Curriculum vitae

Personal data

Full name:	Emil Matthias Müller
Date of birth:	08.07.1969
Place of birth:	Herne
Home address:	Springstr. 29 a 37077 Göttingen Germany
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E-mail:	Matthias.Mueller@mpi-bpc.mpg.de
Nationality:	German
Marital status:	unmarried

Current position

02/2002 - present	**Max-Planck Institute for Biophysical Chemistry, Göttingen, Germany** Postdoctoral fellow in the Department for Theoretical and Computational Biophysics, headed by PD Dr. Helmut Grubmüller

Education

01/2002	**PhD in theoretical physics**, Georg-August Universität, Göttingen
07/1998 - 01/2002	PhD thesis: *Towards the Catalytic Mechanism of Acetylcholinesterase* Promoter: PD Dr. Helmut Grubmüller
12/1997	**Diploma in physics**, Ruhr-Universität Bochum
06/1996 - 12/1997	Diploma thesis: *EPR Spectroscopy and Spectra Simulation of Site-Directed Spin-Labeled Lysozyme- and Bacteriorhodopsin-Mutants*, Department of Biophysics, Ruhr-Universität Bochum, Supervisor: Prof. Dr. Heinz-Jürgen Steinhoff
09/1989 - 12/1997	**Study of physics**, Ruhr-Universität Bochum

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Research interests

	- Using and developing computational techniques to study dynamics and function of proteins and protein-ligand interactions at the atomic level - Applying computational techniques to identify and optimize lead compounds in proteins
past	- EPR spectra simulation from molecular dynamics simulations for structure refinement and function analysis - targeted molecular dynamics (TMD) simulations
present	- accelerated molecular dynamics techniques for the study of chemical reactions - free energy perturbation calculations - large-scale molecular dynamics simulations and related techniques to study protein ligand interactions and to improve the efficiency and accuracy of molecular docking - 'first principles docking' - structure-based ligand design
future directions	- combine bio-informatics, chem-informatics, molecular docking and molecular dynamics techniques to improve knowledge-based strategies for structure-based drug design (e.g. virtual screening)

Work experience and teaching

06/1998	Università degli Studi di Roma 'Tor Vergata' , Italy *Research visit at the Department of Biology, Prof. A. Desideri, EPR spectra simulation from molecular dynamics simulation*
03/1998 - 04/1998	Max-Planck Institute für Molecular Physiology, Dortmund *build an ICM module for the characterization of protein interfaces*
01/1998 - 02/1998	Department of Biophysics, Bochum *teaching: modelling software package INSIGHTII*
04/1997 - 07/1997	Department of Biophysics, Bochum *teaching: graphics and modelling software packages*
03/1995 - 12/1996	Department of Biochemistry of Plants, Bochum *Targeted molecular dynamics simulation of RuBISCO*

Referee assistance for journals

Journal of Molecular Modelling

Biophysical Journal

ChemBioChem

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Further training

09/2002	Haeraeus summer school in Halle *Computational Material Sciences*
09/2000	Summer school in Vienna *Drug design*
09/1995	Haeraeus summer school in Chemnitz *Computational physics*
01/1989 - 05/1989	Course of instruction of Handwerkskammer Münster *Principals of electrical engineering*

Skills

languages	German (mother tongue), English (fluent), Italian (basic knowledge)
IT (experienced)	Standard software (MS Office, CorelDraw, Origin, PhotoImpact, ...), Operating systems (Windows98, Windows XP, Linux, IRIX, ...), Modelling software (INSIGHTII, Pymol, ...), Shell programming
IT (basic knowledge)	FORTRAN77, C, Python Modelling software (Sybyl)

Military service

07/1988 - 09/1989	Topographiebatterie 800 in Münster

Activities

Handball (for 22 years up to semiprofessional level),
Coach of youth handball teams (for 7 years),
Fitness training,
Chess

