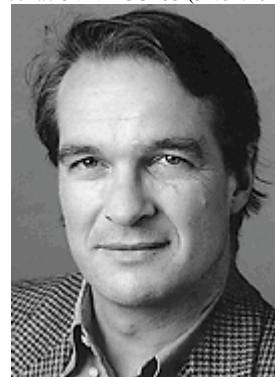


CURRICULUM VITAE

(C3)

Personal/CV VAGU-C3 (31.01.2012)

Name van Gunsteren, Willem F.
Date of birth August 7, 1947
Place of birth Wassenaar, The Netherlands
Nationality Dutch
Sex male
Civil Status married, two children



Address
home Krähbühlstrasse 49
8044 Zürich
Switzerland
phone 41-44-262 1747
office Laboratory of Physical Chemistry
ETH Zürich, HCI G237
CH-8093 Zürich
Switzerland
phone 41-44-632 5501/02
FAX 41-44-632 1039
email: wfvgn@igc.phys.chem.ethz.ch
homepage: www.igc.ethz.ch

Education

<i>Institution</i>	<i>Degree</i>	<i>Year</i>	<i>Scientific Field</i>
Free University, Amsterdam	B.Sc.	1968	Physics
Free University, Amsterdam	Meester	1974	Law
Free University, Amsterdam	Ph.D.	1976	Nuclear Physics
University of Groningen	(Postdoc)	1976-1978	Molecular Physics
Harvard University	(Postdoc)	1978-1980	Molecular Physics

Honors

- Doctorate Cum Laude (1976)
- Royal Dutch - Shell Prize for Doctoral Research (1975)
- Royal Dutch Union of Chemists gold medal for research (1987)
- Degussa - Stiftungsgastprofessur für Chemie und Medizin, Johann Wolfgang Goethe - Universität, Frankfurt (1988)
- Visiting Professor, University of Science and Technology of China, Hefei (1993-1997)
- Corresponding member, Royal Dutch Academy of Arts and Sciences (1995)
- 73th Priestly Lecturer Penn State University (1999)
- Visiting Professor, University of Florence (2000)
- 10th Huygens Lecturer Dutch Science Foundation (2001)
- Visiting Professor, University of Leiden (2002)
- Max-Planck Forschungspreis für Chemie und Pharmazie (2002)
- Visiting Professor, École Normale Supérieure, Paris (2007)
- Distinguished Lecturer, CMMS, University of Pittsburgh (2009)
- Golden Tricycle award for most family friendly group leader, ETH Zürich (2009)

Major research interest

Development of methodology to simulate the behaviour of biomolecular systems

Research and/or Professional Experience

- March 1980 - Senior Lecturer, Department of Physical Chemistry,
May 1987 University of Groningen, The Netherlands
- May 1987 - Professor of Physical Chemistry, University of
Sept. 1990 Groningen, The Netherlands
- Sept. 1987 - Professor of Computational Physics, Free University,
Aug. 1992 Amsterdam, The Netherlands
- Nov. 1987 - Sabbatical leave, University of California,
Sept. 1988 San Francisco, USA
- Sept. 1990 - Professor of Computer-Aided Chemistry, ETH Zürich,
Zürich, Switzerland
- March 1997 - Sabbatical leave, University of Oxford,
Oct. 1997 Oxford, U.K.

Teaching duties

courses on

- Mathematical and Computational Methods in Chemistry
- Statistical Mechanics
- Computational Physics
- Advanced Programming
- Computer Science
- Computer Simulation in Chemistry, Biology and Physics

supervised PhD theses: 42

Organisational experience and duties

- *September 1982*
one of two organisers of a three-week workshop on nucleotide binding to proteins (15 participants) at CECAM, University of Paris IX, Orsay, France
- *May 1984*
one of two organisers of a one-week workshop on molecular dynamics and protein structure (140 participants) at the University of North Carolina, Chapel Hill, USA
- *September 1984*
one of two organisers of a three-day CECAM discussion meeting on the design of drugs and vaccines (35 participants) in Amersfoort, The Netherlands
- *August 1985*
organiser of a three-day CECAM discussion meeting on the calculation of free energy in macromolecular systems (17 participants) in Amersfoort, The Netherlands

