gunsteren
   Time-Averaging Crystallographic Refinement: Possibilities and Limitations
   Using α-Cyclodextrin as a Test System

181. C.D. Berweger, W.F. van Gunsteren and F. Müller-Plathe
   Force field parametrisation by weak coupling. Re-engineering SPC water

182. 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

   Internal Mobility of the Basic Pancreatic Trypsin Inhibitor in Solution: A Comparison of NMR Spin Relaxation Measurements and Molecular Dynamics Simulations

184. T.C. Beutler, D.R. Béguelin and W.F. van Gunsteren
   Free energy of cavity formation in solvent: Computational, methodological and physical aspects

185. P.H. Hünenberger, A.E. Mark and W.F. van Gunsteren
   Computational Approaches to Study Protein Unfolding: Hen Egg White Lysozyme as a Case Study
   Proteins 21 (1995) 196-213

186. A.E. Mark and W.F. van Gunsteren
   Free Energy Calculations in Drug Design: A Practical Guide
187. 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

188. H. Bekker, H.J.C. Berendsen and W.F. van Gunsteren
   Force and virial of torsional-angle dependent potentials

189. 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

190. 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

191. 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

192. I.G. Tironi, R. Sperb, P.E. Smith and W.F. van Gunsteren
   A generalized reaction field method for molecular dynamics simulations

193. T.C. Beutler and W.F. van Gunsteren
   Umbrella sampling along linear combinations of generalized coordinates. Theory and application to a glycine dipeptide

   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

195. 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

196. B.A. Luty, I.G. Tironi and W.F. van Gunsteren
   Lattice-sum Methods for Calculating Electrostatic Interactions in Molecular Simulations

197. W.F. van Gunsteren, T. Huber and A.E. Torda
   Biomolecular Modelling: Overview of Types of Methods to Search and Sample Conformational Space

198. 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 23 (1995) 49-62
199. 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

Computer simulation of protein motion  

201. F. Müller-Plathe, H. Liu and W.F. van Gunsteren  
Conceptual Hierarchies in Polymer Electrolyte Simulations - 
From Quantum Chemistry to Molecular Dynamics  

202. P.E. Smith and W.F. van Gunsteren  
Reaction field effects on the simulated properties of liquid water  
Molecular Simulation 15 (1995) 233-245

203. P.H. Hünlenberger, A.E. Mark and W.F. van Gunsteren  
Fluctuation and Cross-Correlation Analysis of Protein Motions 
Observed in Nanosecond Molecular Dynamics Simulations  

204. 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

205. F. Müller-Plathe and W.F. van Gunsteren  
Computer simulation of a polymer electrolyte: Lithium iodide in amorphous poly(ethylene oxide)  

206. 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

207. 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

208. 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) 301-3

209. 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

210. 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  

211. 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
212. 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

213. 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

214. F. Fraternali and W.F. van Gunsteren
An Efficient Mean Solvation Force Model for Use in Molecular Dynamics Simulations of Proteins in Aqueous Solution

215. 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

216. W.F. van Gunsteren, A.P. Nanzer and A.E. Torda
Molecular simulation methods for generating ensembles or trajectories consistent with experimental data

217. 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

218. 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

219. 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

220. 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

221. H. Liu, F. Müller-Plathe and W.F. van Gunsteren
A Combined Quantum/Classical Molecular Dynamics Study of the Catalytic Mechanism of HIV-Protease

222. C.A. Schiffer and W.F. van Gunsteren
Structural Stability of Disulfide Mutants of Basic Pancreatic Trypsin Inhibitor: A Molecular Dynamics Study
Proteins 26 (1996) 66-71

223. 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
224. A.P. Nanzer, T. Huber, A.E. Torda and W.F. van Gunsteren
Molecular dynamics simulation using weak-coupling NOE distance restraining

225. 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

A.E. Torda, A.P. Nanzer and W.F. van Gunsteren
Restrained molecular dynamics of RGD-containing cyclic peptides using time-averaged NOEs

Protein Structure Prediction Force Fields: Parametrization with Quasi-Newtonian Dynamics
Proteins 27 (1997) 367-384

228. H. Kovacs, A.E. Mark and W.F. van Gunsteren
Solvent Structure at a Hydrophobic Protein Surface
Proteins 27 (1997) 395-404

Dynamical Studies of Peptide Motifs in the Plasmodium falciparum Circumsporozoite Surface Protein by Restrained and Unrestrained MD Simulations

