

Curriculum Vitae: Bert de Groot

Personal data

Full name: Berend Lammert de Groot
Date of birth: August 24 1971
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Education and professional experience

1989-1994 Chemistry studies at the university of Groningen, the Netherlands. Specialisation: Biophysical chemistry. Supervisor: prof. H.J.C. Berendsen.
1994-1998 PhD student at the university of Groningen, the Netherlands, the department of biophysical chemistry. Promotor: prof. H.J.C. Berendsen. Subject: Native state protein dynamics studied by a variety of computer simulation techniques.
1998-2003 Postdoctoral fellow in the theoretical molecular biophysics group headed by Dr. Helmut Grubmüller, at the Max-Planck Institute for Biophysical Chemistry, Göttingen, Germany. Subject: Structure and function of aquaporins, studied by Molecular Dynamics and other computational techniques.
1997-2005 Extensive research visits to Rome university, EMBL Heidelberg, the Basel Biocentre and Nijmegen university.
2004- Head of the computational biomolecular dynamics group, Max-Planck Institute for Biophysical Chemistry, Göttingen, Germany.
2009 apl. Professor in physics, university of Göttingen.

Teaching and advanced training

- Computational Biophysics I and II for third and fourth year physics and chemistry students, university of Göttingen, since 2006;
- Advanced simulation course (lectures+practicals) "Computersimulation biomolekularer Prozesse" for third year physics and chemistry students, university of Göttingen, 2004-2006;
- education of first and second year chemistry and physics students in practical courses university of Groningen, 1994-1998;
- participation in several courses/workshops/masterclasses among which C/C++ programming, protein folding, molecular modelling, advanced techniques in Molecular Dynamics, in Shanghai, Nijmegen, Utrecht, Basel, Groningen, Göttingen.

Research interests

Protein structure-dynamics-function relationships, studied by computational techniques. In particular:

- large-scale molecular dynamics simulations and related techniques for the study of biomolecular dynamics at the atomic level tailored to unravel the functional mechanism of proteins and other biological macromolecules and complexes.
- reduced dimensionality methods not only to analyse molecular dynamics simulation trajectories but also to develop novel simulation techniques tailored at enhancing simulation efficiency;
- the use of molecular dynamics simulations and related techniques in the elucidation and refinement of macromolecular structures based on experimental data (x-ray, NMR, EM);
- development and application of alternative simulation approaches, like the CONCOORD method, to address questions that because of size and/or timescale issues are not accessible by conventional molecular dynamics simulations;
- conformational sampling and free energy approaches to structure based drug design.

Computing experience

Author of CONCOORD, an efficient method to predict (protein) conformational freedom from geometric constraints. Contributed essential dynamics sampling and normal modes to the gromacs molecular dynamics simulation suite, contributed several routines to the WHAT IF molecular modelling and visualisation package. Broad experience on different UNIX systems, extensive programming experience.

Languages

Dutch (mother tongue), English (fluent), German (fluent).

Referee assistance for journals and funding agencies

Journals: Algorithms, Angewandte Chemie, BBA Biomembranes, BMC Structural Biology, BMC Biochemistry, Biophysical Journal, Biopolymers, Chembiochem, Chemphysche, Chemmedchem, Chemical Physics Letters, Drug Discovery Today, Journal of Biological Physics, European Biophysics Journal, JACS, Journal of Chemical Theory and Computation, Journal of Computational Chemistry, Journal of Computer aided molecular design, Journal of Medicinal Chemistry, Journal of Molecular Biology, Journal of Molecular Graphics and Modelling, Journal of Molecular Modeling, Journal of Physical Chemistry, Journal of Structural Biology, Molecular Systems Biology, Nucleic Acids Research, Proceedings of the National Academy of Sciences U.S.A., Proteins: Structure, function and genetics, Protein Science, Science.

Funding agencies: DFG, NSF, NWO, STW, ISF.

Grants

1. "Computer simulation of enzymatic processivity" - Funded by the Deutsche Forschungsgemeinschaft (DFG GR 2079/1),
2. "Single file water transport across peptidic nanopores" - funded by the Deutsche Forschungsgemeinschaft (DFG GR 2079/2),
3. "Validation of the Plasmodium aquaglyceroporin as a drug target" - Funded by the EU (FP6-2003-LIFESCIHEALTH-3 - 012189), together with H. Grubmüller,
4. Marie Curie Research Training Network "Aqua(glycero)porins", funded by the EU.
5. "An integrated strategy for the in silico prediction and clinical evaluation of the cardiotoxicity of drug candidates", Funded by TI Pharma.
6. "Receptor ligand binding: complex structure prediction and affinity evaluation" - Funded by the Deutsche Forschungsgemeinschaft (DFG GR 2079/4),
7. "Spontaneous and induced aggregation of peptides" - Funded by the Deutsche Forschungsgemeinschaft (GRK 782)
8. European Drug Initiative for Channels and Transporters (EDICT), funded by the EU.
9. "Lipid-protein interactions in membrane embedded channels probed by atomistic molecular dynamics simulations" within the collaborative research center SFB 803 "Functionality Controlled by Organisation in and between Membranes", funded by the DFG.