- *1986* -
Author and organiser of the Groningen Molecular Simulation (GROMOS) software for biomolecular simulation, which is used in hundreds laboratories in more than 60 countries on all continents.
- *1991* -
organiser of the yearly international Biomos meeting on biomolecular simulation (30 - 40 participants) at Burg Arras, Germany,
- *September 1992*
one of three organisers of a five-day workshop on protein folding and stability (51 participants) in Ascona, Switzerland
- *1993 - 2005*
Head Competence Centre for Computational Chemistry, Zürich
- *April 1993*
one of two organisers of a two-day CECAM discussion meeting on the generation of amorphous polymer structures (17 participants) at CECAM, Orsay, France
- *April 1994*
one of four organisers of a five-day workshop on membranes, theory, simulation and experiment (48 participants) in Ascona, Switzerland
- *1995 - 1997*
Head Institute of Physical Chemistry, ETH Zürich
- *1997 - 2005*
President Informatikkommission ETH Zürich
- *November 1997*
one of nine organisers of a three-day joint workshop of the GDCh and C4 ETHZ on the use of computers in chemistry (93 participants) in Männedorf, Switzerland
- *1997* -
Delegate of the President of the ETH for nominations of professors
- *May 1999*
one of three organisers of a five-day workshop on computational sciences and engineering (80 participants) in Ascona, Switzerland
- *September 1999*
one of six organisers of a two-day conference on biomolecular structure, dynamics and function (172 participants) in Groningen, The Netherlands
- *2000 - 2002*
Head Department of Chemistry, ETH Zürich (~40M Euro turnover)
- *2001*
Responsible for festivities regarding the opening of the new chemistry laboratory of the ETH Zürich (~10'000 visitors)

- 2005
Responsible for 150th anniversary festivities of the Department of Chemistry and Applied Biosciences, ETH Zürich (~10'000 visitors)
- Member of the University Council of Vienna
- 2006-2008
Head Department of Chemistry and Applied Biosciences, ETH Zürich (~50M Euro turnover)
- 2006
Chair of the Gordon Research Conference on Computational Chemistry (one week with 150 participants) in Les Diablerets, Switzerland
- 2008 -
Member Strategiekommission ETH Zürich
- 2009
Organiser of a symposium on computational science and engineering (140 participants) in Zürich, Switzerland

Scientific duties

- Member of the Editorial Board of the European Biophysical Journal
- Founder and Director of a software house for scientific computer software, Biomos b.v., since 1986
- Member of the Editorial Board of the journal Molecular Simulation
- Member of the Editorial Board of the Journal of Biomolecular NMR
- Member of the Editorial Board of the Journal of Computational Chemistry
- Member of the University Council of the University of Vienna, Austria
- Member of the Editorial Board of the journal Angewandte Chemie

Invited lectures

1982

- Biophysical Society (Oxford, U.K.)
- Burroughs Wellcome (London, U.K.)
- Rheinisch Westphalische Technische Hochschule (Aachen, Germany)
- University of Alberta (Edmonton, Canada)
- University of California (San Francisco, U.S.A.)
- University of North-Carolina (Chapel Hill, U.S.A.)
- Harvard University (Cambridge, U.S.A.)

1983

- Swedish Agricultural University (Uppsala, Sweden)
- Birkbeck College (London, U.K.)
- Rheinisch Westphalische Technische Hochschule (Aachen, Germany)

1984

- University of Science and Technology of China (Hefei, China)
- Polish Academy of Sciences (Warsaw, Poland)
- University of North Carolina (Chapel Hill, U.S.A.)

- Fysisch Laboratorium, R.U.U. (Utrecht, The Netherlands)

1985

- Institut Laue Langevin (Grenoble, France)
- University of Frankfurt (Frankfurt, Germany)
- Stichting Academisch Rekencentrum Amsterdam (Amsterdam, The Netherlands)
- KNCV (Twente, The Netherlands)
- Royal Swedish Academy of Sciences (Stockholm, Sweden)
- German and Swedish Biophysical Societies (Lübeck, Germany)
- New York Academy of Sciences (New York, U.S.A.)
- Du Pont (Wilmington, U.S.A.)
- KNAW (Amsterdam, The Netherlands)

1986

- Fysisch Laboratorium V.U. (Amsterdam, The Netherlands)
- Molecular Graphics Society (Cap d'Agde, France)
- International Union of Crystallography (Garmisch-Partenkirchen, Germany)

1987

- Molecular Graphics Society (York, U.K.)
- ICI (Macclesfield, U.K.)
- University of Frankfurt (Frankfurt, Germany)
- SON (Lunteren, The Netherlands)
- Material Science Center (Vlieland, The Netherlands)
- Colloquium de Protides (Brussels, Belgium)
- BIOSON (Groningen, The Netherlands)
- Gesellschaft Deutscher Chemiker (Baden-Baden, Germany)
- Unilever (Vlaardingen, The Netherlands)
- Shell (Amsterdam, The Netherlands)
- FEBS (Ljubljana, Yugoslavia)
- Max-Planck Institut für Biochemie (München, Germany)
- Freie Universität (Berlin, Germany)
- University of Minnesota (Minneapolis, U.S.A.)
- University of Science and Technology of China (Hefei, China)
- University of New South Wales (Sydney, Australia)
- Australian National University (Canberra, Australia)
- Ludwig Institute for Cancer Research (Melbourne, Australia)
- University of Chicago (Chicago, U.S.A.)
- Alliant (Princeton, U.S.A.)

