SCANZ NEWSLETTER

SOCIETY OF CRYSTALLOGRAPHERS IN AUSTRALIA AND NEW ZEALAND

No 59, December 2004

http://www.sca.asn.au/

FROM THE PRESIDENT

Dear SCANZ members,

Seasons greetings to everyone!

The year has flown by and I am sure that, like me, many of you have not yet had time to register for the Crystal24 meeting. Don't forget to do this soon though, as the early registration deadline is looming (14 January for registration and Abstracts, 24 December for the accommodation package). Further information about the SCANZ conference is included below, and student members will be particularly interested in the SCANZ and IUCr funding schemes.

One of the tasks that has kept me busy over the past few months is the collation of an article for the IUCr newsletter on Crystallography in Australia And New Zealand. This document is almost ready to send off to the Union, and I hope you will enjoy reading the finished product. I would like to take this opportunity to thank all who contributed to the article. It is not possible in this limited space to thank everyone individually, but you will see that your hard work will be paid off in double since we plan to publish the longer versions of each section in the SCANZ newsletter. Our editor, Geoff Jameson, has opted to begin in this issue with the section on Fibre Diffraction by Jim Metson, Ward Robinson and Allan White.

The Australian Synchrotron continues to occupy the time of many of us, most recently with the establishment of beamline advisory panels for the facility. It is intended that the outcomes of the panels will be made available to the community and I hope that everyone will take the opportunity to provide feedback. The SCANZ conference in March will provide a suitable general forum for this, another good reason to register early! Meanwhile the building to house the Synchrotron is moving along according to schedule and engineers are expected to move into the building, to begin work on the next stage of the facility, in the first quarter of 2005.

On a final sad note, the crystallography world was saddened to hear of the recent deaths of two world-renowned crystallographers - Maurice Wilkins and Carl-Ivar Brändén – whose obituaries are included below.

Best wishes to everyone for a prosperous, happy and safe 2005,

Jenny Martin

FROM THE SECRETARY

Notice is given that the SCANZ Annual General Meeting will be held during SCANZ 24 at the Marylands Country House, Marysville. Members are invited not only to attend but to submit to the Secretary items for the agenda.

AWARDS

Jamie Rossjohn

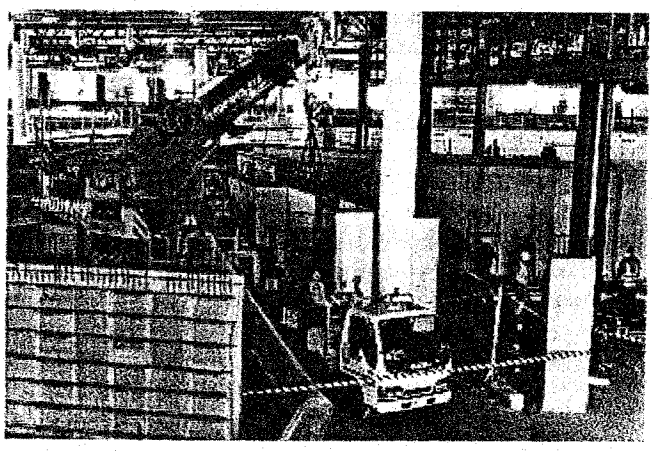
The Science Minister's Prize for Life Scientist of the Year was awarded at a ceremony in Canberra on 8 September to Jamie Rossjohn. Dr Jamie Rossjohn, a leader in structural biology and X-ray crystallography at Monash University, uses overseas synchrotron facilities to investigate the structure of proteins and how they work in the human body.

"Synchrotron science has had a huge impact on my research productivity. I travel to overseas synchrotrons two to three times a year, and I'm looking forward very much to the arrival of the Australian Synchrotron facility to enhance my productivity and that of my team," Dr Rossjohn said.

Dr Rossjohn leads a team of sixteen researchers at Monash University's Protein Crystallography unit. His research has thrown light on aspects of asthma, Alzheimer's disease, multiple sclerosis, organ rejection, drug resistances, the performance of anti-cancer drugs and bacterial toxins.

