

BIOGRAPHIES

Robert A. Alberty

I graduated from the University of Nebraska in 1943, did research on blood plasma at the University of Wisconsin, received my PhD in 1947, and became an Instructor at the University of Wisconsin. I became interested in enzyme kinetics and was a postdoc with Linus Pauling at CalTech in 1950–51. Back at the University of Wisconsin we isolated fumarase, determined the rate equations for both the forward and reverse reactions, and confirmed the Haldane equation, among other things. In 1963 I became Dean of the Graduate School, and in 1967 I became Dean of the School of Science at MIT. I was so deeply involved in administration that I had to stop research. When I left the Deanship in 1982, I decided to use computers to study petroleum processing, and that led me to the use of Legendre transforms to define new thermodynamic properties. In 1991 I had my “eureka” moment when I realized that when the pH is used as an independent variable in biochemistry, you should not use the Gibbs energy G , but you need to use a Legendre transform to define a transformed Gibbs energy G' . This led to a IUPAC-IUBMB report in 1994. I have been building a database (BasicBiochemData3) on the thermodynamics of biochemical reactions, and have written two books on the subject, the most recent one in Mathematica.

Rolf Apweiler

is a Team Leader and Senior Scientist at the European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, Cambridge, UK. He studied Biology with a focus on Biochemistry and Molecular Biology in Heidelberg, Germany and Bath, UK, and worked in drug discovery in the pharmaceutical industry. He became involved in Bioinformatics through the Swiss-Prot project in 1987. He received his PhD in 1994 from the Center for Molecular Biology, University of Heidelberg, Germany and joined the European Bioinformatics Institute the same year. Dr Apweiler has coordinated the Swiss-Prot work at the European Bioinformatics Institute since 1994. He also started, among other projects, the TrEMBL protein database, the Integrated resource of protein families, domains and functional sites (InterPro), Gene Ontology Annotation (GOA), the Integr8 web portal, the Genome Reviews, and the UniProt resource (the successor of the Swiss-Prot, TrEMBL and PIR projects). These projects have organised large amounts of protein information, provided comparisons between proteomes and aim to produce dynamic, controlled vocabularies that can be applied to all organisms. In addition, Dr Apweiler has been in charge of the EMBL nucleotide sequence database since 2001. Dr Apweiler served on many review and editorial boards and published more than hundred peer-reviewed articles and numerous book chap-

ters. Rolf Apweiler has also a long-standing interest in data standards and nomenclature as exemplified in his engagement in the IUBMB Nomenclature Committee, the HUGO gene nomenclature committee, and in the HUPO Proteomics Standards Initiative.

URLs:

<http://www.ebi.ac.uk/seqdb/>

<http://www.uniprot.org>

<http://www.ebi.ac.uk/interpro/>

<http://www.ebi.ac.uk/integr8>

<http://www.ebi.ac.uk/GOA/>

<http://www.ebi.ac.uk/embl/>

<http://www.ebi.ac.uk/GenomeReviews/>

Jildau Bouwman

Jildau Bouwman was educated in neuroscience at the vrije Universiteit Amsterdam. She did a molecular biology internship in synapse development and an electrophysiological internship on receptor subunit switches during development. In 1999 she started with a PhD studentship at the Rudolf Magnus Institute for neurosciences in Utrecht. In 2004 she started her recent position as post-doc in the department of Molecular Cell Physiology at the Vrije Universiteit Amsterdam. She is involved in the “Vertical Genomics” project. The eventual goal of the project is to be able to predict how a change in gene expression can influence metabolic fluxes.

Richard Cammack

is Professor of Biochemistry at King's College, University of London. He graduated from the University of Cambridge with a BA in Natural Sciences in 1965 and PhD in Enzymology, under Malcolm Dixon in 1968. He has over 200 publications on mechanisms of electron transfer and enzyme catalysis, particularly in iron-sulfur proteins such as hydrogenases and aromatic dioxygenases. He is currently using EPR spectroscopy to study the role of iron in health and disease. He is past Chairman (2000–2005) of the Nomenclature committee of the International Union of Biochemistry and Molecular Biology (IUBMB) and Joint commission on Biochemical Nomenclature (JCBN), and Editor-in-Chief of the second edition of the Oxford Dictionary of Biochemistry and Molecular Biology.