1988

- KNCV (Amsterdam, The Netherlands)
- Bayer (Leverkusen, Germany)
- Florida State University (Tallahassee, U.S.A.)
- UCSD (San Diego, U.S.A.)
- Alliant (Amsterdam, The Netherlands)
- Int. School of Crystallography (Erice, Italy)
- Gordon Research Conf. on Comput. Chemistry (Plymouth, U.S.A.)
- 14th Biochemistry Congress (Prague, Czechoslovakia)
- Molecular Graphics Society (San Francisco, U.S.A.)
- CARB (Rockville, U.S.A.)
- NIH (Bethesda, U.S.A.)
- Du Pont (Wilmington, U.S.A.)
- Wyeth-Ayerst (Princeton, U.S.A.)
- Wesleyan University (Middletown, U.S.A.)
- State University (Utrecht, The Netherlands)
- BASF (Ludwigshafen, Germany)

- Swiss Crystallographic Society (Lausanne, Switzerland)
- Hoffmann-La Roche (Basel, Switzerland)
- Gesellschaft für Biotechnologische Forschung (Braunschweig, Germany)
- J.W. Goethe University (Frankfurt, Germany)
- Hoechst (Frankfurt, Germany)

1989

- University of Oxford (Oxford, U.K.)
- University of Cambridge (Cambridge, U.K.)
- CCP4/CCP5 Meeting, SERC (Daresbury, U.K.)
- Eidg. Technische Hochschule (ETH) (Zürich, Switzerland)
- University of Utrecht (Utrecht, The Netherlands)
- GERM XI (Bordeaux, France)
- Sandoz (Basel, Switzerland)
- ICSN (Gif sur Yvette, France)
- Bio-Expo 89 (Paris, France)
- Int. School of Crystallography (Erice, Italy)
- Alfred Benzon Symposium (Copenhagen, Denmark)
- 32nd IUPAC Congress (Stockholm, Sweden)
- CECAM Meeting (Ermelo, The Netherlands)
- German, Swiss, Austrian and Yugoslavian Biophysical Societies (Todtmoos)
- Alliant (Tokyo, Japan)
- CBI (Tokyo, Japan)
- Philips (Eindhoven, The Netherlands)
- Dutch Biophysical Society (Groningen, The Netherlands)
- Janssen Pharmaceuticals (Tilburg, The Netherlands)
- Technische Universität (München, Germany)
- SON (Lunteren, The Netherlands)

1990

- CECAM Meeting (Orsay, France)
- Rhône-Poulenc (Vitry, France)
- Agricultural University (Wageningen, The Netherlands)
- University of Houston (Houston, U.S.A.)
- Texas A&M University (College Station, U.S.A.)
- Howard Hughes Medical Institute (Dallas, U.S.A.)
- Austrian Chemical Society (Vienna, Austria)
- University of Vienna (Vienna, Austria)
- Biostructure (Strasbourg, France)
- Second Naples Workshop on Bioactive Peptides (Anacapri, Italy)
- DSM (Vaals, The Netherlands)
- C4 Symposium (Zuerich, Switzerland)
- University of Michigan (Ann Arbor, U.S.A.)
- Eli Lilly (Indianapolis, U.S.A.)
- 10th Int. Biophysics Congress (Vancouver, Canada)
- UCSF (San Francisco, U.S.A.)
- 4th Symposium Protein Society (San Diego, U.S.A.)
- IBM Workshop on Polymer Science (Oberlech, Austria)
- European Physical Society (Amsterdam, The Netherlands)
- Czechoslovakian Academy of Sciences (Podebrady, Czechoslovakia)
- Molecular Graphics Society (York, United Kingdom)
- IBM, Intl. Business Machines Corp. (Rüschlikon, Switzerland)
- Eidg. Technische Hochschule (ETH) (Zürich, Switzerland)
- Max-Planck Institut für Biochemie (Martinsried, Germany)
- University of Zürich (Zürich, Switzerland)

- Hoffmann-La Roche (Basel, Switzerland)

