Biographies

Timothy Clark

was born in southern England and studied chemistry at the University of Kent at Canterbury, where he was awarded a first class honors Bachelor of Science degree in 1969. He obtained his Ph.D. from the Queen's University Belfast in 1973 after working on the thermochemistry and solid phase properties of adamantane and diamantane derivatives. After two years as an Imperial Chemical Industries Postdoctoral Fellow in Belfast, he moved to Princeton University as a NATO Postdoctoral Fellow working for Paul Schleyer in 1975. He then followed Schleyer to the Institut für Organische Chemie of the Universität Erlangen-Nürnberg in 1976. He is currently technical Director of the Computer-Chemie-Centrum in Erlangen. His research areas include the development and application of quantum mechanical methods in inorganic, organic and biological chemistry, electron-transfer theory and the simulation of organic and inorganic reaction mechanisms. He is the author of 250 articles in scientific journals and two books and is the editor of the Journal of Molecular Modeling and founding director of Cepos InSilico Ltd., a company jointly owned by the Universities of Erlangen, Southampton, Portsmouth and Aberdeen.

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* (3 rd edition, Portland Press, 2004). Since moving to Marseilles he has been particularly interested in multi-enzyme systems, including the regulation of metabolic pathways. At present his main interest is in the definition of life and the capacity of living organisms for self-organization. In addition his principal areas of research, he has long had an interest in biochemical aspects of evolution, and his semi-popular book in this field, *The Pursuit of Perfection*, was published by Oxford University Press in 2004.

Antoine Danchin

trained as a mathematician and a physicist Antoine became an experimental microbiologist in the early seventies. The main goal of his research has always been to try and understand how bacterial genes can function collectively in the cell, as a pre-requisite to understand the path from commensalism to pathogenicity. To this aim, he started in 1985 a collaboration with computer scientists for evaluation of artificial intelligence techniques to the study of integrated problems in molecular genetics. This convinced him that it was time to investigate genomes as wholes, provided that an important effort in computer sciences was initiated in parallel. Early in 1987 he proposed that a sequencing program should be undertaken for *Bacillus subtilis*, the model of Gram positive bacteria. This proposal was actualized by an European joint effort on this genome, starting in 1988. The complete sequence has been published in 1997.

The first significant and unexpected discovery of this work was, in 1991, that many genes (at that time half of the genes) were of completely unknown function. As a further outcome of this work, it has been discovered that genomes are structures that are much more ordered than previously suspected, and that there probably exists a strong interaction between the organisation of the genes in the genome and the cell's architecture.

Antoine has published more than 500 articles and four books (300 in international scientific journals), including a book on the origin of life, and a book on genomes (*The Delphic Boat*, Harvard University Press, 2003). He has a continuous interest in philosophy, and in exchanges with other civilisations (formation of a Chinese-European University Without Walls in 1990), and has published many articles on subjects in epistemology and ethics. This was at the root of his interest to promote genome research in Hong Kong, where he has created the HKU-Pasteur Research Centre in 2000 at the Faculty of Medicine. He stayed in Hong Kong for three years and set up there a working seminar with the Department of Mathematics of Hong Kong University to discuss epistemological and ethical problems raised by the recent status of Biology in human knowledge.

Alexander Heckel

Born:	26th February 1972, Lindau (Lake Constance), Bavaria, Germany
1992 – 1997	Chemistry studies at the University of Constance, Diploma thesis with Prof. Dr. R. R. Schmidt (*Solid-Phase Synthesis of Oligosaccharides*)
1997 – 2001	Ph.D. thesis at the ETH Zurich with Prof. Dr. D. Seebach (*Enantioselective Heterogeneous Catalysis with TADDOL and Salen on Silica Gel*)
2001 – 2003	Postdoctoral Fellow at the California Institute of Technology with Prof. Dr. P. B. Dervan (Recognition of DNA with Minor Groove Binders)

2003 – 2007	Independent Studies at the University of Bonn Mentor: Prof. Dr. M. Famulok
since 2007	W2-Professor at the University of Frankfurt, Cluster of Excellence Macromolecular Complexes

Research Interests:
Photochemistry in living organisms, Nucleic acid nanoarchitectures

Scholarships and Awards:

1992 – 1996	Hundhammer-Fellowship (Bavarian Government)
1997	Prize for best diploma in chemistry at the University of Constance
1998 – 1999	Kekulé-Fellowship (Fonds der Chemischen Industrie)
2001 – 2003	Feodor Lynen-Fellowship (Alexander von Humboldt-Foundation)
2003 – 2006	Liebig-Fellowship (Fonds der Chemischen Industrie)
2006	Thieme Journal Award
since 2006	Emmy Noether Fellowship (DFG)

