

BIOGRAPHIES

Sir Tom L. Blundell FRS, FMedSci

- 1961 Open Scholarship in Natural Sciences, Brasenose College, Oxford University.
- 1964 First Class Honours, Senior Hulme Scholarship, Brasenose College, Oxford University.
- 1967 D.Phil., Oxford University.
- 1967 College Lecturer, Hertford College, Oxford University.
- 1968 Junior Research Fellow in Molecular Biophysics, Linacre College, Oxford University.
- 1973 Lecturer, Biological Sciences, Sussex University.
- 1976 Professor, Department of Crystallography, Birkbeck College, University of London.; sometime Dean of Science
- 1989 Director, Imperial Cancer Research Fund Unit of Structural Molecular Biology
- 1991 Director General, Agricultural and Food Research Council
- 1994 Chief Executive, BBSRC (till 1996)
- 1995 Professorial Fellow, Sidney Sussex College, Cambridge University
- 1995 Sir William Dunn Professor of Biochemistry, University of Cambridge.
- 1996 Head of Department of Biochemistry, University of Cambridge.
- 2003 Chair, School of Biological Sciences, Cambridge (until 2007)

Tom Blundell's research interests are in the definition of the architecture of macromolecules and their assemblies and the relation to biological function and diseases including cancer. Techniques used in his laboratory include biochemistry, protein crystallography and bio-computing. He has used X ray crystallography to define the structures of multiprotein complexes involved in DNA repair, conformations of polypeptide hormones, growth factors and their receptors, the architecture of cellular signalling systems, the structures of enzymes that are important drug targets and the three dimensional structures of vertebrate lens proteins, the crystallins.

These interests have led to work on rational approaches to drug design. Tom has pioneered methods of structure-based design in 1970s, 1980's and early 1990's. In the past decade he has developed high throughput and fragment-based approaches to drug discovery and co-founded a successful company Astex.

Tom Blundell has published over 400 research papers (over 30 in Nature and Science).

Nediljko Budisa

studied Chemistry, Biology, Molecular Biology and Biophysics at the University of Zagreb (Croatia). He made his PhD work in the laboratory of Robert Huber at the Max-Planck-Institute of Biochemistry in Martinsried and defended his PhD thesis (summa cum laude) in 1997 at the Technical University, Munich. During PhD work he initiated an independent project on protein design and engineering by an expanded amino acid repertoire. These works were further elaborated and extended during his Postdoctoral work (1997-2000) in Martinsried in the laboratories of Robert Huber and Luis Moroder. Later on, during 2000, he succeeded to establish a departmental research team for protein engineering and in parallel made habilitation work (finished 2005) at the Technical University in Munich. He started an independent research Group 'Molecular Biotechnology' at the Max-Planck-Institute of Biochemistry after receiving the prestigious BioFuture Award of the German Ministry for Research and Education in 2004.

Nediljko Budisa's research at the interface of chemistry and biology is mainly concerned with the possibilities to generate novel generic classes of amino acids by using synthetic chemistry, bio-computing and target-engineered metabolic circuits. Such novel amino acids should enable an expansion of the genetic code in the context of a reprogrammed protein translation. The final goal is to create designer molecules and cells carrying out novel properties optimized for user-defined environments or to engineer a genetic code such that proteome-wide substitutions/insertions of synthetic amino acids can yield a synthetic life with new chemical possibilities.

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.

Tim 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.

Jonathan Clayden

was born in Uganda in 1968, grew up in eastern England and in 1989 received a degree in Natural Sciences from the University of Cambridge. He carried out research on asymmetric chemistry of phosphine oxides under the supervision of Dr Stuart Warren and was awarded a PhD in 1993. After a period in the laboratories of Prof. Marc Julia at the Ecole Normale Supérieure in Paris he began his independent academic career as a lecture at the University of Manchester in 1994. He was appointed to a professorship in Manchester in 2001. He has published over 100 papers, and his research interests encompass various areas of synthesis and stereochemistry, particularly where conformational control is important. His current research projects are addressing the themes of asymmetric synthesis, dearomatising reactions, atropisomerism, organolithium chemistry, and remote stereocontrol.

He is co-author (with Nick Greeves, Stuart Warren and Peter Wothers) of the textbook *Organic Chemistry*, (Oxford Univ. Press 2001), and his book *Organolithiums: Selectivity for Synthesis* was published by Pergamon in 2002. He has received the Royal Society of Chemistry's Meldola (1997) and Corday Morgan (2003) medals, along with the GlaxoSmithKline Prize for Innovative Organic Chemistry (1998), the AstraZeneca Prize (2001), the Pfizer Prize (2001) and the Novartis Young European Investigator Award (2004). He was Royal Society Leverhulme Trust Senior Research Fellow 2003-4, and has been visiting professor at the Universities of Rouen, Bordeaux and Strasbourg. He is editor in chief of *Beilstein Journal of Organic Chemistry*.