230. I.G Tironi, B.A. Luty and W.F. van Gunsteren
Space-time correlated reaction field: A stochastic dynamical approach to the dielectric continuum

231. 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

232. F.A. Hamprecht, W.R.P. Scott and W.F. van Gunsteren
Generation of Pseudonative Protein Structures for Threading
Proteins 28 (1997) 522-529

233. W.F. van Gunsteren and A.E. Mark
Computational Chemistry: Abschied vom Experiment?
ETH-Bulletin 266 (1997) 18-19

Experimental and Theoretical Approach to Hydrogen-Bonded Diastereomeric Interactions in a Model Complex

235. T. Huber, A.E. Torda and W.F. van Gunsteren
Structure Optimisation Combining Soft-Core Interaction Functions, the Diffusion Equation Method and Molecular Dynamics

236. 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
237. C.D. Berweger, W.F. van Gunsteren and F. Müller-Plathe
Finite Element Interpolation for Combined Classical/Quantum Mechanical
Molecular Dynamics Simulations

238. P.H. Hünenberger and W.F. van Gunsteren
Empirical classical interaction functions for molecular simulation

239. S.R. Billeter and W.F. van Gunsteren
A modular molecular dynamics/quantum dynamics program for non-adiabatic
proton transfers in solution

240. K. Park and W.F. van Gunsteren
Parameter Optimization for Calculation of Proton Chemical Shift in Protein

241. K. Park and W.F. van Gunsteren
Solution Structure of Bovine Pancreatic Trypsin Inhibitor using NMR Chemical Shift Restraints

242. 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

243. X. Daura, A.E. Mark and W.F. van Gunsteren
Parametrization of Aliphatic CH₅ United Atoms of GROMOS96 Force Field

244. W.F. van Gunsteren and A.E. Mark
Validation of molecular dynamics simulation

245. 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

246. W.F. van Gunsteren, H. Liu and F. Müller-Plathe
The elucidation of enzymatic reaction mechanisms by computer simulation:
Human Immunodeficiency Virus protease catalysis

247. 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

248. S.R. Billeter and W.F. van Gunsteren
Protonizable Water Model for Quantum Dynamical Simulations

249. T. Huber and W.F. van Gunsteren
SWARM-MD: Searching Conformational Space by Cooperative Molecular Dynamics
250. X. Daura, B. Jaun, D. Seebach, W.F. van Gunsteren and A.E. Mark
Reversible Peptide Folding in Solution by Molecular Dynamics Simulation

251. 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

252. 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

253. W.R.P. Scott, A.E. Mark and W.F. van Gunsteren
On using time-averaging restraints in molecular dynamics simulation

254. W.F. van Gunsteren, X. Daura and A.E. Mark
GROMOS force field

255. 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,

256. 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
(eds.), Springer-Verlag Berlin, (1999), pp. 149-162

257. X. Daura, K. Gademann, B. Jaun, D. Seebach, W.F. van Gunsteren and A.E. Mark
Peptide Folding: When Simulation Meets Experiment
(German version is also available)

258. X. Daura, R. Suter and W.F. van Gunsteren
Validation of molecular simulation by comparison with experiment: Rotational reorientation
of tryptophan in water

259. X. Daura, W.F. van Gunsteren and A.E. Mark
Folding-Unfolding Thermodynamics of a β-Heptapeptide From Equilibrium Simulations
Proteins 34 (1999) 269-280

260. 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

261. R. Walser, A.E. Mark and W.F. van Gunsteren
On the validity of Stokes' law at the molecular level

T. Huber, P. Krüger and W.F. van Gunsteren
The GROMOS Biomolecular Simulation Program Package
263. 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 36 (1999) 77-86

Aspects of Modeling Biomolecular Structure on the Basis of Spectroscopic or Diffraction Data

265. C.A. Schiffer and W.F. van Gunsteren
Accessibility and Order of Water Sites in and Around Proteins: A Crystallographic Time-Averaging Study
Proteins 36 (1999) 501-511

266. 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 36 (1999) 542-555

267. C.D. Berweger, W.F. van Gunsteren and F. Müller-Plathe
The Photoisomerization of cis-Stilbene Does not Follow the Minimum Energy Path
(German version is also available)