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Publications and patents

Refereed international journals

2004 F. J. M. Detmers, B. L. de Groot, E. M. Müller, A. Hinton, S. L. Flitsch, H. Grubmüller, and P. M. T. Deen, *Quaternary ammonium compounds as aquaporin water channel blocker: specificity, potency and putative site of action*, (submitted)

2004 E. M. Müller, H. Schill, A. de Meijere, and H. Grubmüller, *Thermal rearrangement/fragmentation of [3]rotane: A Computer-Aided Experimental Study*, (in preparation)

2002 E. M. Müller, A. de Meijere, and H. Grubmüller, *Predicting unimolecular chemical reactions: Chemical flooding*, Journal of Chemical Physics. **116**, 897–905 (2002)

2000 H.-J. Steinhoff, M. Müller, C. Beier, and M. Pfeiffer, *Simulation and EPR spectroscopy of nitroxide side chains in bacteriorhodopsin*, Journal of Molecular Liquids. **84**, 17–27 (2000)

1996 G. F. Wildner, J. Schlitter, and M. Müller, *RUBISCO, an old Challenge with new Perspectives*, Zeitschrift für Naturforschung. **51c**, 263–276 (1996)

Patents

2004 P. M. T. Deen, F. J. M. Detmers, S. Hohmann, S. Nielsen, J. Frøkiær, A. Engel, P. J. L. Werten, K. H. Grubmüller, B. L. de Groot, E. M. Müller, S. L. Flitsch, and F. K. Brown
Use of Quaternary Ammonium Compounds as Specific Blockers of Transport through Aquaporin, Compositions Comprising the Compounds and Method of Selecting the Compounds.

Others

2004 A. de Meijere, H. Schill, S. I. Kozhushkov, R. Walsh, E. M. Müller, and H. Grubmüller, *Cyclopropylidenes, Bicyclopropylidenes, Venylcarbenes - Some Modes of Formation and Preparative Applications*, Russian Chemical Bulletin. **53(3)**, 947–959 (2004)

2002 M. Müller, *Molekulardynamik-Simulationen zum Katalysemechanismus der Acetylcholinesterase*, Dissertation (PhD thesis)

2000 M. Müller, and H. Grubmüller, *Systematic Search for a 'Back Door' in Acetylcholinesterase*, (meeting abstract)European Biophysical Journal, **29**, 282 (2000)

1997 M. Müller, *ESR-Spektroskopie und Spektrensimulation von ortsspezifisch spinmarkierten Lysozym- und Bakteriorhodopsinmutanten*, Diplomarbeit

Conference contributions

Talks

08/2004 μ-TheoChem: Modelling and Understanding in Theoretical Chemistry, Lucca
Inhibition of human Aquaporin 1: A Molecular Dynamics Study

06/2004 BI Structural Research and Computational Chemistry Meeting, Biberach
Molecular Dynamcis Simulations: Can they Contribute to structure-based drug design?

05/2004 Darmstädter Molecular Modelling Workshop, Erlangen
Molekulardynamik Simulationen zur Inhibierung von humanem Aquaporin 1

02/2004 EU-Meeting: Action, Kopenhagen
Preliminary MD-Simulation Results for hAQP1 Inhibition with TEA

12/2003 EU-Meeting: Aquaplugs, Nijmegen
Preliminary MD-Simulation Results for hAQP1 Inhibition with TEA

09/2003 Workshop: Methods of Molecular Modelling and Simulation, Heidelberg,
'Conformational Flooding': A Method to Predict Product States in Biological and Chemical Reactions

05/2003 EU-Meeting: Aquaplugs, Aarhus
Preliminary MD-Simulation Results for hAQP1 Inhibition with TEA

03/2003 Methods in Biomolecular Simulation, Schloss Ringberg/Rottach-Egern,
'Conformational Flooding': A Method to Predict Product States in Biological and Chemical Reactions

11/2002 16. CIC-Workshop, Kleinmachnow/Berlin,
'Chemical Flooding': Eine neue Methode zur Vorhersage chemischer Reaktionen

