BIOGRAPHIES

Konrad Bleicher

09/85-02/95	PhD Organic Chemistry, Tübingen University; Prof. E. Bayer
10/00-today	Hoffmann-La Roche, Basel, Switzerland; Scientific Specialist, Head of Combinatorial Chemistry
04/99-09/00	Hoffmann-La Roche, Basel, Switzerland; Senior Scientist, Member of New Lead Chemistry Initiative Responsibility to build up a high throughput synthesis and purification platform for the generation of large compound libraries
10/97-04/99	Hoffmann-La Roche, Basel, Switzerland; Research Scientist Parallel Synthesis Group CNS Support of various CNS projects using parallel synthesis techniques
09/96-11/97	Novartis, East Hanover, USA; Dr. J. Wareing Postdoctoral Fellow Combinatorial Chemistry Resin and Linker synthesis for solid supported combinatorial chemistry
04/95-09/96	Sandoz, Basel, Switzerland; Dr. R.Giger Postdoctoral Fellow Combinatorial Chemistry Solid supported synthesis of compound collections using Chiron's multipin technology

Konrad Bleicher is author of ca. 25 patents and scientific publications.

Virginia Cornish

graduated summa cum laude from Columbia University with a B.A. in Biochemistry in 1991, where she did undergraduate research with Professor Ronald Breslow in the Chemistry Department. She then moved west to do research with Professor Peter Schultz in the Chemistry Department at the University of California at Berkeley as an NSF Predoctoral Fellow. In Professor Schultz's laboratory she helped develop a new methodology for incorporating synthetic amino acids into proteins using the protein biosynthetic machinery. In 1996, she became an NSF Postdoctoral Fellow in the Biology Department at M.I.T. under the guidance of Professor Robert Sauer. At M.I.T. she initiated an independent project that is the basis for the directed evolution program in her laboratory at Columbia. Virginia joined the Chemistry Department at Columbia in 1999, working at the interface of chemistry and biology.

Her laboratory brings together modern methods in synthetic chemistry and DNA technology to co-opt biological systems for the synthesis of new materials, understanding the function of these systems by challenging their specificity at the molecular level. Her research has been recognized by numerous awards including a Sloan Foundation Fellowship, a Beckman Young Investigator Award, and a NSF Career Award.

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.

Kevin Davies

is the Editor-in-Chief of *BioIT World*, the monthly magazine covering information technology and life sciences published by IDG. He is the author of Cracking the Genome, an accessible and comprehensive account of the conclusion of the Human Genome Project.

Davies graduated from Oxford University and obtained in Ph.D in genetics from the University of London. After conducting postdoctoral research at MIT and Harvard Medical School, he joined the editorial staff of the prestigious British science journal *Nature* in 1990. In 1992, Kevin founded *Nature Genetics*, the world's leading genetics and genomics journal. He later served as the science editor at the Howard Hughes Medical Institute in Chevy Chase, Maryland, the largest medical philanthropy in the United States. Prior to launching *BioIT World*, Davies served as editor-in-chief of Cell Press.

Davies' latest book, Cracking the Genome, has been translated into 15 languages. He is also the author (with Michael White) of *Breakthrough: The Race to Find the Breast Cancer Gene*.

Ernesto Freire

is the Henry Walters Professor in the Department of Biology at The Johns Hopkins University. He is also Professor in the Department of Biophysics. Dr. Freire has been at Johns Hopkins since 1986. He obtained his Ph.D. in Biophysics at the University of Virginia. Dr. Freire has served in numerous scientific boards, scientific advisory committees, editorial boards, and is a member of the Biophysical Society, American Chemical Society, American Association for the Advancement of Science and Protein Society.

Dr. Freire has pioneered the application of thermodynamic methods to the development of new molecular design algorithms aimed at engineering drugs that exhibit extremely high affinity, selectivity and maintain their effectiveness in the face of mutations causing drug resistance and genomic diversity. Dr. Freire has authored over 170 scientific publications and holds several patents.