Athel Cornish-Bowden

carried out his undergraduate studies at Oxford, obtaining his doctorate with Jeremy R. Knowles in 1967. After three post-doctoral years in the laboratory of Daniel E. Koshland, Jr., at the University of California, Berkeley, he spent 16 years as Lecturer, and later Senior Lecturer, in the Department of Biochemistry at the University of Birmingham. Since 1987

he has been Directeur de Recherche in three different laboratories of the CNRS at Marseilles. Although he started his career in a department of organic chemistry virtually all of his research has been in biochemistry, with particular reference to enzymes, including pepsin, mammalian hexokinases and enzymes involved in electron transfer in bacteria. He has written several books relating to enzyme kinetics, including *Analysis of Enzyme Kinetic Data* (Oxford University Press, 1995) and *Fundamentals of Enzyme Kinetics* (3rd edition, Portland Press, 2004). Since moving to Marseilles he has been particularly interested in multi-enzyme systems, including the regulation of metabolic pathways. More generally, he has long had an interest in biochemical aspects of evolution, and his semi-popular book in this field, *The Pursuit of Perfection*, will be published by Oxford University Press in 2004.

Kirill N. Degtyarenko

Born in Moscow region, Russia in 1967.

In 1989, graduated from the Russian State Medical University, Medico-Biological Faculty (M.D.; M.Sc. in Biochemistry). Since 1986, he worked under guidance of Prof. Valentin Uvarov, first at the Department of Biochemistry, MBF and later at the Institute of Biomedical Chemistry, Moscow.

In 1992, he defended his Ph.D. thesis on Molecular Evolution of the P450 Superfamily at the Institute of Biomedical Chemistry (supervisors: Prof. Alexander Archakov and Valentin Uvarov).

He spent one year at the International Centre for Genetic Engineering and Biotechnology, Trieste, Italy, before joining the Department of Biochemistry and Molecular Biology, the University of Leeds, UK in 1995. Since 1998, Kirill has been working at the European Bioinformatics Institute, Hinxton (near Cambridge).

Martin Field

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| 1982 | Undergraduate degree (BA) from St.Catharine's College, Cambridge in Natural Sciences. |
| 1982 – 1985 | PhD at the University of Manchester in quantum chemistry. |
| 1985 – 1989 | Postdoctorate at the University of Harvard – theoretical studies of enzymatic reaction mechanisms and protein dynamics. |
| 1989 – 1992 | Posts at the University of Geneva and at the NIH, Bethesda, Maryland. |
| 1992+ | Group leader of the modeling and simulation laboratory at the Institut de Biologie Structurale in Grenoble. |

Martin's general research involves using molecular modeling and simulation approaches for studying problems of biological interest. Specific interests include the development and application of hybrid potential techniques for studying enzymatic reaction mechanisms and other condensed phase processes.

Wilfred R. Hagen

is a Professor of Enzymology in the Department of Biotechnology at Delft University of Technology in Delft, The Netherlands. The central research theme in his group is the role of metal ions in redox biocatalysis. Fred Hagen completed his PhD on EPR of metalloproteins at the University of Amsterdam in 1982 with SPJ Albracht and EC Slater. He then took up an EMBO fellowship, and subsequently an NIH fellowship, at the Biophysics Research Division of The University of Michigan in Ann Arbor, to work on g-strain (the theory of EPR spectra from biomacromolecules) with WR Dunham and RH Sands.

In 1984 he returned to The Netherlands to join the Biochemistry Department of C Veeger at Wageningen University to set up a group on metalloproteins. In 1995 he was appointed to a chair of Physical Chemistry at the University of Nijmegen, where he headed the high-frequency EPR spectroscopy group. In 1998 he was also appointed professor of Bioinorganic Chemistry in Wageningen. In 2000 he resigned from both positions and moved to Delft University of Technology to take up the chair of Enzymology in the Department of Biotechnology.

<http://www.bt.tudelft.nl/enz>.