1991

- Sandoz (Basel, Switzerland)
- Ciba-Geigy (Basel, Switzerland)
- Ciba Foundation Symposium (London, U.K.)
- Biozentrum University Basel (Basel, Switzerland)
- Dept. Informatik, ETH Zürich (Zürich, Switzerland)
- French Chemical Society (Obernai, France)
- Gesellschaft Deutscher Chemiker (Frankfurt, Germany)
- Swiss Computational Chemists (Bern, Switzerland)
- Dept. Organic Chemistry, University Basel (Basel, Switzerland)
- AKZO (Arnhem, The Netherlands)
- NATO Workshop on Computation in Biotechnology (Sant Feliu, Spain)
- Workshop on Structure and Function of Mutated Proteins (Florence, Italy)
- EMBO Workshop on NMR Structures of Proteins (Kandersteg, Switzerland)
- Workshop on Molecular Simulation (Ovronnaz, Switzerland)
- Gesellschaft für Biologische Chemie (Bayreuth, Germany)
- Ecole Polytechnique (Palaiseau, France)
- CNRS School of Protein Modelling (Toulouse, France)
- Congresso Nazionale die NMR (Milano, Italy)
- 14iemes Journées Scientifiques Rhône-Poulenc (Lyon, France)
- Johannes Gutenberg-Universität Mainz (Mainz, Germany)
- Utrecht Center for Computational Science (Utrecht, The Netherlands)

1992

- Unilever (Vlaardingen, The Netherlands)
- Société Royale de Chimie (Namur, Belgium)
- Rhône-Poulenc Rorer Recherche-Développement (Vitry, France)
- Universität Ulm (Ulm, Germany)
- Workshop on parallel computers (Ascona, Switzerland)
- Cray symposium (Bern, Switzerland)
- Joint Nordic Spring Meeting Physical Societies (Nyborg, Denmark)
- Novo-Nordisk (Bagsvaerd, Denmark)
- Bayer-Pharma (Wuppertal, Germany)
- Dept. Pharmacy ETH Zürich (Zürich, Switzerland)
- Workshop on supercomputing in science and industry (Ascona, Switzerland)
- Gesellschaft Österreichischer Chemiker (Graz, Austria)
- Siemens Nixdorf (München, Germany)
- Colorado State University (Fort Collins, USA)
- 3rd Keck Symposium (Houston, USA)
- Indian Institute of Science (Bangalore, India)
- Dept. Physics, University of Lausanne (Lausanne, Switzerland)
- Unilever (Vlaardingen, The Netherlands)
- Schering (Berlin, Germany)
- Technische Universität (Berlin, Germany)

1993

- Dept. Biochemistry, University of Zürich (Zürich, Switzerland)
- Keystone Symposium 1993 (Taos, USA)
- Workshop on Protein Dynamics & Thermodynamics (Jerusalem, Israel)
- CECAM Workshop on Starting Structures for Polymer Simulation (Paris, France)
- Max-Planck-Institut für Biochemie (Martinsried, Germany)
- Schwerpunktprogramm Informatik Workshop (Bern, Switzerland)

- Agouron Institute (San Diego, USA)
- Nalbandov-Beckman Institute Symposium (Urbana-Champaign, USA)
- Parallel Computational Biology Workshop (Urbana-Champaign, USA)
- Symposium on Macromolecular Structure & Function (Toronto, Canada)
- 12th Annual Conference of the Molecular Graphics Society (Interlaken, Switzerland)
- Société Vaudoise des Sciences Naturelles (Lausanne, Switzerland)
- Zeneca Pharmaceuticals (Macclesfield, United Kingdom)
- 22nd FEBS Meeting (Stockholm, Sweden)
- 7th Rhine-Knee Crystallographers Meeting (Délémont, Switzerland)
- Universitat Polytechnica de Catalunya (Barcelona, Spain)
- Leiden University (Leiden, The Netherlands)

1994

- Unilever Ltd (Vlaardingen, The Netherlands)
- EMBL (Heidelberg, Germany)
- Karolinska Institutet (Stockholm, Sweden)
- Int. Young Scientist meeting on Biotechnology (Ascona, Switzerland)
- Asean Molecular Biology Organisation (Osaka, Japan)
- Protein Engineering Research Institute (Osaka, Japan)
- Chemistry, Biology, Informatics Forum (Tokyo, Japan)
- Protein Engineering and Molecular Design Forum (Tokyo, Japan)
- University of Groningen (Groningen, The Netherlands)
- European Workshop COST-Chemistry (Como, Italy)
- Rhone-Poulenc (Vitry, France)
- 1st Eur. Conf. Comput. Chem. (Nancy, France)
- Ciba-Geigy (Basel, Switzerland)
- Thomae (Biberach, Germany)
- Center for Adv. Res. in Biotechnology (Rockville, USA)
- NIH (Bethesda, USA)
- Univ. of North Carolina (Chapel Hill, USA)
- Rhône-Poulenc/Rorer (Collegeville, USA)
- Bristol-Myers-Squibb (Princeton, USA)
- DuPont-Merck (Wilmington, USA)
- Unilever Ltd. (Vlaardingen, The Netherlands)
- XVI-th Int. Conf. Magn. Res. in Biol. Syst. (Eindhoven, The Netherlands)
- NOVUM Conf. Protein Motion (Stockholm, Sweden)
- Groningen Biomolecular Sciences Institute (Groningen, The Netherlands)
- Royal Society Meeting on Protein Folding (London, U.K.)
- Zeneca Pharmaceuticals (Macclesfield, U.K.)
- Conference at the Institute Juan March (Madrid, Spain)
- Conference at Unilever Ltd. (Vlaardingen, The Netherlands)
- University of Amsterdam (Amsterdam, The Netherlands)