Supervised Ph.D. Theses (past and current)

- Harshad Joshi - 1.2004 - 5.2007
- Daniel Seeliger - 3.2004 - 1.2008
- Marcus Kubitzki - 7.2004 - 12.2007
- Jochen Hub - 8.2004 - 1.2008
- Guillem Portella - 9.2004 - 4.2008
- Camilo Aponte - 9.2007 -
- Dirk Matthes - 2.2008 -
- Martin Vesper - 1.2009 -
- Sören Wacker - 1.2009 -
- Jan-Henning Peters - 3.2009 -
- Vytautas Gapsys - 1.2010 -

Group homepage: http://www.mpibpc.gwdg.de/groups/de_groot

Publications in peer-reviewed journals

(h-index: 30)

1. R.M. Scheek, N.A.J. van Nuland, B.L. de Groot and A. Amadei; "Structure from NMR and molecular dynamics: distance restraining inhibits motion in the essential subspace", *J. Biomol. NMR.* 6:106-11 (1995)
2. A. Amadei, A.B.M. Linssen, B.L. de Groot, D.M.F. van Aalten and H.J.C. Berendsen; "An efficient method for sampling the essential subspace of proteins.", *J. Biomol. Struct. Dyn.* 13:615-626 (1996)
3. B.L. de Groot, A. Amadei, D.M.F. van Aalten and H.J.C. Berendsen; "Towards an exhaustive sampling of the configurational spaces of the two forms of the peptide hormone guanylin", *J. Biomol. Struct. Dyn.* 13 : 741-751 (1996)
4. N.A.J. van Nuland, J.A. Wiersma, D. van der Spoel, B.L. de Groot, R.M. Scheek and G.T. Robillard; "Phosphorylation-induced torsion-angle strain in the active center of HPr, detected by NMR and restrained molecular dynamics refinement", *Prot. Sci.* 5: 442-446 (1996)
5. B.L. de Groot, D.M.F. van Aalten, A. Amadei and H.J.C. Berendsen; "The consistency of large concerted motions in proteins in Molecular Dynamics simulations", *Biophys. J.* 71: 1707-1713 (1996)
6. B.L. de Groot, A. Amadei, R.M. Scheek, N.A.J. van Nuland and H.J.C. Berendsen; "An extended sampling of the configurational space of HPr from *E. coli*", *Proteins: Struct. Funct. Gen.* 26: 314-322 (1996)
7. D. van der Spoel, B.L. de Groot, S. Hayward, H.J.C. Berendsen and H.J. Vogel; "Bending of the Calmodulin Central Helix: A Theoretical Study", *Prot. Sci.* 5: 2044-2053 (1996)
8. D.M.F. van Aalten, B.L. de Groot, H.J.C. Berendsen and J.B.C. Findlay; "Conformational analysis of retinoids and restriction of their dynamics by retinoid-binding proteins", *Biochem. J.* 319(2): 543-550 (1996)
9. D.M.F. van Aalten, B.L. de Groot, H.J.C. Berendsen, J.B.C. Findlay and A. Amadei; "A Comparison of Techniques for calculating Protein Essential Dynamics", *J. Comp. Chem.* 18:169-181 (1997)
10. B.L. de Groot, D.M.F. van Aalten, R.M. Scheek, A. Amadei, G. Vriend and H.J.C. Berendsen; "Prediction of protein conformational freedom from distance constraints", *Proteins: Struct. Funct. Gen.* 29: 240-251 (1997)
11. D.M.F. van Aalten, D.A. Conn, B.L. de Groot, J.B.C. Findlay, H.J.C. Berendsen and A. Amadei; "Protein dynamics derived from clusters of crystal structures", *Biophys. J.* 73(6): 2891-2896 (1997)
12. B.L. de Groot, S. Hayward, D.M.F. van Aalten, A. Amadei and H.J.C. Berendsen; "Domain Motions in Bacteriophage T4 Lysozyme; a Comparison between Molecular Dynamics and Crystallographic Data" *Proteins: Struct. Funct. Gen.* 31: 116-127 (1998).
13. Johannes P.M. Langedijk, Bert L. de Groot, Herman J.C. Berendsen and Jan T. van Oirschot; "Structural homology of the central conserved region of the attachment protein G of the respiratory syncytial virus with the fourth subdomain of 55 kD tumor necrosis factor receptor", *Virology* 243: 293-302 (1998).
14. B.L. de Groot, G. Vriend and H.J.C. Berendsen; "Conformational changes in the chaperonin GroEL: New insights into the allosteric mechanism", *J. Mol. Biol.* 286: 1241-1249 (1999).