Jonathan W. Essex

is a Reader in the School of Chemistry at the University of Southampton, having been a Royal Society University Research Fellow from 1994-2002. His research interests lie in the application of classical computer simulations to problems of organic & biochemical inter-

est. His research may be broadly divided into three main areas. First, protein-ligand systems have been studied, not only to allow calculation of binding affinities, but also to predict the structures of these complexes. Most recently, he has developed novel and efficient methods for calculating binding free energies based on replica exchange methodology, and also approaches for incorporating receptor flexibility in protein-ligand docking. Second, phospholipid bilayers have been simulated using molecular dynamics computer simulations. Using atomistic models, he has been able to calculate the permeabilities of small molecules and drugs in phospholipid membranes, and he is also developing coarse-grained membrane models based on the Gay-Berne model of liquid crystals. Third, digital signal processing methods have been developed to study conformational change in protein systems. Using this methodology, large-scale conformational motions not accessible over the timescales of conventional simulations, have been observed. These include the movement of the M20 loop of DHFR from the closed to the occluded conformation, and the opening of the flaps in HIV-protease. Dr Essex is the recipient of numerous research grants, from both the Research Councils and industry.

From 2001-2005, Dr Essex was the European Editor of the *Journal of Molecular Graphics & Modelling*, and he currently serves on the Editorial Board of the *Journal of Computer Aided Molecular Design*. He is a member of the EPSRC college (2006-2008), a member of the Hector Project Working Group, and a former Chairman and current committee member of the international *Molecular Graphics & Modelling Society*. Over the last few years he has been invited to speak at a number of national and international conferences, including two CECAM meetings in Lyon, a CERC3 meeting in Portugal, an N+N meeting in Washington DC, an EMBO workshop in Shanghai, and a FEBS course in Tromsø, Norway. He was awarded the 2002 Marlow Medal by the Royal Society of Chemistry.

Richard A. Goldstein

obtained his Ph.D. using experimental and computational methods to study electron transfer in bacterial photosynthesis. After a brief stay teaching Physics in China, he worked with Peter Wolynes developing methods to predict protein tertiary structures. Since moving to a faculty position at the University of Michigan, he has worked on understanding 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 the evolutionary process. Dr. Goldstein is in the process of leaving the University of Michigan and moving to Siena Biotech, a new Biotech company in Siena, Italy, where he will be leading the bioinformatics section.

Stephen J. Haggarty

is an Instructor in Neurology at Harvard Medical/Massachusetts General Hospital and Head of Chemical Neurogenetics at the Broad Institute of Harvard University and MIT. He received a Bachelor of Science degree in Genetics from the University of British Columbia, Vancouver in 1997, and his Ph.D. in Biochemistry in 2003 from Harvard University in the laboratory of Dr. Stuart Schreiber. Dr. Haggarty's uses chemical genomics and molecular approaches to identify novel targets for the development of therapeutics for central nervous system disorders and for the functional characterization of candidate genes linked to neuropsychiatric disorders.

His group has developed high-throughput screening technology for identifying chemical that modulate synapse formation, morphological properties of primary neurons and differentiated stem cells, and neurophysiological activity. The Haggarty group has also developed computational tools for understanding and exploring high-dimensional datasets and networks of chemical-genetic interactions. Collectively these efforts will expand the molecular and cellular 'toolbox' available for understanding a variety of human diseases.

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 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. His interests and responsibilities range from organizing the Beilstein Bozen Workshops with the aim of furthering interdisciplinary communication between chemistry and neighbouring scientific areas to the publication of the Beilstein Journal of Organic Chemistry.

Laurent M. Humeau

Laurent M. Humeau is the Senior Director of Research and Development at VIRxSYS Corporation. He leads a multi-disciplinary group composed of talented researchers with extensive expertise in cell biology, immunology and lentiviral vector design. Dr. Humeau conducted his graduate studies at the Department of Gene Transfer and Cellular Therapy at the Institute Paoli-Calmettes Cancer Center in Marseille, France, and at the DNAX Research Institute in Palo Alto, California. After receiving his Ph.D. in Blood Cell Biology (Summa Cum Laude) in 1997 from the University Denis Diderot, Paris, France, Dr.

Humeau did his post doctoral formation at the University of California at San Francisco, where he focused on *in vitro* multi-lineage hematopoietic stem cell development assays, gene transfer and *in utero* transplantation. Since he joined VIRxSYS Corporation in 2000, Dr. Humeau has been in charge of the development of new and highly efficient transduction procedures that are clinically translatable, as well the development of *in vitro* and/or *in vivo* assays that are used for the generation of data for the clinical trials. His group was also in charge of the design and implementation of the large scale Cell Processing and related quality control procedures currently used in the company phase II clinical trials.

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, 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).

Sjibren Otto

received his M.Sc. (1994) and Ph.D. (1998) degrees cum laude from the University of Groningen in the Netherlands. He worked on physical organic chemistry in aqueous solutions in the group of Prof. Jan B. F. N. Engberts. In 1998 he moved to the United States for a year as a postdoctoral researcher with Prof. Steven L. Regen (Lehigh University, Bethlehem, Pennsylvania) investigating synthetic systems mediating ion transport through lipid bilayers. In 1999 he received a Marie Curie Fellowship and moved to the University of Cambridge where he worked for two years with Prof. Jeremy K. M. Sanders on dynamic combinatorial libraries. In October 2001 he started his independent career as a Royal Society University Research Fellow at the same university. Apart from dynamic combinatorial chemistry his current research interests include molecular networks, drug targeting and molecular recognition at the lipid bilayer interface.