268. 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

269. H. Schäfer, W.F. van Gunsteren and A.E. Mark

270. X. Daura, A.E. Mark and W.F. van Gunsteren
Peptide folding simulations: no solvent required?

271. W.F. van Gunsteren and J. Hermans
Herman Berendsen: Researcher, Teacher, Colleague, Skipper

Structure and Conformation of β-Oligopeptide Derivatives with Simple Proteinogenic Side-Chains: Circular Dichroism and Molecular Dynamics Investigations

273. 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

274. S.R. Billeter and W.F. van Gunsteren
Computer Simulation of Proton Transfers of Small Acids in Water

275. W. Damm and W.F. van Gunsteren
Reversible Peptide Folding: Dependence on the Molecular Force Field Used

276. 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
277. 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

278. X. Daura, E. Haaksma and W.F. van Gunsteren
Factor Xa: Simulation studies with an eye to inhibitor design

279. 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

280. A.M.J.J. Bonvin, A.E. Mark and W.F. van Gunsteren
The GROMOS96 benchmarks for molecular simulation

281. C. Peter, X. Daura and W.F. van Gunsteren
Peptides of Aminoxy Acids: A Molecular Dynamics Simulation Study of Conformational Equilibria under Various Conditions

282. 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 VH Domain into a More Tractable Species

283. 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

284. L.D. Schuler and W.F. van Gunsteren
On the Choice of Dihedral Angle Potential Energy Functions for n-Alkanes
Mol. Sim. 25 (2000) 301-319

285. 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 41 (2000) 299-315

286. H. Schäfer, A.E. Mark and W.F. van Gunsteren
Absolute entropies from molecular dynamics simulation trajectories

Simulations of the Estrogen Receptor Ligand Binding Domain: Affinity of Natural Ligands and Xenoestrogens

288. 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

289. R. Walser and W.F. van Gunsteren
Viscosity Dependence of Protein Dynamics
Proteins 42 (2001) 414-421
290. 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

291. 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

292. 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

Molecular dynamics study of oxygenation reactions catalysed by the enzyme
p-hydroxybenzoate hydroxylase

294. 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

295. 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

296. 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 43 (2001) 45-56

297. J.W. Pitera and W.F. van Gunsteren
The Importance of Solute-Solvent van der Waals Interactions with Interior Atoms of Biopolymers

298. 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

299. 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

300. 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 44 (2001) 509-519

301. 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 43 (2001) 395-402

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

303. 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
304. L.D. Schuler, X. Daura and W.F. van Gunsteren
An Improved GROMOS96 Force Field for Aliphatic Hydrocarbons in the Condensed Phase

305. 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

306. 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

307. W. Czechitzky, 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

308. 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

309. L.D. Schuler, P. Walde, P.L. Luisi and W.F. van Gunsteren
Molecular dynamics simulation of n-dodecyl phosphate aggregate structures

Molecular Dynamics Simulation of Biomolecular Systems
CHIMIA 55 (2001) 856-860

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

312. 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
Mol. Sim. 27 (2001) 215-236

313. J.W. Pitera and W.F. van Gunsteren
One-Step Perturbation Methods for Solvation Free Energies of Polar Solutes

314. 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) 351-
355

315. 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

316. 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
317. J.W. Pitera and W.F. van Gunsteren
A Comparison of Non-bonded Scaling Approaches for Free Energy Calculations
Mol. Sim. 28 (2002) 45-65

A Molecular-Dynamics Simulation Study of the Conformational Preferences of Oligo-(3-hydroxy-alkanoic acids) in Chloroform Solution

319. F.A. Hamprecht, W. Thiel and W.F. van Gunsteren
Chemical Library Subset Selection Algorithms: A Unified derivation Using Spatial Statistics

320. T. Hansson, C. Oostenbrink and W.F. van Gunsteren
Molecular dynamics simulations

321. C. Peter, W.F. van Gunsteren and P.H. Hünenberger
Solving the Poisson equation for solute-solvent systems using fast Fourier transforms

322. 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.

323. 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

324. 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

325. 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 47 (2002) 534-545

326. 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 47 (2002) 469-480

327. L.J. Smith, X. Daura and W.F. van Gunsteren
Assessing Equilibration and Convergence in Biomolecular Simulations
Proteins 48 (2002) 487-496

328. 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

329. 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
330. W.F. van Gunsteren
Computersimulatie van complexe (bio)moleculaire systemen: Mogelijkheden, onmogelijkheden en perspectieven
(only available in Dutch)

331. W.F. van Gunsteren, X. Daura and A.E. Mark
Computation of Free Energy

332. D. Kony, W. Dam, S. Stoll and W.F. van Gunsteren
An Improved OPLS-AA Force Field for Carbohydrates

333. 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?