15. A. Amadei, B.L. de Groot, M.-A. Ceruso, A. Di Nola and H.J.C. Berendsen; "A kinetic model for the internal motions of proteins: Diffusion between multiple harmonic wells," , *Proteins: Struct. Funct. Gen.* 35: 283-292 (1999).
16. J. Bernard Heymann, Matthias Pfeiffer, Volker Hildebrandt, H. Ronald Kaback, Dimitrios Fotiadis, Bert de Groot, Andreas Engel, Dieter Oesterhelt and Daniel J. Müller; "Conformations of the rhodopsin third cytoplasmic loop grafted onto bacteriorhodopsin"; *Structure Fold. Des.* 8(6): 643-653 (2000)
17. Bert L. de Groot, J. Bernard Heymann, Andreas Engel, Kaoru Mitsuoka, Yoshinori Fujiyoshi and Helmut Grubmüller; "The Fold of Human Aquaporin 1"; *J. Mol. Biol.* 300(4): 987-994 (2000)
18. Rainer Ossig, Hans Dieter Schmitt, Bert de Groot, Dietmar Riedel, Sirkka Keränen, Hans Ronne, Helmut Grubmüller, and Reinhard Jahn; "Exocytosis requires asymmetry in the central layer of the snare complex."; *EMBO J.* 19:6000-6010 (2000)
19. Henning Stahlberg, Thomas Braun, Bert de Groot, Ansgar Philippsen, Peter Agre, Mario J. Borgnia, Werner Kühlbrandt, and Andreas Engel; "The 6.9-Å structure of GlpF: A basis for homology modeling of the glycerol channel from *Escherichia coli*"; *J. Struct. Biol.* 132 (2): 133-141 (2000)
20. Bert L. de Groot, Xavier Daura, Alan E. Mark and Helmut Grubmüller; "Essential dynamics of reversible peptide folding: Memory-free conformational dynamics governed by internal hydrogen bonds"; *J. Mol. Biol.*, 390 (1): 299-313 (2001)
21. Bert L. de Groot, Andreas Engel and Helmut Grubmüller; "A refined structure of human aquaporin-1"; *FEBS Lett.* 504:206-211 (2001)
22. Bert L. de Groot and Helmut Grubmüller; "Water permeation across biological membranes: Mechanism and dynamics of aquaporin-1 and GlpF"; *Science*, 294:2353-2357 (2001)
23. Bert L. de Groot, D. Peter Tieleman, Peter Pohl and Helmut Grubmüller; "Water permeation through gramicidin A: desformylation and the double helix; a molecular dynamics study"; *Biophys. J.* 82: 2934-2942 (2002)
24. Mark J. Jedrzejewski, Luciane V. Mello, Bert L. de Groot, and Songlin Li; "Mechanism of hyaluronan degradation by *Streptococcus pneumoniae* hyaluronate lyase: Structures of complexes with the substrate"; *J. Biol. Chem.* 277:28287-28297 (2002)
25. Luciane V. Mello, Bert L. de Groot, Songlin Li, and Mark J. Jedrzejewski; "Structure and flexibility of streptococcus agalactiae hyaluronate lyase complex with its substrate: Insights into the mechanism of processive degradation of hyaluronan"; *J. Biol. Chem.* 277: 36678-36688 (2002)
26. Bert L. de Groot, Andreas Engel and Helmut Grubmüller; "The structure of the Aquaporin-1 water channel: a comparison between cryo-electron microscopy and x-ray crystallography." *J. Mol. Biol.* 325: 485-493 (2003)
27. Bert L. de Groot, Tomaso Frigato, Volkhard Helms and Helmut Grubmüller; "The mechanism of proton exclusion in the aquaporin-1 water channel". *J. Mol. Biol.* 333: 279-293 (2003).
28. Oliver F. Lange, H. Grubmüller, and Bert L. de Groot; "Molecular Dynamics Simulations of Protein G Challenge NMR-Derived Correlated Backbone Motions." *Angew. Chem. Int. Ed.* 44:3394-3399 (2005).
29. Andreas D. Schenk, Paul J.L. Werten, Simon Scheuring, Bert L. de Groot, Shirley A. Müller, Henning Stahlberg, Ansgar Philippsen and Andreas Engel; "The 4.5 Å Structure of Human AQP2." *J. Mol. Biol.* 350: 278-289 (2005).

30. W. Kukulski, A.D. Schenk, U. Johanson, T. Braun, B.L. de Groot, D. Fotiadis, P. Kjellbom and A. Engel; "The 5 Å Structure of Heterologously Expressed Plant Aquaporin SoPIP2;1." *J. Mol. Biol.* 350: 611-616 (2005)
31. Heise H, Luca S, de Groot B. L., Grubmüller H, Baldus M.; "Probing conformational disorder in neurotensin by two-dimensional solid-state NMR and comparison to molecular dynamics simulations." *Biophys J.* 89: 2113-2120 (2005)
32. Gabor Nagy, Ira Milosevic, Dirk Fasshauer, E. Matthias Müller, Bert L. de Groot, Thorsten Lang, Michael C. Wilson and Jakob B. Sorensen; "Alternative Splicing of SNAP-25 Regulates Secretion through Nonconservative Substitutions in the SNARE Domain" *Molecular Biology of the Cell* 16: 5675-5685 (2005).
33. J. B. Sorensen, K. Wiederhold, E. M. Müller, I. Milosevic, G. Nagy, B. L. de Groot, H. Grubmüller, and D. Fasshauer. "Sequential N- to C-terminal SNARE complex assembly drives priming and fusion of secretory vesicles." *EMBO J.* 25:955-966 (2006).
34. Sapar M. Saparov, Jochen R. Pfeifer, Loay Al-Momani, Guillem Portella, Bert L. de Groot, Ulrich Koert and Peter Pohl. "Mobility of a One-Dimensional Confined File of Water Molecules as a Function of File Length." *Phys. Rev. Lett.* 96:148101 (2006).
35. Daniel J. Rigden, James E. Littlejohn, Harshad V. Joshi, Bert L. de Groot and Mark J. Jedrzejewski. "Alternate Structural Conformations of Streptococcus pneumoniae Hyaluronan Lyase: Insights into Enzyme Flexibility and Underlying Molecular Mechanism of Action." *J. Mol. Biol.* 358:1165-1178 (2006).
36. Frank J. M. Detmers, Bert L. de Groot, E. Matthias Müller, Andrew Hinton, Irene B. M. Konings, Mozes Sze, Sabine L. Flitsch, Helmut Grubmüller, and Peter M. T. Deen. "Quaternary Ammonium Compounds as Water Channel Blockers." *J. Biol. Chem.* 281:14207-14214 (2006).
37. Jochen S. Hub and Bert L. de Groot. "Does CO₂ Permeate through Aquaporin-1?" *Biophys. J.* 91:842-848 (2006).
38. Frauke Gräter, Bert L. de Groot, Hualiang Jiang and Helmut Grubmüller "Ligand-Release Pathways in the Pheromone-Binding Protein of *Bombyx mori*" *Structure* 14:1567-1576 (2006).
39. S. Takamori, M. Holt, K. Stenius, E.A. Lemke, M. Grnborg, D. Riedel, H. Urlaub, S. Schenck, B. Brügger, Ph. Ringler, S.A. Müller, B. Rammner, F. Gräter, J. S. Hub, B.L. De Groot, G. Mieskes, Y. Moriyama, J. Klingauf, H. Grubmüller, J. Heuser, F. Wieland, and R. Jahn. "Molecular Anatomy of a Trafficking Organelle." *Cell* 127:831-846 (2006).
40. Guillem Portella, Peter Pohl and Bert L. de Groot. "Invariance of Single-File Water Permeability in Gramicidin-like Peptidic Pores as function of Pore Length." *Biophys. J.* 92:3930-3937 (2007)
41. Marcus B. Kubitzi and Bert L. de Groot. "Molecular Dynamics Simulations using Temperature Enhanced Essential dynamics Replica EXchange (TEE-REX)." *Biophys. J.* 92:4262-4270 (2007).
42. Daniel Seeliger and Bert L. de Groot. "Atomic contacts in protein structures. A detailed analysis of atomic radii, packing and overlaps". *Proteins.* 68: 595-601 (2007).
43. Carsten Kutzner, David van der Spoel, Martin Fechner, Erik Lindahl, Udo W. Schmitt, Bert L. De Groot, Helmut Grubmüller. "Speeding up parallel GROMACS on high-latency networks." *J. Comp. Chem.* 28:2075-2084 (2007).