Martin G. Hicks

is a member of the board of management of the Beilstein-Institut. He received an honours degree in chemistry from Keele University in 1979. There, he also obtained his PhD in 1983 studying synthetic approaches to pyridotropones under the supervision of Gurnos Jones. He then went to the University of Wuppertal as a postdoctoral fellow, where he carried out research with Walter Thiel on semi-empirical quantum chemical methods. In 1985, Martin joined the computer department of the Beilstein-Institut where he worked on the Beilstein Database project. His subsequent activities involved the development of cheminformatics tools and products in the areas of substructure searching and reaction databases. Thereafter, he took on various roles for the Beilstein-Institut, including managing directorships of subsidiary companies and was head of the funding department 2000 – 7. He joined the board of management in 2002 and his current interests and responsibilities range from organizing the Beilstein Bozen Symposia with the aim of furthering interdisciplinary communication between chemistry and neighbouring scientific areas to Beilstein Open Access involving the publication of Open Access journals such as the *Beilstein Journal of Organic Chemistry.*

Douglas B. Kell

1996 – 1970	Top Scholar, Bradfield College, Berks
1975	B.A. (Hons) Biochemistry at St John's College, Oxford. (Class 2-[1] with Distinction in Chemical Pharmacology).
1978	Senior Scholar of St John's College, Oxford, M.A. (Oxon), D.Phil. (Oxon)
1978 – 1980	SRC Postdoctoral Research Fellow
1980 – 81	Postdoctoral Research Assistant
1981 – 1983	SERC Advanced Fellow
1983 – 1988	'New Blood' lecturer in Microbial Physiology, all at the Department of Botany & Microbiology, University College of Wales, Aberystwyth
1988 – 1992	Reader in Microbiology, Dept of Biological Sciences, UCW, Aberystwyth
	Founding Director, Aber Instruments Ltd, Science Park, Aberystwyth
1992	Personal Chair, The University of Wales
1997 – 2002	Director of Research, Institute of Biological Sciences, UWA
2001-	Founding Director, Aber Genomic Computing
2002-	EPSRC/RSC Research Professor of Bioanalytical Science, UMIST
2004-	The University of Manchester
2005-	Director, BBSRC Manchester Centre for Integrative Systems Biology (http://www.mcisb.org/)

Awards and Memberships

1986	Recipient of the Fleming Award of the Society for General Microbiology
1998	Aber Instruments received a Queen's Award for Export Achievement
2004	Royal Society of Chemistry Interdisciplinary Science Award
2005	FEBS-IUBMB Theodor Bücher prize. 2005 Royal Society/Wolfson Merit Award
2005	Royal Society of Chemistry Award in Chemical Biology
2006	Royal Society of Chemistry/Societry of Analytical Chemistry Gold Medal
2000 – 2006	Member, BBSRC Council, BBSRC Strategy Board, NERC Environmental Genomics Committee
2007-	Member, BBSRC Bioscience for Industry Panel; Member, UKPMC Advisory Board
2007 – 2008	Member STFC Science Board

He has published over 350 scientific papers, 24 of which have been cited over 100 times (plus 3 over 90). His H-index is 52.

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 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 the Beilstein symposia, research (proposals) and publication of the proceedings of the symposia. Since 2004 he coordinates the work of the STRENDA commission and promotes along with the commissioners the proposed standards of reporting enzyme data. In 2007 he became involved in the development of a program for the establishment of Beilstein Endowed Chairs for Chemical Sciences and related sciences.

Joseph Lehár

Positions and Employment

1985 – 1987	Teaching Assistant, Massachusetts Institute of Technology, Cambridge, MA
1987 – 1991	Research Assistant, MIT, Cambridge, MA
1991 – 1994	Postdoc. Res. Asst., Institute of Astronomy, Cambridge University, Cambridge, UK
1994 – 2000	Research Associate, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA
2000 – 2002	Research Scientist, Whitehead Institute, Center for Genome Research, Cambridge, MA
2002 – 2004	Team Leader, Computational Biology, CombinatoRx Inc, Cambridge, MA
2004-Present	Director, Computational Biology, CombinatoRx Inc, Cambridge, MA