1995

- WISOR IV Winterschool (Bressanone, Italy)
- Chemische Gesellschaft (Fribourg, Switzerland)
- VW-Stiftung Symposium (Hünfeld, Germany)
- University of Florence (Florence, Italy)
- Workshop on Protein Structure (Ripa d'Orcia, Italy)
- 1st Eur. Symp. Protein Society (Davos, Switzerland)
- Eur. Research Conf. NMR in Molecular Biology (Wildbad-Kreuth, Germany)
- University of Heidelberg (Heidelberg, Germany)
- Summerschool on MC and MD simulation (Como, Italy)
- University of Science and Technology of China (Hefei, China)
- National Supercomputing Research Centre of Singapore (Singapore)

- Centre for Math. Modelling and Computer Simulation (Bangalore, India)
- Indian Institute of Science (Bangalore, India)
- C4 Workshop on computational chemistry (Zürich, Switzerland)

1996

- Rhône-Poulenc Rorer (Vitry, France)
- Gesellschaft Deutscher Chemiker (Konstanz, Germany)
- University of Georgia (Athens, USA)
- Genentech, Inc. (South San Francisco, USA)
- 37th ENC Conference (Pacific Grove, USA)
- University of California (San Francisco, USA)
- Agouron Pharmaceuticals (San Diego, USA)
- University of California (San Diego, USA)
- Amgen Inc. (Thousand Oaks, USA)
- University of Zürich (Zürich, Switzerland)
- Gesellschaft österreichischer Chemiker (GÖCH) (Vienna, Austria)
- University of Vienna (Vienna, Austria)
- NATO workshop on biomolecular structure and dynamics (Loutraki, Greece)
- Gordon Research Conference on computational chemistry (New Hampton, USA)
- WATOC '96: 4th World Congress (Jerusalem, Israel)
- IUPAB: 12th Int. Biophys. Congress (Amsterdam, The Netherlands)
- Amer. Chem. Society: 212th National Meeting (Orlando, USA)
- Firmenich S.A. (Geneva, Switzerland)

1997

- Rhône-Poulenc Rorer (Vitry, France)
- Universität Tübingen (Tübingen, Germany)
- Oxford Centre Molecular Sciences (Oxford, U.K.)
- Workshop on computation of protein structure (Oxford, U.K.)
- Dept. Physical Chemistry, University of Oxford (Oxford, U.K.)
- Humboldt Universität (Berlin, Germany)
- 2nd Int. Symp. Algorithms for Macrom. Modelling (Berlin, Germany)
- Givaudan-Roure S.A. (Dübendorf, Switzerland)
- Zeneca Pharmaceuticals (Macclesfield, U.K.)
- IUPAC: 36th Int. Congress (Geneva, Switzerland)
- 3rd Eur. Research Conf. NMR in Molecular Biology (Oxford, U.K.)
- MGS and WATOC Conference: Modelling '97 (Erlangen, Germany)
- 2nd Int. Conf. on Molecular Structural Biology (Vienna, Austria)
- Int. Workshop on Polyelectrolytes, MPI Pol. Forschung (Mainz, Germany)
- 12. CIC Workshop der GDCh (Männedorf, Switzerland)
- Workshop on MC approach to Biopolymers and Folding, KFA (Jülich, Germany)
- Rheinisch-Westphälische Technische Hochschule (Aachen, Germany)
- Int. Workshop on Bioinformatics, Biozentrum, Univ. Basel (Basel, Switzerland)