SCANZ offers its congratulations and best wishes to Jamie for this very significant award.

AUSTRALIAN SYNCHROTRON



A recent photograph of the interior of the Australian Synchrotron (www.synchrotron.vic.gov.au).

RESEARCH PROFILE

Jenny Martin has been collating for the IUCr profiles of research in Australasia that uses diffraction techniques. In the light of the death of Maurice Wilkins, who pioneered diffraction studies on DNA, it seemed timely to profile Australasia's research activity on diffraction by and structural analysis of fibrous materials. Subsequent newsletters will profile other areas spanned by SCANZ. The following is the unabridged version prepared by Rick Millane.

Fibre Diffraction in Australasia

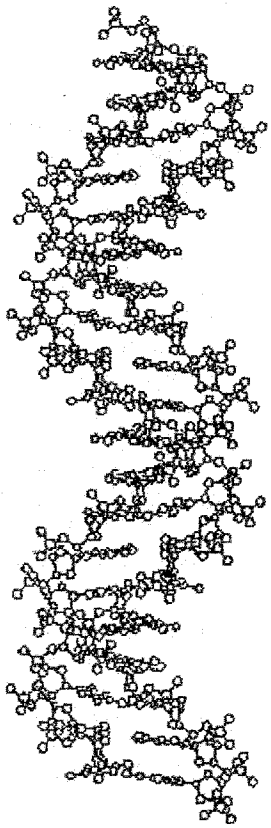
Fibre diffraction analysis (see IUCr Newsletter, Vol. 6, No. 2, 1998) is concerned with obtaining detailed structural information from fibrous specimens; specimens that are oriented and rotationally disordered. The molecules usually have helical symmetry and the rotational disordering leads to cylindrical averaging of the X-ray diffraction intensities in reciprocal space. The challenge is to determine structures from this limited data. A good review of fibre diffraction techniques can be found in International Tables for Crystallography Vol. B, pp. 466-481 (2001). This technique has a long history and in its early forms played an important role in determination of the structures of cellulose, DNA and some polypeptides.

Fibre diffraction has some significant history in Australia dating back to Bruce Fraser and Tom MacRae at the Wool Textile Research Laboratory, Division of Protein Chemistry, CSIRO in Melbourne in the 1950s. They used X-ray diffraction to study natural fibres, and produced particularly important structural results on collagen and keratin. They were also one of the first groups to use computers to analyse fibre diffraction patterns. The book "Conformation in Fibrous Proteins and Related Synthetic Polypeptides" by Fraser and MacRae in 1971 was an important reference in this area. One of Bruce's early collaborators, David Parry, is now at Massey University in New Zealand and is a world authority on fibrous proteins.

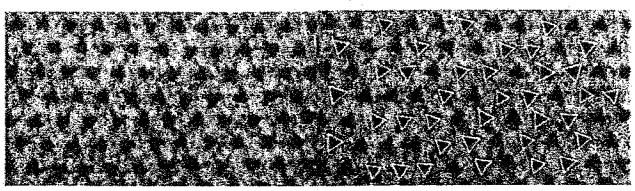
One of fibre diffraction's most influential recent practitioners, Gerald Stubbs, now at Vanderbilt University in the U.S., hails from Tasmania. Gerald did his undergraduate at ANU and graduate work at Oxford under Tony North. Gerald has pioneered the application of fibre diffraction methods to high-resolution studies of large structures, particularly helical viruses, and developed methods such as MDIR (multidimensional isomorphous replacement) and layer-line splitting. Gerald now leads the FiberNet consortium in the U.S. (www.fibernet.us).