334. X. Daura, A. Glättli, P. Gee, C. Peter and W.F. van Gunsteren
The Unfolded State of Peptides

335. R. Baron, D. Bakowies, W.F. van Gunsteren and X. Daura
β-Peptides with Different Secondary-Structure Preferences: How Different Are Their Conformational Spaces?

336. 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

337. 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
Mol. Sim. 29 (2003) 123-138

338. H. Yu, T. Hansson and W.F. van Gunsteren
Development of a simple, self-consistent polarizable model for liquid water

A consistent potential energy parameter set for lipids: Dipalmitoylphosphatidylcholine as a benchmark of the GROMOS96 45A3 force field

340. 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

341. 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

342. 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
343. 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

344. 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?

345. 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 54 (2003) 116-127

346. C. Oostenbrink and W.F. van Gunsteren
Free energies of binding of polychlorinated bifenyls to the estrogen receptor from a single simulation
Proteins 54 (2004) 234-246

347. N.F.A. van der Vegt and W.F. van Gunsteren
Entropic Contributions in co-Solvent Binding to Hydrophobic Solutes in Water

348. 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

349. 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

Computer simulation studies on the solvation of aliphatic hydrocarbons in 6.9 M aqueous urea solution
Erratum: Computer simulation studies on the solvation of aliphatic hydrocarbons in 6.9 M aqueous urea solution

351. 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

352. C. Peter, C. Oostenbrink, A. van Dorp, W.F. van Gunsteren
Estimating entropies from molecular dynamics simulations

On the transferability of the SPC/L water model to biomolecular simulation

354. 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

Effect of methylation on the stability and solvation free energy of amylase and cellulose fragments: A molecular dynamics study
356. 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

357. I. Chandrasekhar, C. Oostenbrink and W.F. van Gunsteren
Simulating the Physiological Phase of Hydrated Dipalmitoylphosphatidylcholine Bilayers: The Ester Moiety

358. 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

359. R. Baron, D. Bakowies and W.F. van Gunsteren
Carbopeptoid folding: effects of stereochemistry, chain length and solvent
Angew. Chem. 116 (2004) 4147-4151

360. 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

361. 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

362. 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

363. A. Glättli, D. Seebach and W.F. van Gunsteren
Do valine side-chains have an influence on the folding behavior of β-substituted β-peptides?

364. M. van den Bosch, M. Swart, W.F. van Gunsteren and G.W. Canners
Simulation of the Substrate Cavity Dynamics of Quercetinase

365. H. Yu and W.F. van Gunsteren
Charge-on-spring polarizable water models revisited: From water clusters to liquid water to ice

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

367. C. Oostenbrink and W.F. van Gunsteren
Methane clustering in explicit water: Effect of urea on hydrophobic interactions

368. 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 58 (2005) 439-449

369. 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
370. 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

371. 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

Gunsteren and G.W. Caners
Calculation of the redox potential of the protein azurin and some mutants

373. C. Oostenbrink and W.F. van Gunsteren
Free energies of ligand binding for structurally diverse compounds

374. C. Oostenbrink, T.A. Soares, Nico F.A. van der Vegt and W.F. van Gunsteren
Validation of the 53A6 GROMOS force field

375. 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

The relative stability of homochiral and heterochiral alanine dipeptides. Effects of perturbation pathways and
force-field parameters on free energy calculations

377. 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

378. C. Oostenbrink and W.F. van Gunsteren
Efficient calculation of stacking and pairing free energies in DNA from molecular dynamics simulations

379. B. Zagrovic, E.J. Sorin, I.S. Millett, W.F. van Gunsteren, S. Doniach and V.S. Pande
Unusual compactness of a polyproline type II structure

380. A. Aemisseger, V. Kräutler, W.F. van Gunsteren and D. Hilvert
A Photoinducible β-Hairpin

381. V. Kräutler, A. Aemisseger, P.H. Hünenberger, D. Hilvert, T. Hansson, W.F. van Gunsteren
Use of molecular dynamics in the design and structure determination of a photoinducible β-Hairpin

382. 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
Mol. Sim. 31 (2005) 543-548
383. 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