Jan-Hendrik Hofmeyr

is Professor in the Department of Biochemistry at the University of Stellenbosch, South Africa. He obtained his Ph.D. in 1986 at the University of Stellenbosch after collaborating with Henrik Kacser (one of the founders of metabolic control analysis) and the enzymologist Athel Cornish-Bowden. Jannie and his colleagues Jacky Snoep and Johann Rohwer form the Triple-J Group for Molecular Cell Physiology, a research group that studies the control and regulation of cellular processes using theoretical, computer modelling and experimental approaches. He has made numerous fundamental contributions to the development of metabolic control analysis and computational cell biology, and with Athel Cornish-Bowden developed both co-response analysis and supply-demand analysis as a basis for understanding metabolic regulation. He is a Fellow of the Academy of Science of South Africa and, with the other Triple-Js, chairs the International Study Group for BioThermoKinetics. He recently won the Harry Oppenheimer Fellowship Award, South Africa's most prestigious science award.

Hermann-Georg Holzhütter

became professor in 1998 and head of the research group "Theoretical Systemsbiology" at the Institute of Biochemistry of the Medical School (Charité) of the Humboldt-University in Berlin. His academic roots extend back to the late 60s/early 70s when he studied Physics at the Humboldt-University. In 1976, he was awarded his Ph.D. for his research on the theory of transport in small gap semiconductors and in 1986 he received his

habilitation (Dr. rer. nat. habil.) for theoretical studies on the dynamics and evolution of enzymatic networks. Today, his research topics are enzyme kinetics and the modelling of complex enzymatic networks with an immunological focus.

Carsten Kettner

studied biology at the University of Bonn and obtained his diploma at the University of Göttingen in the group of Prof. Gradmann which had the pioneering and futuristic name – “Molecular Electrobiology”. This group consisted of people carrying out research in electrophysiology and molecular biology in fruitful cooperation. In this mixed environment, he studied transport characteristics of the yeast plasma membrane using patch clamp techniques. In 1996 he joined the group of Dr. Adam Bertl at the University of Karlsruhe and undertook research on another yeast membrane type. During this period, he successfully narrowed the gap between the biochemical and genetic properties, and the biophysical comprehension of the vacuolar proton-translocating ATP-hydrolase. He was awarded his Ph.D for this work in 1999. As a post-doctoral student he continued both the studies on the biophysical properties of the pump and investigated the kinetics and regulation of the dominant plasma membrane potassium channel (TOK1). In 2000 he moved to the Beilstein-Institut to represent the biological section of the funding department. Here, he is responsible for the organization of symposia (sic!), research (proposals) and development of new products considering the ideas of the Beilstein-Institut, such as a medical plant database, considering the ideas of the Beilstein-Institut. He also co-ordinates the work of the STRENDA commission which is concerned with the standardization of enzyme data (see also www.strenda.org).

Ursula Kummer

After finishing her Abitur in Baden-Baden, Ursula Kummer studied Biochemistry, Physics and Chemistry in Tübingen, Germany and Eugene, Or, USA. She received a MSc in Chemistry at the University of Oregon, Eugene, Or, USA, a Vordiplom in Physics, a Diplom in Biochemistry and a PhD in Biochemistry at the University of Tübingen. Her PhD thesis which combined experimental and computational studies was finished in 1996 and dealt with the Nonlinear Dynamics of Enzymatic Systems. After postdoctoral time in Tübingen she joined the EML in Heidelberg where she became group leader in 2000. Since then her group, the Bioinformatics and Computational Biochemistry Group has been working on development of methodologies for the simulation, modeling and analysis of biochemical networks and on their application. Ursula Kummer is one of the coordinators of the BIOMS center in Heidelberg.

Nicolas Le Novere

started his career in the team of Jean-Pierre Changeux at the Pasteur Institute in 1992. He investigated, using both experimental and bioinformatics methods, the structure and function of cerebral nicotinic acetylcholine receptors until 1999. After a post-doc in the team of Dennis Bray at the University of Cambridge, where he worked on the modelling of bacterial chemotaxis, he came back to France as a CNRS research fellow. He is now Group Leader at the European Bioinformatics Institute, the british outstation of the EMBL. He shares his efforts between the modelling of neuronal signalling and the development of tools and services for Computational Systems Biology. Nicolas Le Novere is co-author of 50 scientific publications. He received in 2004 the Jean-Marie Le Goff award, of the French Academy of Science, for his work concerning the bioinformatics analysis of Ligand-Gated Ion channels.

