UNIVERSITÄT BAYREUTH

Faculty of Biology, Chemistry and Earth Sciences / Department of Chemistry
Bioinformatics/Structural Biology
Prof. Dr. G. Matthias Ullmann

Curriculum Vitae

Job History

10/2003 - present	Professor (Structural Biology/Bioinformatics, University of Bayreuth, Faculty of Biology, Chemistry and Geo-sciences,)
01/2001 - 09/2003	Group Leader in the Emmy-Noether Program of the DFG at the Chair for Computational Molecular Biophysics at the IWR of the Ruprecht-Karls-Universität Heidelberg

Education

01/1999 - 12/2000	Postdoc at The Scripps Research Instiute in the group of Prof. David A. Case in collaboration with Prof. Louis Noodlemann and Prof. Donald Bashford
12/1998	Ph. D. at the Department of Chemistry of the Free University Berlin
1996 - 1998	Ph. D. study at the Free University Berlin in the group of Prof. E. W. Knapp (Theoretical and Computational Molecular Biophysics)
1994 - 1995	Diploma thesis at the Free University Berlin in the group of Prof. E. W. Knapp (Theoretical and Computational Molecular Biophysics)
1990 - 1995	Studies of Biochemistry at the Friedrich-Schiller University Jena and at the University Witten/Herdecke

Awards and other responsibilities

1991 - 1995	Scholar of the German National Merit Foundation (Studienstiftung)
1996 - 1998	Ph. D. Scholar of the Boehringer Ingelheim Fonds
1999 - 2000	Postdoctoral Fellowship of the Deutsche Forschungsgemeinschaft (DFG)
2001 - 2003	Groupleader in the Emmy-Noether Program of the Deutsche Forschungsgemeinschaft (DFG)
since 2010	Member of the international scientific board of the University of Science and Technology of Hanoi (USTH)
seit 2013	Mitglied des Gutachter Pannel “Sciences Exactes et Naturelles-1” (SEN-1) des Fund for Scientific Research - FNRS

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Research Focus

In our research, we investigate the function of proteins involved in various biological energy transduction pathways. Many of these proteins are metalloproteins or cofactor-containing proteins. To study these proteins and processes, we apply a variety of theoretical methods including continuum electrostatics calculations, molecular dynamics simulations and quantum chemical calculations. Moreover, we develop methods to analyze and simulate the energetics and kinetics of charge and exciton transfer processes. Our work is at the interface of theoretical biophysics and biochemistry, bioinformatics and computational biology, bioinorganic chemistry, and structural biology

- **Docking of Electron Transfer Proteins**
- **Understanding the Protonation and Redox Behavior of Proteins**
- **Kinetics of Charge and Exciton Transfer in Proteins**
- **Density Functional Calculations of Enzyme Mechanisms**
- **Effect of Membrane Potentials on Proteins**

Publications

1. **Mikolaj Feliks, Berta M. Martins, and G. Matthias Ullmann.** Catalytic Mechanism of the Glycyl Radical Enzyme 4-Hydroxyphenylacetate Decarboxylase from Continuum Electrostatic and QC/MM Calculations. *J. Amer. Chem. Soc.*, **135**: *14574-14585*, 2013

2. **R. Thomas Ullmann and G. Matthias Ullmann.** GMCT : A Monte Carlo Simulation package for macromolecular receptors. *J. Comput. Chem.*, **33**: *887-900*, 2012

3. **Silke A. Wieninger, Engin H. Serpersu and G. Matthias Ullmann.** ATP Binding Enables Broad Antibiotic Selectivity of Aminoglycoside Phosphotransferase(3)-IIIa: An Elastic Network Analysis. *J. Mol. Biol.*, **409** : *450-465*, 2011

4. **Elisa Bombarda and G. Matthias Ullmann.** Continuum electrostatic investigations of charge transfer processes in biological molecules using a microstate description. *Faraday Discussions*, **148**: *173-193*, 2011

5. **Elisa Bombarda and G. Matthias Ullmann.** pH-dependent pK_a Values in Proteins - A Theoretical Analysis of Protonation Energies with Practical Consequences for Enzymatic Reactions. *J. Phys. Chem. B*, **114** : *1994-2003*, 2010

6. **Astrid R. Klingen, Hildur Palsdottir, Carola Hunte, and G. Matthias Ullmann.** Redox-linked Protonation State Changes in Cytochrome bc_1 Identified by Poisson-Boltzmann Electrostatics Calculations. *Biochem. Biophys. Acta Bioenergetics*, **1767**, *204-221*, 2007

7. **Elisa Bombarda, Torsten Becker, and G. Matthias Ullmann.** The Influence of the Membrane Potential on the Protonation of Bacteriorhodopsin: Insights from Electrostatic Calculations into the Regulation of Proton Pumping. *J. Amer. Chem. Soc.* , **128**, *12129-12139*, 2006

8. **G. Matthias Ullmann.** Relations between Protonation Constants and Titration Curves in Polyprotic Acids: A Critical View. *J. Phys. Chem. B,* **107**, *1263-1271*, 2003

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9. **G. Matthias Ullmann, Louis Noodleman, and David A. Case.** Density Functional Calculation of pK_a values and Redox Potentials in the Bovine Rieske Iron-Sulfur Protein. *J. Biol. Inorg. Chem.* **7**, *632-639*, 2002

10. **Alexey Onufriev, David A. Case, and G. Matthias Ullmann.** A Novel View of pH Titration in Biomolecules. *Biochemistry (New Concepts)* **40**, *3413-3419*, 2001

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