1998

- Technische Universität München (München, Germany)
- IRRMA simulation course, EPFL (Lausanne, Switzerland)
- Bristol-Myers-Squibb (Princeton, USA)
- Merck-DuPont (Wilmington, USA)
- National Institutes of Health (NIH) (Washington D.C., USA)
- 3rd Johns Hopkins Protein Folding Meeting (Berkeley Springs, USA)
- Eur. Conf. on Comput. Chem. (Chambery, France)
- Biomedical Centre, Uppsala University (Uppsala, Sweden)
- Rhône-Poulenc Rorer (Lyon, France)
- Cours 3^{ème} Cycle en Physique, EPFL (Lausanne, Switzerland)
- CECAM Workshop on implicit solvent models (Lyon, France)

- Symp. on large scale computing, Lund University (Lund, Sweden)
- Cours 3ème Cycle en Physique, EPFL (Lausanne, Switzerland)
- CECAM Workshop on hybrid methods (Lyon, France)
- Gordon Research Conference (Kingston, USA)
- University of Florence (Florence, Italy)
- 6th Naples Workshop on Bioactive Peptides (Capri, Italy)
- EMBO Workshop on Proteins (EMBL, Heidelberg, Germany)
- 34th Symposium for Theoretical Chemistry (Gwatt, Switzerland)
- University of Tübingen (Tübingen, Germany)
- Workshop on protein folding (Madrid, Spain)

1999

- IMS Int. Workshop on Protein Stability and Folding (Okazaki, Japan)
- Oxford Centre Molecular Sciences (Oxford, U.K.)
- Int. School of Struct. Biology and Magn. Resonance (Erice, Italy)
- Gordon Conf. on Comput. Aspects of NMR (Il Ciocco, Italy)
- Kansas State University (Manhattan, USA)
- Workshop on Treatment of Electrostatic Interactions (Santa Fe, USA)
- COST Workshop (Geneva, Switzerland)
- Course Advanced Computing in NMR Spectr. (Florence, Italy)
- Conf. on Understanding Biomol. Struct., Funct., Dyn. (Groningen, The Netherlands)
- Penn State University (State College, USA)
- Univ. of the Sciences in Philadelphia (Philadelphia, USA)
- Univ. of Science and Technology of China (Hefei, China)
- Sino-Swiss Workshop on Bioinformatics (Beijing, China)
- University of Utrecht (Utrecht, The Netherlands)

2000

- National Institute for Medical Research (London, U.K.)
- University of Florence (Florence, Italy)
- 18-th Molecular Graphics Society Meeting (York, U.K.)
- IBM Research Laboratory (Rüschlikon, Switzerland)
- Uppsala University (Uppsala, Sweden)
- VW Symposium on Conformational Control (Kloster Banz, Germany)
- Conference Computational Biophysics 2000 (Nice, France)
- Gordon Research Conference on Biopolymers (Newport, USA)
- IBM Tomas Watson Research Laboratory (Yorktown Heights, USA)
- Gordon Research Conference on Computational Chemistry (Oxford, U.K.)
- University of Barcelona (Barcelona, Spain)
- XIX-th Int. Conf. Magn. Res. in Biol. Sci. (Florence, Italy)
- 7-th Biophysics Summerschool (Rovinj, Croatia)

2001

- University of Massachusetts Medical School (Worcester, USA)
- Wesleyan University (Middletown, USA)
- Bristol-Myers-Squibb (Princeton, USA)
- National Institutes of Health (Bethesda, USA)
- University of California (San Francisco, USA)
- IBM Workshop on Protein Folding (San Diego, USA)
- 221-th ACS meeting (San Diego, USA)
- Annual Meeting Swiss Physical Society (Dübendorf, Switzerland)
- Gesellschaft Deutscher Chemiker (Mülheim, Germany)
- Leiden University (Leiden, The Netherlands)
- Gesellschaft Deutscher Chemiker (Göttingen, Germany)
- Boehringer Ingelheim (Biberach, Germany)
- SIMU conference (Konstanz, Germany)

- University of Queensland (Brisbane, Australia)
- ComBio2001 (Canberra, Australia)
- 7-th Australian Molecular Modelling Workshop (Canberra, Australia)
- Sydney Protein Meeting (Sydney, Australia)
- Ludwig Institute for Cancer Research (Melbourne, Australia)
- NWO/Huygens-lezing (Den Haag, The Netherlands)