Thomas S. Leyh

is a Professor of Biochemistry at the Albert Einstein College of Medicine (USA). He is deeply interest in all levels of protein function: structure, dynamics, ground- and transition-state structure and energetics, ligand-binding, allostery, the conformational coupling of energetics, and the higher-order organization of catalysis in the cell. His current projects, many of which are structurally grounded, include numerous enzymes that are loosely centered around biomedically relevant issues in sulfur metabolism, isoprenoid biosynthesis and antibiotic development. Dr. Leyh reviews manuscripts for numerous journals, and has been a Member of the Editorial Board of the *Journal of Biological Chemistry*. He has served as a Member of the *Molecular Biochemistry* Study Section at the NSF, and the NIH *Biochemistry* Study Section where he served as Chairman. He is currently a Member of the *Molecular Structure Function A* Study Section at the NIH. He recently spearheaded an NIH workshop on Functional Genomics, which lead to a new NIH-sponsored program. Dr. Leyh a member of the *Strenda Commission*.

Steffen Neumann

studied "Computing in the Natural Sciences" at Bielefeld University, where he focused on Pattern Recognition, Distributed Systems and Bioinformatics, combined with Neurobiology, -psychology and Cybernetics. In 1994/95 he took part in the Erasmus exchange program at Dublin City University (DCU). From 1999 to 2003 he was assistant researcher in the group of Prof. Gerhard Sagerer, where he completed his Ph. D. on Protein Docking. In 2004 Steffen Neumann held a Post Doc Position in the Plant Data Warehouse Group at the Institute of Plant Genetics and Crop Plant Research (IPK) in Gatersleben, before he became head of the Bioinformatics and Mass Spectrometry Group at the Leibniz Institute of Plant Biochemistry (IPB) in Halle.

The Group is developing a Platform for Metabolomics Research, standardisation and exchange formats and integrating data from other -omics fields.

Scott Pegg**Education**

University of California, San Francisco, 1996–2001

Ph. D. in Pharmaceutical Chemistry, 2001

Area of Specialization: Bioinformatics and Computer-aided Molecular Design

University of California, Berkeley, 1990–1995

B. A. in Molecular and Cell Biology & Computer Science, with honors

Research

Current Research: Dept. of Biopharmaceutical Sciences, UCSF

- Computational methods of describing enzyme function, particularly the explicit role of enzyme structure-function relationships.
- Computational methods for the development of biosynthetic routes to small molecules.

Postdoctoral Research: Dept. of Biopharmaceutical Sciences, UCSF 2001–2003 (research advisor: Dr. Patricia C. Babbitt).

- Construction of the Structure-Function Linkage Database, providing links between protein sequence, structure, and specific chemical function.

Doctoral Research: Dept. of Pharmaceutical Chemistry, UCSF, 1996–2001 (research advisors: Dr. Irwin D. Kuntz and Dr. Patricia C. Babbitt).

- Development of a genetic algorithm for the de-novo design of small molecule ligands.
- Development and analysis of a methodology for detection of remote protein homologies in sequence databases.
- Analysis of docking simulations using protein homology models.

Teaching

Instructor: Bioinformatics Algorithms, U.C. San Francisco, 2001–present.

Lecturer: Introduction of Bioinformatics, U.C. San Francisco, 2001–present.

Awards and Honors

Eino Nelson Prize for Graduate Research Achievement, U.C.S.F., 1999

NIH Biotechnology Training Grant, 1997

U.C. Regents Graduate Fellowship, 1996

Computer Science Departmental Achievement Award, 1995

NCAA Student Athlete Award (waterpolo), 1994

Johann Rohwer

is Associate Professor in the Department of Biochemistry at Stellenbosch University, South Africa. He obtained his Ph.D. in 1997 from the University of Amsterdam, working on the control and regulation of the bacterial phosphotransferase system under the supervision of Hans Westerhoff. He then joined Stellenbosch University, where he and his colleagues Jannie Hofmeyr and Jacky Snoep constitute the "Triple-J Group for Molecular Cell Physiology", a research group that studies the control and regulation of cellular processes using theoretical, numerical and experimental approaches.