Johann Gasteiger

(Johnny), studied chemistry at the University of Munich, ETH and the University of Zürich and received his Doctorate in Organic Chemistry from the University of Munich in 1971. Following a postdoctoral fellowship at the University of California in Berkeley in 1971-1972 Johnny taught at the Technical University of Munich. In 1994 he moved to the University of Erlangen-Nuremberg where he co-founded the "Computer-Chemie-Centrum". He is one of the founders of Chemoinformatics in Germany and has produced more than 250 scientific publications in this field Johnny was consultant to the Beilstein Institute and to FIZ CHEMIE BERLIN, where he was the project manager for the development of the ChemInformRX reaction database. He is a past chairman (1994-1996) of the Division "Chemistry-Information-Computer" of the German Chemical Society, and has served as Vice-Chairman of the Working Party "Computational Chemistry" of the Federation of European Chemical Societies (1986-2002). In 1991 Johnny was awarded with the Gmelin-Beilstein Medal of the German Chemical Society for Achievements in Computer Chemistry and in 1997 he received the Herman-Skolnik-Award of the Division of Chemical Information of the American Chemical Society.

Richard Goldstein

obtained his Ph.D. using experimental and computational methods to study electron transfer in bacterial photosythesis. After a brief stay teaching Physics in China, he worked with Peter Wolynes developing methods to predict protein tertiary structures. He then spent eight years on the faculty at the University of Michigan. He left academia briefly to become Head of Bioinformatics at Siena Biotech, and then moved to the Mathematical Biology Division at the National Institute for Medical Research in Mill Hill, London. His research focuses on the relationship between a protein's structure, function, and other properties and the evolutionary processes through which these properties emerged. These efforts have included methods of identifying and aligning distant protein homologs, examining the evolutionary record of related sets of proteins in order to determine characteristics of specific proteins, developing better models for phylogenetic reconstruction, and using simplified theoretical and computational models to develop deeper insights into how proteins can be understood in their evolutionary context.

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, he 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 in the areas of substructure searching and reaction databases, and products such as Current Facts and CrossFire. After brief sojourns as the managing director of the Beilstein Verlagsgesellschaft in 1997 and subsequently the Beilstein GmbH from 1998 - 2000, he returned home to the Beilstein-Institut as head of the funding department in 2000.

He is particularly interested in furthering interdisciplinary communication between chemistry and neighbouring scientific areas and has been organizing the Beilstein Bozen Workshops since 1988.

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!), administering research (proposals) and funding, as well as, the development of new projects and products for the Beilstein-Institut.

Hugo Kubinyi

studied chemistry in Vienna, Austria. After his Ph.D. thesis at the Max Planck Institute of Biochemistry in Munich he continued as a PostDoc at the German Cancer Research Centre in Heidelberg. In 1966 he joined Knoll AG, later a subsidiary of BASF AG, and in 1985 he moved to BASF AG. Since 1987, until his retirement in summer 2001, he was responsible for the Molecular Modelling, X-ray Crystallography and Drug Design group of BASF, since early 1998 also for Combinatorial Chemistry in the Life Sciences.

He is Professor of Pharmaceutical Chemistry at the University of Heidelberg, former Chair of The QSAR and Modelling Society, and IUPAC Fellow. From his scientific work resulted five books on QSAR, 3D QSAR, and Drug Design (the German book "Wirkstoffdesign" received the 1999 Book Award of the FCI, Association of Chemical Industry) and about 90 publications. He is a member of several Scientific Advisory Boards, coeditor of the Wiley-VCH book series "Methods and Principles in Medicinal Chemistry", and member of the Editorial Boards of several scientific journals.

Steve Ley

is BP (1702) Professor of Organic Chemistry at the University of Cambridge, and Fellow of Trinity College. He is Immediate Past President of the Royal Society of Chemistry and was made a CBE in January 2002.

He was appointed to the staff at Imperial College in 1975 and became head of department in 1989. He was elected to the Royal Society (London) in 1990, and came to Cambridge in 1992.