Other Experience and Professional Memberships

1997 – 2000	Teaching Fellow, Harvard University, Cambridge, MA
1999	Visiting Scholar, Inst. of Astronomy, Cambridge University, Cambridge, UK
2000 – 2001	Consulting Scientist, NetGenics Inc., Cleveland, OH
2001 – 2002	Consulting Scientist, BioSift, Inc., Cambridge, MA
2002	Consulting Scientist, US Genomics, Inc., Woburn, MA
2002–Present	Adjunct Assistant Professor, Boston University, Boston, MA

Honors

1980	National Merit Scholarship Program, Finalist
1985	Brandeis University, Magna cum Laude with Highest Honors
1985	Brandeis University, Physics Faculty Prize
1990	Sigma Xi, MIT Chapter, Elected to membership
2000	Harvard University, CUE Certificate of Distinction in Teaching

Steven V. Ley

Steve Ley is currently the BP (1702) Professor of Chemistry at the University of Cambridge, and Fellow of Trinity College, Cambridge, UK. He studied for his Ph.D. at Loughborough University working with Harry Heaney and then carried out postdoctoral work in the USA with Leo Paquette at Ohio State University. In 1974 he returned to the UK to continue postdoctoral studies with Sir Derek Barton at Imperial College. He was appointed to the staff at Imperial College in 1975 and was promoted to Professor in 1983, and Head of Department in 1989. In 1990 he was elected to the Royal Society (London). In1992 he moved to his current post at Cambridge and from 2000 – 2002 he was also President of the Royal Society of Chemistry.

Professor Ley's work involves the discovery and development of new synthetic methods and their application to biologically active systems. The TPAP catalytic oxidant that is now used worldwide and cited extensively was one of his inventions. His group has published extensively on the use of iron carbonyl complexes, organoselenium chemistry, the use of microwaves in organic chemistry, biotransformations for the synthesis of natural products, and strategies for oligosaccharide assembly. To date more than 115 major natural products have been synthesised by the group. The group is currently developing new methods and techniques in particular the use solid-supported reagents in a designed sequential and multi-step fashion, and in combination with advances in the use of scavenging agents and catch and release techniques and for flow microreactor systems. Interesting advances have been made in the design of new catalysts especially for asymmetric synthesis.

Professor Ley has published over 630 papers and his achievements have been recognised by 32 major awards which include the Hickinbottom Research Fellowship, the Corday Morgan Medal and Prize, the Pfizer Academic Award, the Royal Society of Chemistry Synthesis Award for 1989, the Tilden Lectureship and Medal, the Pedler Medal and Prize, the Simonsen Lectureship and Medal and the Aldolf Windaus Medal of the German Chemical Society and Göttingen University, the Royal Society of Chemistry Natural Products Award, the Flintoff Medal, the Paul Janssen Prize for Creativity in Organic Synthesis, the Rhône-Poulenc Lectureship and Medal of the Royal Society of Chemistry and the Glaxo-Wellcome Award for Outstanding Achievement in Organic Chemistry.

Other notable accolades have been the Royal Society of Chemistry Haworth Memorial Lectureship, Medal and Prize and The Royal Society Davy Medal and the German Chemical Society August-Wilhelm-von Hofmann Medal together with the Pfizer Award for Innovative Science. In 2003 he was awarded the American Chemical Society Ernest Guenther Award in the Chemistry of Natual Products together with the Royal Society of Chemistry Industrially-sponsored award in Carbohydrate Chemistry, the Chemical Industries Association Innovation of the Year Award and the iAc Award; both jointly with AstraZeneca, Avecia and Syngenta. In 2004 he received the Messel Medal Lecture of the Society of Chemical Industry and the Alexander-von-Humboldt Award.

Recently his work has been acknowledged by the presigous Yamada-Koga Prize in 2005 and the Nagoya Gold Medal (Banyu Life Science Foundation International, Japan) and the Robert Robinson Award and Medal (Royal Society of Chemistry) in 2006 and in 2007 the Award for Creative Work in Synthetic Organic Chemistry (American Chemical Society) and the Karrer Gold Medal, University of Zurich.

Professor Ley has been the recipient of 74 named lectureships and given 303 special invited lectures. He has served on 42 national and international committees, 43 editorships and many industrial science advisory boards. He has been awarded honorary degrees and fellowships from the universities of Loughborough, Salamanca, Imperial College, London, Huddersfield and Cardiff.

