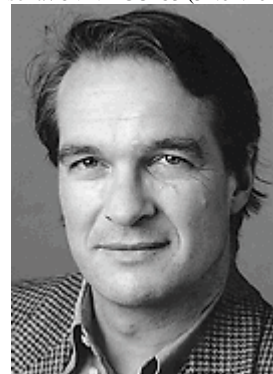


## CURRICULUM VITAE

(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



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*home* Krähbühlstrasse 49  
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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 (Ovornaz, 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)
- 1<sup>st</sup> 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)
- 1<sup>st</sup> 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)
- 37<sup>th</sup> 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: 4<sup>th</sup> World Congress (Jerusalem, Israel)
- IUPAB: 12<sup>th</sup> Int. Biophys. Congress (Amsterdam, The Netherlands)
- Amer. Chem. Society: 212<sup>th</sup> 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)
- 2<sup>nd</sup> Int. Symp. Algorithms for Macrom. Modelling (Berlin, Germany)
- Givaudan-Roure S.A. (Dübendorf, Switzerland)
- Zeneca Pharmaceuticals (Macclesfield, U.K.)
- IUPAC: 36<sup>th</sup> Int. Congress (Geneva, Switzerland)
- 3<sup>rd</sup> Eur. Research Conf. NMR in Molecular Biology (Oxford, U.K.)
- MGS and WATOC Conference: Modelling '97 (Erlangen, Germany)
- 2<sup>nd</sup> 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)
- 3<sup>rd</sup> 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<sup>ème</sup> 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)
- 6<sup>th</sup> Naples Workshop on Bioactive Peptides (Capri, Italy)
- EMBO Workshop on Proteins (EMBL, Heidelberg, Germany)
- 34<sup>th</sup> 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)
- 7<sup>th</sup> Annual Meeting Swedish Structural Biology (Tallberg, Sweden)
- Summerschool Biomolecular Structure and Dynamics (Otočec, Slovenia)
- Astra Zeneca (Macclesfield, U.K.)
- Oxford University (Oxford, U.K.)
- 11<sup>th</sup> Intl. Congress of Quantum Chemistry (Bonn, Germany)
- Technical University Delft (Delft, The Netherlands)
- 8<sup>th</sup> 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)
- 2<sup>nd</sup> 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)
- 1<sup>st</sup> 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)
- 12<sup>th</sup> 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)
- 23<sup>rd</sup> Symposium of the Protein Society (Boston, USA)
- Mediterranean Institute for Life Sciences (Split, Croatia)
- 3<sup>rd</sup> 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)
- 2<sup>nd</sup> Workshop on Molecular Kinetics, (Berlin, Germany)

2012

- NCCR course on biomolecular modelling (Kandersteg, Switzerland)