44. Jochen S. Hub, Tim Salditt, Maikel C. Rheinstädter, and Bert L. de Groot "Short range order and collective dynamics of DMPC bilayers. A comparison between molecular dynamics simulations, x-ray, and neutron scattering experiments". *Biophys. J.* 93: 3156-3168 (2007).
45. Daniel Seeliger, Jürgen Haas, and Bert L. de Groot. "Geometry-based Sampling of Conformational Transitions in Proteins." *Structure* 15: 1482-1492 (2007).
46. Jochen S. Hub and Bert L. de Groot. "Mechanism of selectivity in aquaporins and aquaglyceroporins" *Proc. Nat. Acad. Sci.* 105:1198-1203 (2008).
47. Claudia Hartmann, Mohamed Chami, Ulrich Zachariae, Bert L. de Groot, Andreas Engel and Markus G. Grütter. "Vacuolar protein sorting: Two different functional states of the AAA-ATPase Vps4p." *J. Mol. Biol.* 377:352-363 (2008).
48. Matthias E. Müller, Jochen S. Hub, Helmut Grubmüller and Bert L. de Groot. "Is TEA an inhibitor for human Aquaporin-1?" *Pflügers Archiv.* 456:663-669 (2008).
49. Ulrich Zachariae, Robert Schneider, Phanindra Velisetty, Adam Lange, Daniel Seeliger, Sören J. Wacker, Yasmin Karimi-Nejad, Gert Vriend, Stefan Becker, Olaf Pongs, Marc Baldus and Bert L. de Groot. "The molecular mechanism of toxin-induced conformational changes in a potassium channel: relation to C-type inactivation." *Structure* 16:747-754 (2008).
50. Marcus B. Kubitzki and Bert L. de Groot. "The Atomistic Mechanism of Conformational Transition in Adenylate Kinase: a TEE-REX Molecular Dynamics Study." *Structure*, 8:1175-1182 (2008).
51. Nils-Alexander Lakomek, Korvin F. A. Walter, Christophe Fares, Oliver F. Lange, Bert L. de Groot, Helmut Grubmüller, Rafael Brüschweiler, Axel Munk, Stefan Becker, Jens Meiler and Christian Griesinger. Self-consistent residual dipolar coupling based model-free analysis for the robust determination of nanosecond to microsecond protein dynamics *J. Biomol. NMR.* 41: 139-155 (2008)
52. Oliver F. Lange, Nils-Alexander Lakomek, Christophe Farès, Gunnar F. Schröder, Korvin F. A. Walter, Stefan Becker, Jens Meiler, Helmut Grubmüller, Christian Griesinger, Bert L. de Groot. "Recognition dynamics up to microseconds revealed from RDC derived ubiquitin ensemble in solution". *Science*, 320:1471-1475 (2008).
53. Guillem Portella, Jochen S. Hub, Martin D. Vesper, and Bert L. de Groot. "Not only enthalpy: large entropy contribution to ion permeation barriers in single-file channels". *Biophys. J.* 95: 2275-2282 (2008).
54. Rainer A. Böckmann, Bert L. de Groot, Sergej Kakorin, Eberhard Neumann, Helmut Grubmüller. "Kinetics, Statistics, and Energetics of Lipid Membrane Electroporation Studied by Molecular Dynamics Simulations" *Biophys. J.* 95: 1837-1850 (2008).
55. Nils-Alexander Lakomek, Oliver F. Lange, Korvin F.A. Walter, Christophe Fares, Dalia Egger, Peter Lunkenheimer, Jens Meiler, Helmut Grubmüller, Stefan Becker, Bert L. de Groot and Christian Griesinger. "Residual dipolar couplings as a tool to study molecular recognition of ubiquitin." *Biochemical Society Transactions* 36: 1433-437 (2008).
56. Alexander Benedix, Caroline M. Becker, Bert L. de Groot, Amedeo Caffisch, Rainer A. Böckmann. "Predicting Free Energy Changes Using Structural Ensembles". *Nature Methods.* 6: 3-4 (2009).
57. Harshad V. Joshi, Mark J. Jedrzejewski and Bert L. de Groot. "Domain motions of hyaluronan lyase underlying processive hyaluronan translocation." *Proteins.* 76:30-46 (2009).