04/2002 Molecular Modelling Workshop, Darmstadt,
Predicting unimolecular chemical reactions: Chemical flooding

05/2001 Computer Simulation and Theory of Biomolecules, Hünfeld,
Predicting unimolecular chemical reactions: Chemical flooding

Posters

08/2004	μ-TheoChem: Modelling and Understanding in Theoretical Chemistry, Lucca *Inhibition of human Aquaporin 1: A Molecular Dynamics Study* *Predicting unimolecular chemical reactions: Chemical flooding*
06/2004	2004 ISQBP President's Meeting, Como *Inhibition of human Aquaporin 1: A Molecular Dynamics Study* *Predicting unimolecular chemical reactions: Chemical flooding*
05/2004	Darmstädter Molecular Modelling Workshop, Erlangen *Inhibition of human Aquaporin 1: A Molecular Dynamics Study*
05/2004	Computer Simulation and Theory of Marcomolecules 2004, Hünfeld *Inhibition of human Aquaporin 1: A Molecular Dynamics Study*
04/2004	Fourth Annual Structure-Based Drug Design, Boston *Inhibition of human Aquaporin 1: A Molecular Dynamics Study*
07/2003	Modelling Chemical Reactivity: from gas-phase to solution and enzymes, Nancy, *A Systematic Search for a 'Back Door' in Acetylcholinesterase* *Predicting unimolecular chemical reactions: Chemical flooding* *Prediction of Rearrangement and Fragmentation Reactions: [3]Rotane as an Example*
07/2003	European Biophysics Congress 2003, Alicante, *A Systematic Search for a 'Back Door' in Acetylcholinesterase* *Predicting unimolecular chemical reactions: Chemical flooding* *Prediction of Rearrangement and Fragmentation Reactions: [3]Rotane as an Example*
02/2003	295. Haeraeus-Seminar: Biological Physics of Proteins – Structure, Flexibility and Function, Bad Honnef, *A Systematic Search for a 'Back Door' in Acetylcholinesterase* *Predicting unimolecular chemical reactions: Chemical flooding*
11/2002	16. CIC-Workshop, Kleinmachnow/Berlin, *Predicting unimolecular chemical reactions: Chemical flooding* *Prediction of Rearrangement and Fragmentation Reactions: [3]Rotane as an Example*

09/2002	Jahrestagung der biophysikalischen Gesellschaft, Dresden, *A Systematic Search for a 'Back Door' in Acetylcholinesterase* *Predicting unimolecular chemical reactions: Chemical flooding* *Prediction of Rearrangement and Fragmentation Reactions: [3]Rotane as an Example*
04/2002	Molecular Modelling Workshop, Darmstadt, *A Systematic Search for a 'Back Door' in Acetylcholinesterase* *Predicting unimolecular chemical reactions: Chemical flooding* *Prediction of Rearrangement and Fragmentation Reactions: [3]Rotane as an Example* (**Award for the best poster:** ***A Systematic Search for a 'Back Door' in Acetylcholinesterase***)
04/2002	Computer Simulation and Theory of Biomolecules, Hünfeld, *A Systematic Search for a 'Back Door' in Acetylcholinesterase* *Predicting unimolecular chemical reactions: Chemical flooding* *Prediction of Rearrangement and Fragmentation Reactions: [3]Rotane as an Example*
05/2001	Computer Simulation and Theory of Biomolecules, Hünfeld, *A Systematic Search for a 'Back Door' in Acetylcholinesterase* *Predicting unimolecular chemical reactions: Chemical flooding*
05/2001	Molecular Modelling Workshop, Darmstadt, *A Systematic Search for a 'Back Door' in Acetylcholinesterase* *Predicting unimolecular chemical reactions: Chemical flooding*
09/2000	3. European Biophysics Congress 2000, München , Poster: *A Systematic Search for a 'Back Door' in Acetylcholinesterase*