Steve's research involves the discovery and development of new synthetic methods and their application to biologically active systems. His group has published extensively on the synthesis of natural products and to date more than 100 target compounds have been synthesised. The group is also developing new ways of making complex carbohydrates and developing new strategies for combinatorial chemistry. Steve Ley's work of 530 papers has been recognised by 14 major prizes and awards, the most recent of which was the Ernest Guenther Award from the American Chemical Society.

Thomas S. Leyh

received a Ph. D. in biophysics from the University of Pennsylvania in 1983. He joined the faculty at the Albert Einstein College of Medicine in New York in 1989, where he is currently a Professor of Biochemistry. Prof. Leyh is a mechanistic enzymologist with a long-standing interest in sulfur biochemistry, GTPase function, and the conformational coupling of energetics. His group has recently demonstrated that enzymes in the cysteine biosynthetic pathway self-organize into a multifunctional protein complex out of which emerges new catalytic function that orchestrates the activities of the complex. John Andreassi, Ph. D., is a postdoctoral fellow working with Dr. Leyh to initiate the genomic enzymology program.

Alex MacDonald

is a Ph.D pharmacokineticist and bioengineer. He is currently working as a senior scientist at Roche Pharma Research in Basel, Switzerland, in the non-clinical modelling and simulation group. His expertise in physiologically-based pharmacokinetic and pharmacodynamic modelling and pre-clinical pharmacokinetics. His previous experience includes modelling and simulation scientist positions at Novartis Pharma AG and with the UK government. Prior to gaining his Ph.D Alex worked for a number of years as a control systems design engineer in the automotive industry.

Jason Micklefield

received a PhD in Organic Chemistry from the University of Cambridge in 1993 working with Prof Sir Alan R. Battersby to complete the first total synthesis of Haem d1. This was followed by a NATO postdoctoral fellowship at the University of Washington in Seattle, USA, with Prof Heinz G. Floss, investigating enzyme mechanisms. In 1995 he became a Lecturer in Organic Chemistry at Birkbeck College, University of London, before moving to the University of Manchester Institute of Science and Technology in 1998 where he is now a Reader in Organic and Biological Chemistry. His current research interests are at the chemistry-biology interface and include the synthesis, conformational analysis and biophysical evaluation of modified nucleic acids and oligonucleotide mimics. His other research programmes are concerned with engineering the biosynthesis of nonribosomal peptide secondary metabolites and the use of biotransformations in synthesis.

Keith Russell

was born in the UK and obtained his PhD from the University of Cambridge, UK with Dr. A. B. Holmes in 1984 in the area of synthetic organic chemistry. He was then awarded a NATO fellowship to do post doctoral studies with Professor L. A. Paquette at Ohio State University (1984-1986). In 1986, he took up a position as a Senior Research Chemist in the Medicinal Chemistry Department of AstraZeneca Pharmaceuticals in Alderley Park. In 1989 he transferred to the Medicinal Chemistry Department in the Wilmington, DE research site of AstraZeneca Pharmaceuticals in the USA, where he is now Director of Chemistry in the CNS Discovery Area. Keith has worked in a number of areas of medicinal chemistry. He was a key player in the team that discovered ZD6169 and ZD0947, the first bladder selective potassium channel openers aimed at urge urinary incontinence. He led the Tachykinin team to deliver a selective N_{K1} antagonists for depression, a dual $N_{K1}N_{K2}$ antagonist for asthma, as well as the early stages of the NK2 antagonist project aimed at urge incontinence. He has contributed to several development teams and co-led a Global Tackykinin R&D Project aimed at increasing the efficiency of the R to D transition process. Keith has been a major force behind the introduction and application of automation, intranet, combinatorial chemistry and other new chemical technologies into AstraZeneca drug discovery. More recently, Keith has spearheaded an initiative in "Chemical Genetics" aimed at more fully integrating chemistry activities throughout the entire discovery value chain. An ACS and AAAS member, he is the author of over 30 peer-reviewed publications and is an inventor on over 25 patents emanating from his work at AstraZeneca. Keith is a reviewer for Journal of the American Chemical Society and Bioorganic and Medicinal Chemistry Letters.