2002

- University of Konstanz (Konstanz, Germany)
- Wacker GmbH (München, Germany)
- IBM and NeSC Workshop on Protein Science (Edinburgh, Scotland)
- Lund Life Sciences Symposium (Lund, Sweden)
- Symposium New Chemistry ETH Zürich (Zürich, Switzerland)
- University of Pernambuco (Recife, Brazil)
- Workshop on Modeling in Biophysics (Rio de Janeiro, Brazil)
- University of Sao Paulo (Sao Paulo, Brazil)
- University of Sao Paulo (Ribeirao Preto, Brazil)
- University of Leiden (Leiden, The Netherlands)
- COST-D9 Workshop (Smolenice, Slovakia)
- University of Groningen (Groningen, The Netherlands)
- Gordon Research Conf. on Comput. Chemistry (New London, USA)
- SFC Eurochem Conference (Toulouse, France)
- Exploring Modern Comput. Chemistry (Nottingham, UK)
- WATOC'02 (Lugano, Switzerland)
- Bijvoet Seminar, University of Utrecht (Utrecht, The Netherlands)
- Ehrenfest Colloquium, University of Leiden (Leiden, The Netherlands)
- 44th Symp. of Soc. for Histochemistry (Vlissingen, The Netherlands)
- NCCR Symposium Uni Zürich (Zürich, Switzerland)

2003

- Sharif University of Technology (Tehran, Iran)
- University of Tehran (Tehran, Iran)
- Tarbiat Modarres University (Tehran, Iran)
- University of Leiden (Leiden, The Netherlands)
- University of Bordeaux (Bordeaux, France)
- 7th Annual Meeting Swedish Structural Biology (Tallberg, Sweden)
- Summerschool Biomolecular Structure and Dynamics (Otočec, Slovenia)
- Astra Zeneca (Macclesfield, U.K.)
- Oxford University (Oxford, U.K.)
- 11th Intl. Congress of Quantum Chemistry (Bonn, Germany)
- Technical University Delft (Delft, The Netherlands)
- 8th Biophysics Summerschool (Rovinj, Croatia)
- National Institutes of Health (Bethesda, USA)

2004

- Conf. on Theory and Applic. of Comput. Chemistry (Gyeongju, S.Korea)
- ETH-Kolloquium Naturwiss. und Unterricht (Zürich, Switzerland)
- Free University (Amsterdam, The Netherlands)
- Workshop Intrinsic Reactivity of New Molec. Materials (Nice, France)
- Intl. Meeting Molec. Graphics and Modelling Society (Manchester, U.K.)
- EMBO Course Methods for Protein Simulation and Drug Design (Shanghai, China)
- University of Science and Technology of China (Hefei, China)
- University of Beijing (Beijing, China)
- 2nd Eur. Conf. on Chemistry towards Biology (Seggau/Graz, Austria)
- Pantok Dialogos (Zürich, Switzerland)

2005

- WATOC Congress (Capetown, South Africa)
- Kolloquium Naturwiss. at University Basel (Basel, Switzerland)
- Glaxo-Smith-Kline (Stevenage, UK)
- Pfizer (Sandwich, UK)
- Royal Dutch Acad. Sciences (Amsterdam, The Netherlands)
- Symposium Frontiers in Comput. Biology, NIH (Washington, USA)
- Kolloquium Phys. Chemie ETH (Zürich, Switzerland)
- Dutch Polymer Institute, Tech. Univ. Eindhoven (Eindhoven, The Netherlands)
- Sika Technologies AG, (Zürich, Switzerland)
- Boehringer (Wien, Austria)
- Symposium Theoretical Chemistry (Innsbruck, Austria)
- Parrinello Symposium (Monte Verita, Ascona, Switzerland)
- FEBS Course Theo. Mod. of ligand binding and enzymatic catalysis (Tromsø, Norwegen)
- Intl. Conf. on Diff. Eq. from Theory to Comput. Sci. and Eng. (Zürich, Switzerland)
- Rotary Club (Zug, Switzerland)
- Conf. Biol. Dynamics: from molecules to cells (Amsterdam, The Netherlands)

2006

- Chemische Gesellschaft Darmstadt (Darmstadt, Germany)
- Univ. Heidelberg (Heidelberg, Germany)
- Organon N.V. (Oss, The Netherlands)
- University of Vienna (Vienna, Austria)
- Technical University of Munich (Munich, Germany)
- Kolloquium Rechnergestützte Wissenschaften, ETH Zürich (Zürich, Switzerland)
- University of Basel (Basel, Switzerland)
- Max Gruber Lecture, University of Groningen (Groningen, The Netherlands)
- University of Ljubljana (Ljubljana, Slovenia)
- Summer school Varenna (Varenna, Italy)
- 1st European Chemistry Congress (Budapest, Hungary)
- IFPSC Workshop, 3M Headquarters (St Paul, USA)