Rick Millane's group at the University of Canterbury in New Zealand uses fibre diffraction techniques together with the theory of diffraction by disordered lattices to study systems that are both rotationally disordered and subject to various forms of lattice or substitution disorder within the constituent microcrystallites. Diffraction from these specimens consists of Bragg diffraction with amplitudes that are modulated by the disorder and diffuse diffraction between the reciprocal lattice points. Such problems arise in a variety of contexts including artificially prepared fibre specimens such as those of nucleic acids and polysaccharides, and naturally occurring assemblies such as in vertebrate muscle. Rick, while originally from New Zealand, developed many of these techniques during a long stint at Purdue University in the U.S., starting as a post-doc under Struther Arnott. It is interesting to note that both Mitchell Guss and Neil Isaacs also post-docs under Struther. Rick returned to New Zealand in 2001 and is now a member of the Editorial Board of *Acta Crystallographica Section A*.

Artificial fibre specimens often exhibit lattice, rotational and "screw" disorder, and the Millane group has developed descriptions of the diffraction from such systems and incorporated them into structure determination. For example, the figure below shows the structure of the synthetic polynucleotide poly(dA).poly(dT) in which the effect of the disorder has been incorporated into the structure determination (see Fibre Diffraction Review, Vol. 10, 57-62, 2002). Integral to this work is the study of diffraction by disordered crystals (see IUCr Newsletter, Vol. 9, No. 2 p. 7 2001), which is related to the work described by Richard Welberry in the section on Diffuse Scattering.



A current project in the Millane group, in collaboration with John Squire at Imperial College, London, is analysis of disorder in the myosin filament array that occurs in many higher vertebrate muscles. A lack of knowledge on the precise characteristics of this disorder and its effects on the x-ray diffraction has so far been an impediment to rigorous application of fibre diffraction analysis to muscle. This is a fascinating system because the disorder (in the orientations of the myosin filaments) is complex, but one has the advantage of direct imaging of the disorder by electron microscopy. Methods for determining the orientations of the filaments from rather noisy electron micro-graphs have been developed, and current efforts are to model the disorder and develop a description of the diffraction. The figure below shows a small section of an electron micrograph of frog muscle (left) and a determination and classification of the myosin filament orientations (right).



(Left) Small section of frog muscle micrograph and (Right) classification of myosin filament orientations.

There is a variety of other activity in fibre diffraction and disordered materials in New Zealand. These include studies

of cellulose microfibril orientation in wood (Ward Robinson, University of Canterbury), use of reflection high-energy electron diffraction (RHEED) to study crystal orientation and growth in compound semiconductor thin films (Steve Durbin, University of Canterbury), and a variety of industrial applications to cement, fertilisers and soils.

Rick Milllane

Postscript: A. Lindo Patterson (of the Patterson function) was born in Nelson, New Zealand, in 1902. His family moved to Canada when he was one-and-a-half years old, and to London when he was 14.

FUTURE CONFERENCES and WORKSHOPS

(See also next item for student travel awards)

SCANZ Meeting, CRYSTAL-24

Tuesday 29th March to lunchtime Friday 1 April, 2005
Marysville, Victoria

Marysville is a picturesque village verging on state forest and at the foot of Lake Mountain (a popular X-country skiing area) and is located about 90km from Melbourne (across the Great Divide and past many renowned wineries of the Yarra Valley). There are many scenic walks through rainforest including the "Beeches Walk" and to towering mountain ash emanating from around Marysville.

Provisional deadlines:

Registration:	14 January 2005
Abstracts deadline:	14 January 2005
Accommodation:	Favourable accommodation rates at the venue (the Marylands) will be available to those who book early (a 30% deposit will be required). The deadline for this is 24 December.

Conference dinner is included in accommodation cost for those staying at Marylands but will be extra ($55) for those staying elsewhere.

Costs:

Full:	A$450 (late A$525)
Student/retired:	A$250 (late A$300)

A Registration Form was enclosed in the last Newsletter. For more information and for on line registration please visit the SCANZ website (http://www.sca.asn.au/) or go directly to http://xrsi.cmit.csiro.au/Crystal24/).