Eric Meggers

Professional Preparation

1999 – 2002	The Scripps Research Institute Postdoctoral fellow with Prof. Peter G. Schultz a) Development of the concept of metallo-base pairing in DNA. b) Phage display methodology for the ribosomal incorporation of unnatural amino acids into proteins.
1999	Univ. of Basel, Switzerland, Ph.D. in Organic Chemistry

1995 University of Bonn, Germany, Diploma in Chemistry

Appointments

2002 – June 2007 Assistant Professor, Department of Chemistry, University of Pennsylvania

July 2007 – present Professor, Philipps-University of Marburg

July 2007 – present Adjunct Assistant Professor, Wistar Institute, Philadelphia, USA

Awards and Honors

1994 – 1995 Fellowship from the Theodor-Laymann Foundation

1996 Award from the Heinrich-Hörlein-Memory Foundation

1995 – 1999 Fellowship from the Swiss National Science Foundation

1999 – 2000 Feodor Lynen Fellowship of the Alexander von Humboldt Foundation

2000 – 2001 Emmy Noether Fellowship from the DFG

2002 Camille and Henry Dreyfus New Faculty Award

2003 Synthesis-Synlett Journal Award

2006 – 2008 Alfred P. Sloan Research Fellow

2006 Camille Dreyfus Teacher-Scholar Award

2007 NanXiang Fellowship from Xiamen University, China

Justin K. M. Roberts

studied Agricultural and Forest Sciences at Oxford University (B.A., 1978) while performing research in plant biochemistry at ARC Letcombe Laboratory with D.T. Clarkson. On completion of his undergraduate training, he joined P.M. Ray's laboratory in Biological Sciences at Stanford University, primarily conducting research in O. Jardetzky's Stanford Magnetic Resonance Laboratory to measure intracellular pH gradients in plant cells (Ph.D. 1982). His post-doctoral work applying NMR to plant metabolism continued at Stanford until 1985, when he joined the Department of Biochemistry, University of California, Riverside as an assistant professor. He has been a Professor of Biochemistry at UCR since 1995, serving as Chairman 2001 – 4.

A predominant focus of his research has been nucleotide metabolism, from the pool sizes and physical states of nucleotides in plant cells, to rates of nucleotide turnover to, most recently, aspects of protein-nucleotide recognition in the context of functional and structural genomics in *Mycobacterium tuberculosis*.

Gisbert Schneider

studied biochemistry at the Free University (FU) of Berlin, Germany. From 1991 to 1994 he prepared his doctoral thesis on machine learning systems for peptide *de novo* design as a fellow of the Fonds der Chemischen Industrie. From 1994 to 1997 he performed post-doctoral research at the FU Berlin, the University of Stockholm, Sweden, the Massachusetts Institute of Technology, Cambridge, MA, USA, and the Max-Planck-Institute of Biophysics in Frankfurt, Germany. In 1997 he joined the pharmaceuticals division of F. Hoffmann-La Roche AG in Basel, Switzerland, where he became Head of Cheminformatics. Since 2002 he is a full professor of Chem- and Bioinformatics (Beilstein Endowed Chair for Cheminformatics) at Johann Wolfgang Goethe-University in Frankfurt, Germany, where he concentrates on the development and application of software methods for virtual screening and molecular design. He has published more than 150 scientific papers, books and patents and is author of two textbooks on molecular design. He is editor of the journal "QSAR and Combinatorial Science", and member of the editorial advisory boards of several journals in the field of chemical biology and drug discovery.

Peter H. Seeberger

received his Vordiplom in 1989 from the Universität Erlangen-Nürnberg, where he studied chemistry as a Bavarian government fellow. In 1990 he moved as a Fulbright scholar to the University of Colorado where he earned his Ph.D. in biochemistry under the guidance of Marvin H. Caruthers in 1995. After a postdoctoral fellowship with Samuel J. Danishefsky at the Sloan-Kettering Institute for Cancer Research he became Assistant Professor at the Massachusetts Institute of Technology in 1998 and was promoted to Firmenich Associate Professor of Chemistry with tenure in 2002. In June 2003 he assumed a position as Professor for Organic Chemistry at the Swiss Federal Institute of Technology (ETH) in Zurich, Switzerland and a position as Affiliate Professor at the Burnham Institute in La Jolla, CA.

Professor Seebergers research has been documented in over 170 articles in peer-reviewed journals, fourteen issued patents and patent applications, more than 90 published abstracts and more than 360 invited lectures. Among other awards he received the Technology Review Top 100 Young Innovator Award (1999), MITs Edgerton Award (2002), an Arthur C. Cope Young Scholar Award and the Horace B. Isbell Award from the American Chemical Society (2003), Otto-Klung Weberbank Prize.