384. C. Oostenbrink, D. Juchli, W.F. van Gunsteren
Amine hydration: A united-atom force field solution

385. H. Yu and W.F. van Gunsteren
Accounting for polarization in molecular simulation

386. 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

van Gunsteren.
On the influence of charged side-chains on the folding-unfolding equilibrium of β-peptides - A molecular
dynamics simulation study

388. M. Christen and W.F. van Gunsteren
An approximate but fast method to impose flexible distance constraints in molecular dynamics simulations

389. D. Trzesniak, A. Glättli, B. Jaun and W.F. van Gunsteren
Interpreting NMR Data for β-peptides using Molecular Dynamics Simulations

390. C. Oostenbrink and W.F. van Gunsteren
Calculating zeros: non-equilibrium free energy calculations

391. 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

392. P.J. Gee and W.F. van Gunsteren
Numerical simulation of the effect of solvent viscosity on the motions of a β-peptide heptamer

393. P.J. Gee and W.F. van Gunsteren
Acetonitrile revisited: a molecular dynamics study of the liquid phase

Orientation and conformational preference of leucine-enkephalin at the surface of a hydrated
dimyristoylphosphatidylcholine bilayer: NMR and MD simulation

395. P.J. Gee and W.F. van Gunsteren
Terminal-group effects on the folding behaviour of selected β-peptides
Proteins 63 (2006) 136-143

396. B. Zagrovic and W.F. van Gunsteren
Comparing atomistic simulation data with the NMR experiment: How much can NOE’s actually tell us?
Proteins 63 (2006) 210-218
397. 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

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

399. P.J. Gee and W.F. van Gunsteren
Numerical simulation of the pressure-denaturation of a helical beta-peptide heptamer solvated in methanol

400. 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

401. 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

Biomolecular modelling: goals, problems, perspectives
Angew. Chem 118 (2006) 4168-4198

403. 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 Journal 91 (2006) 1460-1470

404. 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

405. 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

406. 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

407. M. Christen, A.-P.E. Kunz, W.F. van Gunsteren
Sampling of rare events using hidden restraints

408. D. Trzesniak, R.D. Lins, W.F. van Gunsteren
A protein under pressure: Molecular dynamics simulation of the Arc repressor
Proteins 65 (2006) 136-144

409. M. Christen and W.F. van Gunsteren
Multigraining: an algorithm for simultaneous fine-grained and coarse-grained simulation of molecular systems
410. D. Trzesniak, W.F. van Gunsteren
Pathway dependence of the efficiency of calculating free energy and entropy of solute-solute association in water

411. D. Trzesniak, A.-P.E. Kunz, W.F. van Gunsteren
A comparison of methods to compute a potential of mean force

412. D. Trzesniak, B. Jaun, R.I. Mathad, W.F. van Gunsteren
Simulation of an all-β3-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. (DOI: 10.1002/bip.20601)

Molecular Dynamics Study of the Stabilities of Consensus Designed Repeat Proteins

414. 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

415. 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 β-type variant and the Apo state
Proteins 65 (2006) 702-711

416. 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

417. 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

418. C. Oostenbrink, M.M.H. van Lipzig and W.F. van Gunsteren

419. 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

420. B. Zagrovic, W.F. van Gunsteren
Computational analysis of the mechanism and thermodynamics of inhibition of phosphodiesterase 5A by synthetic ligands

421. 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

422. D. Trzesniak, N.F.A. van der Vegt, W.F. van Gunsteren
Analysis of neo-pentan-urea pair potentials of mean force in aqueous urea

423. 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)
424. C.D. Christ, W.F. van Gunsteren
Enveloping Distribution Sampling: A method to calculate free energy differences from a single simulation

425. 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
Proteins 16 (2007) 1101-1118

426. W.F. van Gunsteren, Z. Gattin
Simulation of folding equilibria

427. M. Christen, C. Christ, W.F. van Gunsteren
Free energy calculations using flexible-constrained, hard-constrained and non-constrained MD simulations

Configurational entropy elucidates the role of salt-bridge networks in protein thermostability

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

430. 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

431. M. Christen, W.F. van Gunsteren
On searching in, sampling of, and dynamically moving through conformational space of biomolecular systems: a review

432. 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

Analysis of the driving forces for biomolecular solvation and association

434. N. Schmid, B. Zagrovic, W.F. van Gunsteren
Folding-unfolding equilibrium of a methylene substituted beta-peptide

435. 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

436. 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
437. M.A. Cuendet, W.F. van Gunsteren
On the calculation of velocity-dependent properties in molecular dynamics simulations using the leap-frog integration algorithm