2007

- J. W. Goethe University (Frankfurt, Germany)
- University of Leiden (Leiden, The Netherlands)
- University of Heidelberg (Heidelberg, Germany)
- Ecole Normale Supérieure (Paris, France)
- Institut de Biologie Physico-Chimique (Paris, France)
- Darmstädter Molecular Modelling Workshop (Erlangen, Germany)
- BIG seminar series, University Lausanne (Lausanne, Switzerland)
- Bioinformatics Institute, Biomed. Res. Council (Singapore)
- Nanyang Technical University (Singapore)
- National Institute of Chemistry (Ljubljana, Slovenia)
- Rudjer Boskovic Institute (Zagreb, Slovenia)
- Course on free energy calculation (Zürich, Switzerland)
- 12th European Conf. on the spectroscopy of biological molecules (Bobigny, France)
- Conference on biomolecular simulation and experiment (Manchester, UK)
- University of Leeds (Leeds, UK)
- University of Oxford (Oxford, UK)
- Birkbeck College, University of London (London, UK)
- Symposium on light-induced dynamics of biopolymers (Munich, Germany)

2008

- NCCR course on biomolecular modelling (Kandersteg, Switzerland)
- Zing conference on computational biophysics (Antigua and Barbuda)
- Kolloquium Rechnergestützte Wissenschaften, ETH (Zürich, Switzerland)
- CASP 7.5 conference (Madrid, Spain)

- Ludwig-Maximilians University (Munich, Germany)
- Theoretical Biochemistry Conference (Stockholm, Sweden)
- Workshop Computational Biology and System Biology (Jülich, Germany)
- Pfizer Ltd. (Sandwich, UK)
- NCCR structural biology seminar (Zürich, Switzerland)
- National Yang-Ming University (Taipei, Taiwan)
- Academia Sinica (Taipei, Taiwan)
- Biomolecular Modelling Retreat (Stradbroke Island, Australia)
- WATOC conference (Sydney, Australia)
- TACC conference (Shanghai, China)
- University of Science and Technology of China (Hefei, China)
- CAS-SSSTC workshop (Zürich, Switzerland)

2009

- Deutsche Chemische Gesellschaft (Berlin, Germany)
- University of Chicago (Chicago, USA)
- Cornell Medical College (New York, USA)
- University of Pittsburgh (Pittsburgh, USA)
- Department of Chemistry, University of Vienna (Vienna, Austria)
- Academy of Science (Linz, Austria)
- Department of Physics, University of Vienna (Vienna, Austria)
- Boehringer GmbH (Vienna, Austria)
- Theoretical and Computational chemistry, University of Vienna (Vienna, Austria)
- Department of Physics, University of Rome La Sapienza (Rome, Italy)
- Biomolecular Simulation Workshop (Stockholm, Sweden)
- 23rd Symposium of the Protein Society (Boston, USA)
- Mediterranean Institute for Life Sciences (Split, Croatia)
- 3rd Adriatic Meeting on Computational Solutions in the Life Sciences (Primosten, Croatia)
- Symp. Frontiers in Macromol. Simulation (Atlanta, USA)

2010

- NCCR course on biomolecular modelling (Kandersteg, Switzerland)
- King's College, University London (London, UK)
- Int. Symp. Theoretical and Comput. Chemistry (Mülheim, Germany)
- Workshop Frontiers in the Life Sciences (Strasbourg, France)
- University of Calgary (Calgary, Canada)
- University of Alberta (Edmonton, Canada)
- ACS - meeting (San Francisco, USA)
- Sino Swiss courses on biomolecular modelling (Hefei, China)
- Chinese Academy of Sciences (Beijing, China)
- Tsinghua University (Beijing, China)
- Int. Soc. Quant. Biology & Pharmacy (Cetraro, Italy)
- Gordon Conf. Comput. Chemistry (Les Diablerets, Switzerland)
- 8-th NCCR Symposium on Structural Biology (Zürich, Switzerland)
- Inst. St. Raffaele (Milano, Italy)
- CECAM workshop on Protein Folding (Lausanne, Switzerland)
- Symp. Frontiers in Simulation (Los Angeles, USA)

2011

- University Göttingen (Göttingen, Germany)
- MPI for Biophysical Chemistry (Göttingen, Germany)
- Univ. Nat. Sci. Vienna (Vienna, Austria)
- Uppsala University (Uppsala, Sweden)
- PSI (Villigen, Switzerland)
- IIQB (Oeiras, Portugal)
- CECAM workshop on thermodynamics (Palaiseau, France)

- LPC colloquium ETH (Zürich, Switzerland)
- GDCh colloquium (Karlsruhe, Germany)
- Biochemical Summerschool (Spetses, Greece)
- University of Cape Town (Cape Town, South Africa)
- WATOC 2011 (Santiago de Compostela, Spain)
- 47-th Symp. Theor. Chemistry (Sursee, Switzerland)
- 2nd Workshop on Molecular Kinetics, (Berlin, Germany)

2012

- NCCR course on biomolecular modelling (Kandersteg, Switzerland)