Johann has contributed to the theoretical development of metabolic control analysis, to its experimental application, and to the development of software tools for computational systems biology. His main research interests are the construction of kinetic models of cellular function, and the application of NMR spectroscopy to the non-invasive study of metabolism in vivo. He has received the President's Award from the South African National Research Foundation and the Silver Medal of the South African Society of Biochemistry and Molecular Biology.

Together with the other Triple-Js, he chairs the BTK: International Study Group for Systems Biology, and he represents his university on the South African National Bioinformatics Network.

Isabel Rojas

Born in Caracas, Venezuela. She graduated as Licentiate in Computer Science at the Universidad Central de Venezuela (UCV) in 1990 and obtained a Master of Science and a Diploma in Computer Science from the Imperial College, UK in 1993. She did her PhD in computer science at the University of Edinburgh, UK, from 1993 to 1997.

Before joining the EML she worked as a database development consultant for a period of 4 years, managing a group of developers as well as training personnel in multiple companies. She has worked as a lecturer in several computer science disciplines in several Universities and High-Education Institutions.

She leads the Scientific Databases and visualisation group at the EML Research since June 1999. The group mainly works on the development and databases to support the study and analysis of biochemical pathways. The development of user interfaces and visualisation methods for better understanding of the data form also part of the group's work. Besides these topics the group works on the development of biological ontologies and methods for the extraction of biological information from text and biochemical databases.

Since end of 2004 the group has been working on the development of the SABIO (System for the Analysis of Biochemical Pathways) – Reaction Kinetics (SABIO-RK) database, a web-accessible system setup to support researchers interested in information about biochemical reactions and their kinetics.

Hartmut Schlüter

- 1981 – 1988: Westfälische-Wilhelms-University, Münster (Chemistry)
- 1988: Diploma (= M. Sc.) in Biochemistry, Faculty of Chemistry, University of Münster
- 1991: Ph. D. (Dr. rer. nat.) in Biochemistry, University of Münster, Faculty of Chemistry,
Thesis supervisor: Prof. Dr. H. Witzel
- 1994: Heinz Maier-Leibnitz prize
- 1995: Gerhard Hess award (DFG)
- 1995: Bennigsen-Foerder prize
- 1991 – 1996: Postdoctoral fellowship at the Medical Faculty of the University of Münster
- 1996: Habilitation (Dr. rer. nat. habil.) in Pathobiochemistry at the Medical Faculty of the University of Münster
- 1996 – 2000: Group leader at the Medical Faculty of the Ruhr-University of Bochum
- 2000-current: Senior Scientist and Head of the Bioanalytical Laboratory of Nephrology, University hospital Benjamin-Franklin, Free University of Berlin, now: Charité – University Medicine Berlin, Campus Benjamin-Franklin, Joint Facility of the Free University of Berlin and the Humboldt-University of Berlin
- 2003-current: (apl.) Professor at the Campus Benjamin-Franklin, Free University of Berlin

Dietmar Schomburg

- 1974: Diplom in Chemistry at the Technical University "Carolo-Wilhelmina" in Braunschweig
- 1976: Dr. rer.nat. in Chemistry (Structural Chemistry of Organo-phosphorus compounds)
- 1985: Habilitation (Dr. rer.nat.habil.) for Structural Chemistry

Scientific Career:

- 1976 – 1978: Post-Doc in the Chemistry Department at Technical University Braunschweig.
- 1978 – 1979: Research Fellow at Harvard University in Cambridge, Mass., U. S. A. in Professor W.N. Lipscomb's and Professor F.H. Westheimer's groups.
- 1979 – 1981: Post-Doctoral Fellow in the Chemistry Department at Braunschweig Technical University
- 1981 – 1983: Assistant Professor (Hochschulassistent), Braunschweig Technical University
-