438. D.P. Geerke, St. Thiel, W. Thiel, W. F. van Gunsteren
A combined QM/MM molecular dynamics study on a condensed-phase S_n2 reaction at saturated nitrogen: the effect of explicitly including solvent polarization

439. M. Christen, B. Keller and W.F. van Gunsteren
Biomolecular structure refinement based on adaptive restraints using local-elevation simulation

440. 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
Mol. Sim. 33 (2007) 1143-1154

441. 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

Atomic model of de novo designed ccf-Met amyloid-like fibrils

443. Z. Gattin, W.F. van Gunsteren
A molecular dynamics study of the ASC and NALP1 Pyrin domains at low pH

444. 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

445. W.F. van Gunsteren, J. Dolenc
Biomolecular simulation: historical picture and future perspectives
Biochem. Soc. Trans. 36 (2008) 11-15, DOI: 10.1042/BST0360011

446. W.F. van Gunsteren, J.Dolenc, A.E. Mark
Molecular simulation as an aid to experimentalists

Structure and dynamics of two β-peptides in solution from molecular dynamics simulations validated against experiment

448. C.D. Christ, W.F. van Gunsteren
Multiple free energies from a single simulation: Extending enveloping distribution sampling to non-overlapping phase-space distributions

449. 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
450. W.F. van Gunsteren, D.P. Geerke
Computer simulation of biomolecular systems: where do we stand?

451. A. Choutko, A. Glättli, W.F. van Gunsteren
Simulation of the outer membrane protein X in a lipid bilayer and in a micelle

452. 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

453. F. Schwab, W.F. van Gunsteren, B. Zagrovic
Computational study of the mechanism and the relative free energies of binding of anticholesterolmic inhibitors to squalene-hopene cyclase

454. M. Winger, W.F. van Gunsteren
Use of molecular dynamics simulation for optimising protein stability: Consensus designed ankyrin repeat proteins

455. N. Schmid, Ch. Bolliger, L.J. Smith, W.F. van Gunsteren
Disulfide bond shuffling in bovine alpha-lactalbumin: MD simulation confirms experiment

456. 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)

457. 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

458. Z. Gattin, J. Schwartz, R.I. Mathad, B. Jaun, W.F. van Gunsteren
Interpreting experimental data by using molecular simulation instead of model building

459. Z. Gattin, W.F. van Gunsteren
Influence of backbone fluorine substitution upon the folding equilibrium of a beta-heptapeptide

460. 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

On the conformational properties of amylose and cellulose oligomers in solution

Force-field dependence of the conformational properties of α, ω-dimethoxypolyethylene glycol
463. D. Wang, B. Jaun, W.F. van Gunsteren
Folding and unfolding of two mixed alpha/beta peptides

464. 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

465. 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. 113 (2009) 11570-11579, DOI: 10.1021/jp903164s

466. 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

467. 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

468. J.R. Allison, W.F. van Gunsteren
A method to explore protein side chain conformational variability using experimental data

469. 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

470. D. Poger, W.F. van Gunsteren, A.E. Mark
A new force field for simulating phosphatidylcholine bilayers

471. 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

472. 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

473. B. Keller, Z. Gattin, W.F. van Gunsteren
What stabilizes the 3_14-helix in β-peptides? A conformational analysis using molecular simulation

474. B. Keller, X. Daura, W.F. van Gunsteren
Comparing geometric and kinetic cluster algorithms for molecular simulation data

475. Z. Gattin, J. Zaugg, W.F. van Gunsteren
Structure Determination of a Flexible Cyclic Peptide Based on NMR and MD Simulation 3J-Coupling
477. N. Schmid, M. Bötschi, W.F. van Gunsteren
A GPU solvent-solvent interaction calculation accelerator for biomolecular simulations using the GROMOS software

478. 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

479. Z. Lin, J.Kornfeld, M. Mächler, W.F. van Gunsteren
Prediction of folding equilibria of differently substituted peptides using one-step perturbation

480. 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

The propensity of aminoisobutyric acid (Aib) to induce helical secondary structure in an alpha-heptapeptide: a computational study

482. D. Wang, T. Merz, W.F. van Gunsteren (C0CP00181C)
The thermal isomerization of the GFP chromophore: a computational study

Molecular Dynamics Simulation of Ester-Linked Hen Egg White Lysozyme Reveals the Effect of Missing Backbone Hydrogen-Bond Donors on the Protein Structure