Joelle N. Pelletier

Joelle Pelletier obtained her PhD with honours at McGill University Biochemistry in 1996. Her doctoral work was recognized by the Bernard-Belleau Research Prize. She undertook postdoctoral work first as a FQRNT Fellow under the guidance of Stephen Michnick at Université de Montréal Biochemistry where their pioneering work on high-throughput detection of protein-protein interactions by PCA gave rise to Odyssey Pharmaceuticals (USA). She went on to Universität Zürich Biochemistry as an NSERC Fellow under the guidance of Andreas Plückthun to develop high-throughput enzyme selection using ribosome display. Hired at the Chemistry Department of Université de Montréal in late 1999 as a FQRNT Research Fellow, her research program in Bio-Organic Chemistry is centred on enzyme engineering. Her research group is multidisciplinary, where chemistry, structural biology, molecular biology and bioinformatics meet to explore the area of ligand selectivity. Joelle is a founding member and current Board member of the Canadian Green Chemistry Network.

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 (design of artificial antigens), the University of Stockholm, Sweden (analysis of mitochondrial targeting sequences), the Massachusetts Institute of Technology, Cambridge, MA, USA (empirical potentials for protein folding simulation), and the Max-Planck-Institute of Biophysics in Frankfurt, Germany (sequence-based prediction of membrane proteins), which was supported by Boehringer-Ingelheim Fonds fellowships. During this time, a common theme of his work was the development and application of artificial neural network models and evolutionary algorithms for amino acid sequence analysis and peptide design. 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 of 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 100 scientific papers and patents, co-edited three multi-author books, and co-authored a textbook on adaptive systems in molecular design. He is editor of the journal "QSAR and Combinatorial Science", and member of the editorial advisory boards of the journals "Chembiochem" and "Current Chemical Biology". Milestones of his research include the combination of artificial neural networks as fitness functions for evolutionary molecular design, and the first automated ligand-based *de novo* design of a novel potassium channel blocker.

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 in New York City he became Assistant Professor at the Massachusetts Institute of Technology in January 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 where he is currently directing research programs with about 30 coworkers. Professor Seebergers research has been documented in over 115 articles in peer-reviewed journals, thirteen issued patents and patent applications, more than 70 published abstracts and more than 250 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), the Award of the European Society of Combinatorial Sciences (2005) and the Carbohydrate Research Award (2005). In 2004 he received the Otto-Klung Weberbank Prize for Chemistry. Peter H. Seeberger is the Editor of the *Journal of Carbohydrate Chemistry* and serves on the editorial advisory boards of seven 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.

Oliver Seitz

was born 1966 in Frankfurt a. M. and studied chemistry at Johannes-Gutenberg University in Mainz. He carried out his doctoral thesis in organic chemistry under the supervision of Professor Horst Kunz (1992-1995). After postdoctoral studies with Professor Chi-Huey Wong at the Scripps Research Institute in La Jolla, California (1996-1997) he started independent work at the Technical University Karlsruhe. In 2000 he moved to the Max-Planck-Institute of Molecular Physiology in Dortmund where he led a group in the Department of Chemical Biology. He was appointed to the Chair of Bioorganic Synthesis at the Institute of Chemistry at Humboldt-Universität zu Berlin in 2003.

Oliver's research interests include the synthesis and modification of nucleic acids, proteins and peptides and carbohydrates as new tools for biological studies. Current research projects involve among others the development of new probes for genotyping, DNA-directed

chemistry, DNA-methyltransferases, cellular signal transduction and proteome profiling. He has been the recipient of Liebig- and Heisenberg Fellowship, of the Bennisgen-Foerder Award and the Lilly-Lecture Award.

Holger Wallmeier

obtained his PhD 1982 in Theoretical Chemistry from the University of Bochum (D) 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 then 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. Since 2003 he works for Sanofi-Aventis Deutschland GmbH.

Marcey L. Waters

earned her bachelors degree in chemistry from the University of California at San Diego in 1992 where she did undergraduate research in physical organic chemistry with Professor Charles Perrin as a Howard Hughes fellow. During this time she also spent two summers doing research in organometallic chemistry with Gerard Parkin at Columbia University as an NSF REU fellow. She completed her PhD in 1997 in organometallic chemistry with Professor William Wulff at the University of Chicago, sponsored in part by an ACS Division of Organic Chemistry fellowship. She then spent two years as an NIH postdoctoral fellow in Professor Ronald Breslows lab at Columbia University working in the area of biomimetic chemistry. She started her independent career at UNC Chapel Hill in 1999 and was promoted to associate professor in 2005. She has continued on in the field of biomimetic chemistry, studying noncovalent interactions in peptide structure and function, and using structured peptides as mimics of protein domains for biomolecular recognition. She has earned several awards during her career, including an NSF Career Award and Sloan Fellowship.