In 2007 he was selected among "The 100 Most Important Swiss 2007" by the magazine "Schweizer Illustrierte", received the Havinga Medal, the Yoshimasa Hirata Gold Medal and the Körber Prize for European Sciences. Peter H. Seeberger is the Editor of the Journal of Carbohydrate Chemistry and serves on the editorial advisory boards of eleven other journals. He is a founding member of the board of the Tesfa-Ilg Hope for Africa Foundation

that aims at improving health care in Ethiopia in particular by providing access to malaria vaccines and HIV treatments. He is a consultant and serves on the scientific advisory board of several companies.

The research in professor Seebergers laboratory has resulted in two spin-off companies: Ancora Pharmaceuticals (founded in 2002, Medford, USA) is currently developing a promising malaria vaccine candidate in late preclinical trials as well as several other therapeutics based on carbohydrates. i2chem (founded in 2005, Cambridge, USA) develops integrated microchemical systems based on silicon microreactors.

Holger Wallmeier

obtained his PhD 1982 in Theoretical Chemistry from the University of Bochum in the Group of Prof. Kutzelnigg with a thesis on relativistic quantum chemistry. In 1984 he took over a position at Hoechst AG in Frankfurt in the Scientific Computing Department of Corporate Research where he worked in computer-assisted drug design, simulation of biomolecular systems, and software development. 1997 he founded the bioinformatics group at Hoechst Research & Technologies GmbH and was appointed head of the Core Technology Area Biomathematics in 1998.

Since than he has initialized and supervised numerous projects in bioinformatics, proteomics, expression analysis, development of bio-analytical software, and text mining. He has published a number of papers in quantum chemistry, structure/activity relationships, and protein structure prediction. 2003 he changed to Sanofi-Aventis doing consulting in the area of biocomputing for Sanofi-Aventis biotech investments and spin-outs of former Aventis Research & Technologies. Since 2008 he works as an independent consultant in the areas of scientific computing and bioinformatics.

Dave A. Winkler

studied chemistry, chemical engineering, and physics at the Monash and RMIT Universities in Melbourne. He completed a PhD in microwave spectroscopy and radioastronomy at Monash University in 1980 as a General Motors postgraduate fellow. He then worked as a tutor and senior research fellow, helping establish the computer-aided drug design group at the Victorian College of Pharmacy under Prof. Peter Andrews, in the early 80s. He subsequently worked as a senior research scientist with the Defence Science and Technology organization in Adelaide for two years, modelling energetic polymer properties.

He joined CSIRO Applied Organic Chemistry in Melbourne as a senior research scientist in 1985 where he worked on the design of biologically active small molecules as drugs and agrochemicals. He was awarded Australian Academy of Science traveling fellowships to Toshio Fujita's lab in Kyoto in 1988, and to Graham Richards' research group in Oxford in 1997. He has remained with CSIRO and his worked a common theme of the application of

computational methods to understanding and designing novel small molecules with biological activity. Major projects during this time involved industry collaborations: development of HBV drugs with AMRAD, crop protection agents with Du Pont, and veterinary drugs with Schering Plough.

His research contributed to the formation of the start up companies such as Betabiotics. He was a member of the Biomolecular Research Institute, headed by Prof. Peter Colman who led the structural biology behind the flu drug Relenza. During has time, at CSIRO, a common theme of his work has been the development and application of Bayesian methods, particularly the Bayesian regularized artificial neural network, to the modelling of biological activity. During the last decade he has worked with a diverse complex systems science group in Australia and internationally. This aimed to understand how complexity concepts such as emergence, criticality, self-organization and self-assembly can contribute to the modelling, understanding and design of complex chemical and biological systems. In the past five years, his research has evolved to encompass biomaterials and regenerative medicine.

He currently leads two research projects; one involved in understanding regulatory processes in stem cells, and how they trigger fate decisions from a complexity perspective; the other is using more traditional molecular modelling methods to design small molecule mimics of cytokines that influence stem cell fate. These projects involve collaboration with the Australian Stem Cell Centre and other international stem cell groups.

Dave is a Fellow and past Chairman of the Board of the Royal Australian Chemical Institute, an Adjunct Professor at Monash University, and is the current President of Asian Federation for Medicinal Chemistry. He has published almost 150 scientific papers, confidential reports, and patents, co-edited three multi-author books, and transferred the Bayesian neural network technology to Bio-RAD as a software product, MolSAR. He a member of the editorial advisory boards of the journals ChemMedChem and Journal of Molecular Graphics and Modelling.