484. 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

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. supp. mat

486. 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

487. Z. Lin, A.P. Kunz, W.F. van Gunsteren
A one-site polarizable model for liquid chloroform: COS/C

488. 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
Mol. Sim. 36 (2010) 708-728, DOI: 10.1080/08927021003752804

489. 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


503. D. Steiner, C. Oostenbrink, F. Diederich, M. Zürcher, W.F. van Gunsteren
Calculation of binding free energies of inhibitors to Plasmepsin II

504. S. Riniker, A.P. Kunz, W.F. van Gunsteren
On the calculation of the dielectric permittivity and relaxation time of molecular models in the liquid phase

505. W. Huang, Z. Lin, W.F. van Gunsteren
Validation of the GROMOS 54A7 force field with respect to β-peptide folding

506. 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

Definition and testing of the GROMOS force-field versions: 54A7 and 54B7

508. 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

509. A. Kuzmanic, D. Kruschel, W.F. van Gunsteren, B. Zagrovic
Dynamics may significantly influence the estimation of interatomic distances in biomolecular X-ray structures

510. 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

511. 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

Biomolecular structure refinement using the GROMOS simulation software
J. Biomolecular NMR. 51 (2011) 265-281, DOI: 10.1007/s10858-011-9534-0

513. 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

GROMOS++ software for the analysis of biomolecular simulation trajectories

515. Z. Lin, W.F. van Gunsteren
Exploring the effect of side-chain substitutions upon the secondary structure preferences of β-peptides
N. Hansen, P. Kraus, H. Sassmannshausen, T. Timmerscheidt, W.F. van Gunsteren
An effective force field for molecular dynamics simulations of dimethyl sulfone

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

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

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 3_10-, α, and π helices

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. supp. mat.

D.A. Niggli, M.O. Ebert, Z. Lin, D. Seebach, W.F. van Gunsteren
Helical content of a β^-octapeptide in methanol: Molecular dynamics simulations explain a seeming discrepancy between conclusions derived from CD and NMR data

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

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

New functionalities in the GROMOS biomolecular simulation software

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

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.R. Allison, S. Riniker, W.F. van Gunsteren
Coarse-grained models for the solvents dimethyl sulfoxide, chloroform and methanol
541. T.S. Hofer, W.F. van Gunsteren
Exploring the properties of small molecule protein binding via molecular simulation: the TRSH – p53 core domain complex

542. 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. supp. mat

543. 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

544. W.F. van Gunsteren, J. Dolenc
Thirty-five years of biomolecular simulation: development of methodology, force fields, and software

Implicit solvation parameters derived from explicit water forces in large-scale molecular dynamics simulations

546. 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

Validation of the GROMOS 54A7 force field regarding mixed α/β peptide molecules

548. D. Wang, W.F. van Gunsteren, Z. Chai
Recent advances in computational actinide chemistry
Progress in Chemistry 7 (2011) 1566-1581 (Chinese version)

549. W.F. van Gunsteren
The seven sins in academic behavior in the natural sciences

550. 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, incl. supp. mat. DOI: 10.1002/pro.2184

Directed evolution of a model primordial enzyme provides insights into the development of the genetic code

552. A. Choutko, W.F. van Gunsteren
Conformational preferences of a β-octapeptide as function of solvent and force-field parameters

553. 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
554. 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) 2-17, DOI: 10.1002/anie.201205408
Angew. Chem. 125 (2013) 2-19, DOI: 10.1002/ange.201205408

555. 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 deca-peptide solvated in supra-molecular coarse-grained water

556. 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

557. 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

558. 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

559. 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

560. 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

561. 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

562. 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

563. 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

564. 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

565. 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
566. 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

567. 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

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. supp. mat.