58. Daniel Seeliger and Bert L. de Groot. "tCONCOORD-GUI: Visually Supported Conformational Sampling of Bioactive Molecules." *J. Comp. Chem.* 30:1160-1166 (2009).
59. Guillem Portella and Bert L. de Groot. "Determinants of water permeability through nanoscopic hydrophilic channels." *Biophys. J.* 96:925-938 (2009).
60. Gerhard Fischer, Urszula Kosinska-Eriksson, Camilo Aponte-Santamaria, Madelene Palmgren, Cecilia Geijer, Kristina Hedfalk, Stefan Hohmann, Bert L. de Groot, Richard Neutze, Karin Lindkvist-Petersson. "Crystal Structure of a Yeast Aquaporin at 1.15Å Reveals a Novel Gating Mechanism." *PLoS Biology.* 7: e1000130 (2009).
61. Christian M. Stegmann, Daniel Seeliger, George M. Sheldrick, Bert L. de Groot and Markus Wahl. "Thermodynamic signature of trapped water molecules in a protein-ligand interaction." *Angewandte Chemie.* 48:5207-5210 (2009).
62. Dirk Matthes and Bert L. de Groot. "Secondary structure propensities in peptide folding simulations: A systematic comparison of molecular mechanics interaction schemes". *Biophys. J.* 97:599-608 (2009).
63. Jochen S. Hub and Bert L. de Groot. "Detection of functional modes in protein dynamics." *PLoS Comput. Biol.* 5: e1000480 (2009).
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65. R. A. Fenton, H. B. Moeller, S. Nielsen, B. L. de Groot, and M. Rützler. "A plate reader-based method for cell water permeability measurement." *Am J Physiol Renal Physiol.* 298: F224-F230 (2010).
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69. Jochen S. Hub, Marcus Kubitzki and Bert L. de Groot. "Spontaneous quaternary and tertiary T-R transitions of human hemoglobin in molecular dynamics simulation." *PLoS Comput. Biol.* 6:e1000774 (2010).
70. Daniel Seeliger and Bert L. de Groot. "Ligand docking and binding site analysis with PyMOL and Autodock/Vina". *J. Computer-aided Molec. Design.* 24:417-422 (2010).
71. Oliver F. Lange, David van der Spoel and Bert L. de Groot. "Scrutinizing Molecular Mechanics Force Fields on the Microsecond Timescale With NMR Data." *Biophys. J.* 99:647-655 (2010).
72. Camilo Aponte-Santamaria, Jochen S. Hub and Bert L. de Groot. "Dynamics and energetics of solute permeation through the Plasmodium falciparum aquaglyceroporin." *PCCP.* 12:10246-10254 (2010).
73. Jochen S. Hub, Fritz Winkler, Mike Merrick and Bert L. de Groot. "Potentials of mean force and permeabilities for carbon dioxide, ammonia, and water flux across a Rhesus protein channel and lipid membranes." *J. Am. Chem. Soc.* 132:13251-13263 (2010).

74. J. J. Lopez Cascales, S. D. Oliviera Costa, Bert L. de Groot and D. Eric Walters. "Binding of Glutamate to the Umami Receptor." *Biophys. Chem.* 152:139-144 (2010).
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76. Jochen S. Hub, Camilo Aponte-Santamaria, Helmut Grubmüller and Bert L. de Groot. "Voltage-regulated water flux through aquaporin channels in silico." *Biophys. J.* 99:L97-L99 (2010).
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Reviews, book chapters and other publications

78. A. Amadei, A.B.M. Linssen, B.L. de Groot and H.J.C. Berendsen; "Essential degrees of freedom of proteins", in "Modelling of Biomolecular Structures and Mechanisms" A. Pullmann et. al. (ed.) pp 85-93 (1995)
79. Bert de Groot; "Native state protein dynamics", PhD Thesis, University of Groningen (1999)
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81. Bert L. de Groot and Helmut Grubmüller; "Aquaporine — Wasserfilter der Zelle"; *BIOforum* 6: 387-389 (2002)
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85. B. L. de Groot and H. Grubmüller; "Aquaporine: Die perfekten Wasserfilter der Zelle"; *BIOspektrum* 4: 384-386 (2004)
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88. Daniel Seeliger and Bert L. de Groot. "Prediction of protein flexibility from geometrical constraints." *Biotech International.* 18:20-22 (2006).
89. Louic S. Vermeer, Bert L. de Groot, Valerie Reat, Alain Milon, Jerzy Czaplicki. "Acyl chain order parameter profiles in phospholipid bilayers: computation from molecular dynamics simulations and comparison with 2H NMR experiments." *Eur. Biophys. J.* 36: 919-931 (2007).