- 1983 – 1986: Head of the x-ray lab at the German Centre for Biotechnology – GBF (Gesellschaft für Biotechnologische Forschung), Braunschweig
- 1987 – 1996: Head of the GBF Department of “Molecular Structure Research.”
- 1989 – 1995: Head of CAPE (Center of Applied Protein Engineering)
- 1990 – 1996: (apl.) Professor at the Technical University Braunschweig
- 1996 – 2007: Full Professor of Biochemistry, University of Cologne
- since 2007: Full Professor of Biochemistry, Technical University of Braunschweig

Jacky Snoep

received his Ph D in 1992 in the fields of microbial physiology and enzymology working on the control of pyruvate catabolism in bacterial systems. He subsequently worked as a postdoctoral fellow, first specializing in molecular techniques to apply control analysis together with Prof. Ingram at the University of Florida and second together with Prof. Westerhoff at the Netherlands Cancer Institute working on theoretical and modelling aspects of biological systems.

Currently Snoep is appointed in Cellular BioInformatics at the Free University of Amsterdam and in Biochemistry at the University of Stellenbosch. He has successfully applied the multidisciplinary approach of combining theory, computer modelling and experiment to understand biological systems to topics as diverse as DNA supercoiling and metabolic engineering of lactic acid bacteria. Since 2001 Snoep has been active in setting up a database for kinetic models that can be interactively run and interrogated over the internet at <http://jjj.biochem.sun.ac.za>.

Matthias Stein

obtained a degree in chemistry and a Ph D in biophysical chemistry from the Technische Universität Berlin. He investigated the enzymatic mechanism of biological hydrogen conversion by means of magnetic resonance spectroscopy and advanced electronic structure calculations. He also obtained a Master of Science degree in theoretical chemistry from the University of Manchester, UK. After his Ph D he worked as an Administrative Manager of the Collaborative Research Centre (SFB) 498 in Berlin. He did a postdoc at the Royal Institute of Technology in Stockholm. He then spend three years in industry and worked for a biotech company in the area of scientific computing and computer-aided drug design. He is currently a Research Associate at the EML Research gGmbH in Heidelberg and is working on the derivation of kinetic parameters from protein structures for simulations in systems biology. The work presented here is part of the German systems biology initiative within the HepatoSys network.

Keith Tipton*Degrees etc.*

B.Sc. (Biochemistry), St Andrews University (1962); M.A. (1965), Ph.D. (1966); Cambridge University; M.R.I.A. (1984)

Main Posts:

University of Cambridge: Demonstrator & Lecturer (1965–1977). Fellow of King's College Cambridge (1965–1977).

University of Dublin: Professor of Biochemistry (1997–present).

Fellow of Trinity College, Dublin (1979–present).

Visiting Professor: Universities of Florence (1976, 1993 & 2003) & Siena (1987 & 1999); Autonomous University of Barcelona (1988–89).

Publications:

Over 250 papers in refereed journals; 35 papers as chapters in books; editor of 19 books, > 150 abstracts; 1 patent, co-author of three books.

Research Interests:

Enzymology: regulation, kinetics, inhibition, isolation, applications and classification. Metabolic analysis and simulation. Neurochemistry: depression, degenerative diseases and 'neuroprotection'. Biochemical Pharmacology: drug design, ethanol.

Jan-Olof Winberg*Education:*

1982, Cand. real., University of Oslo

1990, Dr. philos., University of Oslo.

Positions/graduate employments:

1983–86, Research scholar, Genetic Department, The Norwegian Radium Hospital, Oslo.

1986–1993, Senior research officer and head of the Biochemical section, Genetic Department, University Hospital of Northern Norway, 9038 Tromsø.

1993–, Professor, Department of Biochemistry, IMB, MF, University of Tromsø.

Research activities:

Biochemical and kinetic characterization of alcohol dehydrogenases and matrix metalloproteinases.

In vivo, *ex vivo* and *in vitro* expression of matrix metalloproteinases and their tissue inhibitors in diseases such as epidermolysis bullosa and various types of cancer.

Characterization of factors that are involved in the regulation of matrix metalloproteinases in various types of cancer.

Detection of mutations of collagen type VII in patients with the recessive dystrophic form of epidermolysis bullosa.



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