569. Z. Lin, W.F. van Gunsteren
Enhanced conformational sampling using enveloping distribution sampling

570. Z. Lin, W.F. van Gunsteren
Refinement of the application of the GROMOS 54A7 force field to β-peptides

571. 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

On the sensitivity of peptide nucleic acid duplex formation and crystal dissolution to a variation of force-field parameters

573. 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

574. O.M. Szklarczyk, S.J. Bachmann, W.F. van Gunsteren
A polarisable empirical force field for molecular dynamics simulation of liquid hydrocarbons

575. W. Huang, S. Riniker, W.F. van Gunsteren
Rapid sampling of folding equilibria of β-peptides in methanol using a supramolecular solvent model

576. W. Huang, Z. Lin, W.F. van Gunsteren
The use of enveloping distribution sampling to evaluate important characteristics of biomolecular force fields

577. S.J. Bachmann, W.F. van Gunsteren
Polarisable model for DMSO and DMSO-water mixtures

578. N. Hansen, W.F. van Gunsteren
Practical aspects of free-energy calculations: A review
579. S.J. Bachmann, W.F. van Gunsteren
On the compatibility of polarisable and non-polarisable models for liquid water

580. 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

581. S.J. Bachmann, W.F. van Gunsteren
An improved polarisable water model for use in biomolecular simulation

Pyranose Dehydrogenase Ligand Promiscuity: A Generalized Approach to Simulate Monosaccharide
Solvation, Binding, and Product Formation

583. 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

The key to predicting the stability of protein mutants lies in an accurate description and proper
configurational sampling of the folded and denatured states
suppl. mat.

585. W. Huang, W.F. van Gunsteren
Challenge of representing entropy at different levels of resolution in molecular simulation

586. Z. Lin, S.J. Bachmann, W.F. van Gunsteren
GROMOS polarisable charge-on-spring models for liquid urea: COS/U and COS/U2

587. L.J. Smith, W.F. van Gunsteren, N. Hansen
Characterisation of the flexible lip regions in bacteriophage lambda lysozyme using MD simulations

588. O. Szklarczyk, E. Arvaniti, W.F. van Gunsteren
Polarisable coarse-grained models for molecular dynamics simulation of liquid cyclohexane

589. 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

590. Z. Lin, W.F. van Gunsteren
On the use of a weak-coupling thermostat in replica-exchange molecular dynamics simulations

591. A.P. Eichenberger, W. Huang, S. Riniker, W.F. van Gunsteren
A supra-atomic coarse-grained GROMOS force field for aliphatic hydrocarbons in the liquid phase

592. S.J. Bachmann, W.F. van Gunsteren
Structural and energetic effects of the use of polarisable water to solvate proteins
593. W.F. van Gunsteren  
On the pitfalls of peer review  

594. 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  

595. Z. Lin, W.F. van Gunsteren  
A comparison of pathway independent and pathway dependent methods in the calculation of conformational free enthalpy differences  

596. 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  

597. V.H. Rusu, S.J. Bachmann, W.F. van Gunsteren  
GROMOS polarisable model for acetone  

598. W.F. van Gunsteren  
Going for a PhD: Joys and Pitfalls  

599. 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  

600. L.J. Smith, W.F. van Gunsteren, N. Hansen  
On the Use of Time-Averaging Restraints when Deriving Biomolecular Structure from 1/H-coupling Values Obtained from NMR Experiments  

Deriving structural information from experimentally measured data on biomolecules: a review  
Angew. Chem. 128 (2016) 16222-16244, DOI: 10.1002/ange.201601828

602. W.F. van Gunsteren  
Publication of Research Results: Use and Abuse  
Infozine, Special Issue 1 (2016) 27-28, DOI: 10.3929/ethz-a-010745085

603. 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 S0 order parameters in disordered loops of the protein hGH at low pH  

604. 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  

Validation of Molecular Simulation: An Overview of Issues  
Angew. Chem. 130 (2018) 894-915, DOI:10.1002/ange.201702945
W.F. van Gunsteren
Surfing versus Drilling in Fundamental Research
Infozine, Special Issue 2 (2018) 18-19, DOI:10.3929/ethz-b-000294373

W.F. van Gunsteren
The Roots of Bio-Molecular Simulation: The eight-week CECAM workshop “Models for Protein Dynamics” of 1976

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

In press, submitted or in preparation

M. Pechlaner, A.P. Eichenberger, Z. Lin, V.H. Rusu, W.F. van Gunsteren
A method to apply bond-angle constraints in molecular dynamics simulation

M. Pechlaner, W.F. van Gunsteren
Algorithms to apply dihedral-angle constraints in molecular or stochastic dynamics simulations

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

L.J. Smith, W.F. van Gunsteren, N. Hansen
On the Use of $^3$J-coupling NMR Data to Derive Structural Information on Proteins
J. Biomol. NMR (2019) in preparation

L.J. Smith, W.F. van Gunsteren, N. Hansen
On the Use of Residual Dipolar Coupling NMR Data to Derive Structural Information on Bio-Molecules