90. Steven Hayward and Bert L. de Groot. Normal Modes and Essential Dynamics. in: *Methods in molecular biology, vol 443, Molecular modelling of proteins*. pp. 89-106 (2008).
91. Jochen S. Hub, Helmut Grubmüller and Bert L. de Groot. Dynamics and Energetics of Permeation Through Aquaporins. What Do We Learn from Molecular Dynamics Simulations? In: *Handbook of Experimental Pharmacology. Aquaporins*. Vol. 190: 57-76 (2009).
92. Marcus B. Kubitzki, Bert L. de Groot and Daniel Seeliger. Protein dynamics: from structure to function In: *From Protein Structure to Function with Bioinformatics*. pp. 217-249 (2009).

Invited talks at conferences and workshops

1. BioScience 2010, Forschungszentrum Jülich, Germany, November 15 - 17, 2010. "The dynamics of molecular recognition and aggregation."
2. Epithelial transport Workshop 2010, Strobl, Austria, June 25-27, 2010. "Selectivity, gating and inhibition of aquaporin water channels".
3. 7th transport colloquium, castle Rauischolzhhausen, Germany, May 27-28, 2010. "Selectivity mechanisms in aquaporins".
4. VIII Workshop on Molecular Theories and Simulations, Gaeta, Italy, May 24-26, 2010. "Mechanisms underlying molecular recognition."
5. NBIC thematic meeting Protein structure bioinformatics. University of Nijmegen, the Netherlands, March 1, 2010. "Permeation and inhibition mechanisms in water and ion channels".
6. Workshop: Molecular Simulation of Transport Phenomena in Chemistry and Biology, Saarbrücken, Germany, October 8, 2009. "Molecular mechanisms underlying selectivity, gating and inhibition in aquaporins"
7. TCCM masterclass, Leuven, Belgium, September 15-16, 2009. "Permeation mechanisms across biological membranes." and "Collective transitions in enzyme catalysis and molecular recognition."
8. Novo Nordisk Prize Symposium, Aarhus, September 10-11, 2009. "Permeation, inhibition and gating mechanisms in aquaporin water channels."
9. Membrane protein bioinformatics workshop Stockholm, September 7-8, 2009. "Permeation mechanisms across biological membranes."
10. Biomedical transporters 2009, Thun, CH, August 9-13, 2009. "Permeation mechanisms across biological membranes."
11. Heraeus Summer School 2009: Quantum and Classical Simulation of Biological Systems and their Interaction with Technical Materials, Bremen, June 15-26, 2009. "Permeation mechanisms across biological membranes." and "Collective transitions in enzyme catalysis and molecular recognition."
12. 2nd Conference on Drug Development for the Third World, Trieste, Italy, June 1-5, 2009. "Flexibility and drug design".
13. The young investigators meeting, Estuary Island, Kerala, India, February 24-28, 2009. "Collective transitions in enzyme catalysis and molecular recognition."
14. Regional Biophysics Conference 2009, Linz, Austria, 10-14 February 2009. "Collective transitions in enzyme catalysis and molecular recognition."

15. Gromacs workshop on Advanced Simulation Methods, Göttingen, September 24th-26th, 2008. "Collective transitions in enzyme catalysis and molecular recognition."
16. CECAM workshop Membrane Protein Assembly: Theory and Experiment Lausanne, September 3-6, 2008. "Permeation mechanisms across membranes."
17. ICM meeting, Uppsala, Sweden, April 3-4, 2008. "Water and ion permeation through natural and synthetic membrane channels"
18. Water interfaces in physics, chemistry and biology: a multi-disciplinary approach. 8-13 December 2007, Obergurgl, Austria. "Dynamics and energetics of water permeation across biological channels and model peptidic pores."
19. SFB 613-Symposium, Bielefeld University, Oct. 8.- 9., 2007. "Ion and water permeation through natural and synthetic channels: a single-molecule perspective."
20. Aquaporin 2007,, July 13-17, 2007, Nara, Japan. "Mechanism of selectivity in the aquaporin family of water channels".
21. VIII. Annual Linz Winter Workshop, Advances in Single-Molecule Research for Biology & Nanoscience. February 4-6, 2006, Linz, Austria. "Dynamics and mechanism of aquaporin water channels".
22. SBC-WCN workshop on protein structure/function prediction and comparative genomics. May 28-29 2005, Stockholm, Sweden. "The mechanism of water permeation and proton exclusion in the aquaporin family of water channels".
23. MGMS Annual International Meeting 2005 "Membranes and Membrane Proteins" April 4th - 6th 2005, Oxford, UK. "The mechanism of water permeation and proton exclusion in the aquaporin family of water channels"
24. BioSapiens workshop on membrane proteins January 27-30, 2005, Nijmegen, the Netherlands, "The mechanism of water permeation and proton exclusion in the aquaporin family of water channels"
25. EMBO course "Methods for protein simulations and drug design", September 13-24, 2004, Shanghai, China. "Introduction into molecular dynamics simulations", "Water permeation and proton exclusion in the membrane water channel aquaporin-1", "Principal components analysis"
26. The Biannual International Meeting of the International Society of Quantum Biology and Pharmacology. June 5-8, 2004, Como, Italy. "Dynamics and mechanism of water permeation and proton exclusion in aquaporins"
27. Graduiertenkolleg "Protein-protein interactions in signal transduction", November 7-8, 2003, Regensburg, Germany. "Water permeation and proton exclusion in the membrane water channel aquaporin-1."
28. COST D22 EU Workshop "Membrane Protein interactions", October 30-31, 2003, Madrid, Spain. "Water permeation and proton exclusion in the membrane water channel aquaporin-1"
29. 4th European Biophysics Congress, EBSA 2003, July 5-9, July, Alicante, Spain. "Water permeation across biological membranes: structure, dynamics and mechanism of aquaporin-1 and GlpF"
30. Workshop "Computer Simulation and Theory of Biomolecules", May 9-10, 2003, Hünfeld, Germany. "The mechanism of proton exclusion in the water channel Aquaporin-1"
31. PSB workshop "Membrane structure and function." February 10-11th, 2003, Grenoble, France. "Water permeation across biological membranes: structure, dynamics and mechanism of aquaporin-1 and GlpF"