Gisbert Schneider

born 1965 in Fulda, Germany; studied biochemistry and computer science at the Free University (FU) in Berlin; 1994, PhD in bioinformatics on neural networks and evolutionary algorithms; post-doctoral work on peptide design (with Prof. Wrede, FU Berlin), protein folding simulation (with Prof. Schimmel, M.I.T., Cambridge, USA), analysis of protein targeting signals (with Prof. von Heijne, University of Stockholm, Sweden) and prediction of membrane protein topology (with Prof. Schulten, Max-Planck-Institut Frankfurt, Germany); 1997-2002

F.Hoffmann-La Roche AG, Basel, Switzerland, head of cheminformatics; scientific research on combinatorial drug design, virtual screening, and genome analysis. Current position: Beilstein Professor of Cheminformatics at Johann Wolfgang Goethe-Universität, Frankfurt; research focus on adaptive systems in molecular design.

Nicholas J. Westwood

carried out his doctoral studies in chemical biology at Oxford University under the supervision of Professor Christopher Schofield (1992-1995). He then worked with Professor Philip Magnus FRS as a NATO post-doctoral fellow on synthetic approaches to Taxol (1995-1998), and spent a further 3 years at the Institute of Chemistry and Cell Biology (ICCB) at Harvard Medical School (1998-2001). In Professor Matthew Shair's laboratory, he prepared a collection of 2000+ compounds related in structure to the natural product, galanthamine using solid phase synthesis technology. One member of this library, named secramine, is currently being used to study protein trafficking. He also became interested in high throughput screening technologies during his time in Professor Timothy Mitchison's group at ICCB. A particular focus has been on chemical genetic approaches in cellular microbiology (in a continuing collaboration with Professor Gary Ward at the University of Vermont).

Nick was appointed to a Royal Society University Research Fellowship and lecturer position in Chemical Genetics at the University of St Andrews in 2001. The main research interests of his laboratory remain at the interface of chemistry and biology. His group uses a range of methods in synthetic organic chemistry to address fundamental biological questions. Projects include the chemical characterisation and optimisation of the small molecule tool, blebbistatin, synthetic programmes in diversity oriented synthesis and studies aimed at protein target identification. He has also recently established a HTS facility at St Andrews. He retains an interest in all high throughput synthesis technology and will be on secondment to Pfizer later this year in an EPSRC-funded scheme to improve industrial-academic communication in this research area.

Peter Willett

obtained an Honours degree in Chemistry from Exeter College, Oxford in 1975 and then went to the Department of Information Studies, University of Sheffield where he obtained an MSc in Information Studies. Following doctoral and post-doctoral research on computer techniques for the processing of databases of chemical reactions, he joined the staff of the University of Sheffield as a Lecturer in Information Science in 1979. He was awarded a Personal Chair in 1991 and a DSc in 1997, and is now the Head of the Department. He is a Fellow of the Chartered Institute of Library and Information Professionals, and was the recipient of the 1993 Skolnik Award of the American Chemical Society, of the 1997 Distinguished Lecturer Award of the New Jersey Chapter of the American Society for Information Science, of the 2001 Kent Award of the Institute of Information Scientists, and of the 2002 Lynch Award of the Chemical Structure Association Trust. He is included in Whos Who, is a member of the editorial boards of four international journals, and has been involved in the organisation of many national and international conferences in various aspects of information retrieval. Professor Willett heads a large research group studying novel computational techniques for the processing of chemical and biological information, and has over 400 publications describing this work.

His current interests include: database applications of cluster analysis, evolutionary computing and graph theory; molecular similarity and molecular diversity analysis; the comparison of chemical and biological 3D structures; and the use of citation data for the evaluation of academic research performance.