32. 4th ORCS International symposium on "Development of New Structural Biology Including Hydrogen and Hydration." November 11-12, 2002, Tsukuba, Japan. "Water permeation across biological membranes: structure, dynamics and mechanism of aquaporin-1 and GlpF"
33. Annual Meeting of the German Biophysics Society, September 8-10, 2002, Dresden, Germany "Water permeation across cell membranes: aquaporin-1"
34. 1st Workshop on Molecular Theories and Simulations. May 10-12, 2002, Sperlonga, Italy. "Water permeation across biological membranes: structure, dynamics and mechanism of aquaporin-1 and GlpF"
35. ESS workshop on "Flexibility and Function of Proteins." January 25-27 2002, Heidelberg, Germany. "Water permeation across biological membranes: structure, dynamics and mechanism of aquaporin-1 and GlpF"
36. Workshop "Computational biology and bioinformatics", November 29, 2001, Jena, Germany. "Structure-dynamics-function relationships in proteins probed by computer simulations"
37. Workshop "Computer Simulation and Theory of Biomolecules", May 23-24, 2001, Hünfeld, Germany. "Essential dynamics of reversible peptide folding"
38. CECAM Workshop on "Calculation of concerted motions in biomolecules" October 11-14, 1999, Lyon, France. "Concerted motions in proteins: to what extent does structure determine dynamics?"

Invitations to colloquia and seminars

39. ECROPS seminar, department of biology, university of Erlangen, Germany. January 13, 2011. "Permeation mechanisms across biological membranes"
40. Department seminar, physical chemistry, University of Dortmund, Germany. October 14, 2010. "Spontaneous peptide aggregation in silico".
41. Physiology department seminar, University of Hannover, Germany. September 14, 2010. "Permeation mechanisms across biological membranes"
42. NCMLS Department seminar, university of Nijmegen, the Netherlands, December 1, 2009. "Molecular mechanisms underlying selectivity, gating and inhibition in aquaporins".
43. Department seminar, polymer physics, university of Eindhoven, the Netherlands, November 30, 2009. "Permeation and inhibition mechanisms in water and ion channels."
44. Department seminar, Institute of Physical and Theoretical Chemistry, University of Frankfurt, June 29, 2009. "Collective dynamics underlying enzyme catalysis and molecular recognition".
45. Department seminar, Department of pharmacy, university of Kiel, April 20, 2009. "Permeation mechanisms across membrane channels."
46. Department seminar, Institut für Pharmakologie und Toxikologie, university of Vienna, Austria, January 15, 2009. "Water and ion permeation through natural and synthetic membrane channels."
47. Institute seminar, Max Planck Institute for Biophysics, Frankfurt, December 4, 2008. "Permeation mechanisms across membranes."
48. Institute seminar, department of biology, Darmstadt university, November 27, 2008. "Permeation mechanisms across membranes."

49. Institute seminar Computer-Chemie-Centrum Erlangen, November 17, 2008. "Collective dynamics underlying enzyme catalysis and molecular recognition."
50. Institute seminar Forschungszentrum Jülich, July 4, 2008. "Water and ion permeation through natural and synthetic membrane channels."
51. Institute seminar at the John Innes Centre, Norwich, UK. June 24, 2008. "Collective dynamics underlying enzyme catalysis and molecular recognition."
52. EDICT Kickoff meeting, Düsseldorf, June 18-20, 2008. "Aquaporin channels as drug targets"
53. master course "Molecular simulation of membrane channels", Basel, CH. March 29, 2008.
54. Department seminar, School of Computing Sciences, University of East Anglia, Norwich, UK. Jan 24, 2008.
55. master course "Molecular docking", Manchester, May 15, 2007.
56. Kickoff meeting RTN Network "Aquaglyceroporins", Gothenburg, Nov. 30, 2006; "Dynamics and mechanism of aquaporin water channels".
57. 3. ZKI-Autumn meeting 2006, GWDG, Göttingen, Sept. 26, 2006; "Simulating proteins in action: a challenge for high-performance computing".
58. Seminar at the University of Braunschweig, Jul 28, 2006; "Biomolecular dynamics: from peptide folding to membrane transport"
59. Seminar at Alcon Inc., Ft. Worth, USA, Feb. 17, 2006. "Dynamics and mechanism of aquaporin water channels".
60. Graduate School Seminar, GRK 782, Göttingen, Feb. 2, 2006. "Biomolecular dynamics: from peptide folding to membrane transport"
61. Seminar at the University of Saarbrücken, Sept. 8th, 2005. "Structural variance in solution NMR ensembles."
62. Seminar at the Biozentrum, University of Basel, April 12th, 2005; "The mechanism of water permeation and proton exclusion in the aquaporin family of water channels"
63. Seminar at the Department of Biochemistry and Structural Biology, August 12 2003, University of Edinburgh, UK. "Mechanism of water permeation and proton exclusion in the membrane water channel Aquaporin-1"
64. Seminar at the Department of Cell Physiology, July 16 2003, University of Nijmegen, the Netherlands. "Water permeation across biological membranes: structure, dynamics and mechanism of aquaporin-1 and GlpF"
65. 6th EU biotech ('Aquaplugs') meeting. May 23-25, 2003, Aarhus, Denmark. "The mechanism of proton exclusion in the water channel Aquaporin-1"
66. 5th EU biotech ('Aquaplugs') meeting. October 18, 2002, Hamburg, Germany. "The structure of the Aquaporin-1 water channel: a comparison between cryo-electron microscopy and x-ray crystallography."
67. seminar series: "Meet the expert." July 8-12 2002, CMBI, University of Nijmegen, the Netherlands. "Prediction of protein conformational freedom from distance constraints"

68. Seminar at the Department of Biochemistry, University of Zürich, Switzerland, Prof. A. Caffisch. May 31, 2002. "Structure-dynamics-function relationships in proteins probed by computer simulations"
69. Institute seminar "Doktorandenseminar", Max Planck Institute for biophysical chemistry, Göttingen, Germany. May 8, 2002. "Water permeation across biological membranes: structure, dynamics and mechanism of aquaporin-1 and GlpF"
70. 4th EU biotech ('Aquaplugs') meeting. April 7-11, Haute-Nendaz, Switzerland. "Molecular dynamics simulation of water permeation across Aquaporin-1 and GlpF"
71. Seminar at the Forschungsinstitut für Molekulare Pharmakologie, Berlin, Germany, Dr. P. Pohl. March 19, 2002. "Water permeation across biological membranes probed by computer simulations"
72. Seminar at the Theoretical Chemistry department, Frankfurt University, Frankfurt am Main, Germany, Prof. G. Stock. "Structure-dynamics-function relationships in proteins probed by computer simulations"
73. Seminar at the physical biology department, University of Rio de Janeiro, Brazil, Prof. P. Bisch. January 22, 2002. "Structure-dynamics-function relationships in proteins probed by computer simulations"
74. Institute seminar at the "Embrapa Recursos Genéticos e Biotecnologia", Brasilia, Brazil. January 17, 2002. "Structure-dynamics-function relationships in proteins probed by computer simulations"
75. Institute seminar at the Centre for Molecular and Biomolecular Informatics (CMBI), Nijmegen, the Netherlands, Prof. G. Vriend. December 3, 2001. "Water permeation across biological membranes: structure, dynamics and mechanism of aquaporin-1 and GlpF"
76. 3rd EU biotech ('Aquaplugs') meeting. October 19-20, 2001, Göttingen, Germany. "Water permeation across biological membranes: structure, dynamics and mechanism of aquaporin-1 and GlpF"
77. 2nd EU biotech ('Aquaplugs') meeting. June 1-2, 2001, Edinburgh, UK. "A refined structure of human Aquaporin-1"
78. Department seminar at the biophysics department, Wageningen University, the Netherlands. May 29, 2001. "Structure and dynamics of human aquaporin-1"
79. Department seminar at the Biochemistry department, University of Dundee, Scotland, UK. Dr. D. Van Aalten. February 20, 2001. "Structure and dynamics of human aquaporin-1"
80. 1st EU biotech ('Aquaplugs') meeting. November 3-4, 2000, Amsterdam, the Netherlands. "Progress on the structure of human Aquaporin-1"
81. 4th EU biotech ('Water and Glycerol Channels from the MIP family'), March 18-20, 2000, Haute-Nendaz, Switzerland. "The fold of human aquaporin-1"
82. 3rd EU biotech ('Water and Glycerol Channels from the MIP family') meeting, September 16-17, 1999, Hamburg, Germany. "The structure of AQP1: progress and problems"
83. 2nd EU biotech ('Water and Glycerol Channels from the MIP family') meeting, March 12-14, Gif-sur-Yvette, France. "Novel structure refinement methods at medium resolution"
84. Institute seminar at the Biocenter, Basel University, Switzerland, Prof. A. Engel. December 3, 1998. "Domain Motions in Bacteriophage T4 Lysozyme; a Comparison between Molecular Dynamics and Crystallographic Data"

85. Scientific Meeting of SON Working Group on Proteins, December 8-9, 1997, Lunteren, the Netherlands."Domain Motions in Bacteriophage T4 Lysozyme; a Comparison between Molecular Dynamics and Crystallographic Data"
86. Department seminar at the department of Computational Chemistry and Mathematics, DSM research, Geleen, the Netherlands. April 1996. "Essential dynamics sampling - an efficient way to sample the conformational space of proteins"
87. Department seminar at the department of biochemistry and molecular biology, University 'Tor Vergata', Rome, Italy, Prof. A. Desideri. April 6, 1995. "Essential dynamics sampling of proteins"
88. Presentations at the 5th, 6th and 7th annual Biomos Meeting, Burg Arras, Alf-Mosel, Germany (1995, 1996, 1997).