For more information, please contact Steve Wilkins: Steve.Wilkins@csiro.au

IUCr XX

The twentieth Congress and General Assembly of the International Union of Crystallography will be held in Florence, Italy from 23-31, August 2005 at the Congress Centre. The committee chairpersons are Carlo Mealli (Scientific Program) and Paolo Dapporto (Local Organising Committee). The Congress Centre is located in the very heart of the city, within walking distance of the main tourist attractions and most of the hotels. Further information, including an Interest Form, can be found at the Congress website: http://www.iucr2005.it.

STUDENT TRAVEL AWARDS (to Crystal 24 and IUCr-XX)

The Council of the Society of Crystallographers in Australia and New Zealand is calling for applications from postgraduate students of crystallography for the 'E.N. (Ted) Maslen 1987 Studentships and Scholarships' to fund attendance at two upcoming meetings. Supervisors are urged to inform their students of these travel awards.

Crystal 24, the meeting of the Society of Crystallographers in Australia and New Zealand, will be held in Maryville, Victoria Australia, 29 March - 1 April 2005. Details of the meeting are given in this newsletter or are available from the SCANZ website: http://www.sca.asn.au/ or more directly: http://xrsi.cmit.csiro.au/Crystal24/. ***The deadline for application to SCANZ for travel funds (along with Registration and Abstract submission) is 14 January 2005.***

The XXth Assembly and General Congress of the International Union of Crystallography will be held in Florence, Italy, 23-31 August 2005. Details of the meeting are available in this newsletter or from the Web at the address: http://www.iucr2005.it. ***The deadline for Abstract submission and for application to SCANZ for travel funds is 28 February 2005. Note: The IUCr also has travel funds available. The deadline for abstract submission and application for travel funds from the IUCr is 10 February 2005.***

SCANZ student members from both Australia and New Zealand are invited to apply for the Scholarships, which will make a substantial contribution to the travelling costs. Selections will be based upon merit, geographic distribution and previous and/or future opportunities of the candidates. As the SCANZ Council regards these awards as an important means of introducing young crystallographers to the international scientific community, students awarded Scholarships will be expected to make a presentation of their work at the meeting.

Method of Application. Postgraduate students applying for a 'Maslen 1987 Scholarship' should forward to the Secretary the following:

- An abstract of the presentation sent, or to be sent, to the Congress Secretariat.
- A covering letter from the applicant's supervisor providing a brief reference and verifying that the applicant is a bona fide student at the time of the meeting.
- An indication of what other funding may be available from the applicant's own institution.
- An indication as to whether the applicant has previously received funding from the SCA or SCANZ.

It is strongly recommended that applications be sent by e-mail, though if this is problematic they can be sent by mail or - the least preferred method - fax.

E-mail: G.B.Jameson@massey.ac.nz
Subject: Crystal-24 or IUCR-20 (as appropriate)
Attached: A single WORD file containing the above items

Mail:
Geoffrey B Jameson, Secretary SCANZ
Institute of Fundamental Sciences
Massey University, Private Bag 11 222
Palmerston North, New Zealand

FAX: +64 (0)6 350 5682 (if outside NZ, the (0) is omitted)
If not currently a member of SCANZ: send by ordinary post, a membership application (available from the SCANZ web site) and the appropriate subscription fee by the appropriate deadline to:

Dr Paul D Car, Treasurer of SCANZ
Research School of Chemistry,
The Australian National University,
Canberra, ACT, Australia

PROMOTING SCANZ

Members are reminded that at the last General Meeting of SCANZ at Broome in 2003, $2000 in funds were set aside in 2004 for activities that promoted SCANZ and diffraction sciences in Australasia. The DNA@50 postcards, the Crystal Growing Workshop in Queensland in November 2004, and crystal growing competitions have all benefited from this fund. Please submit applications for the balance of funds allocated for 2004 and for funds allocated for 2005 to the Treasurer, Paul Carr.

SUBSCRIPTIONS

Subscription notices for 2005 are enclosed with this newsletter. (The newsletter editor apologises the notices are not on the traditional blue paper.)

The Treasurer wishes to remind members that annual membership dues for 2004 are to be paid by December 31, 2004. The amount payable is $130 for a corporate member, $25 for a full member and $7 for a student member, with these discounted to $100, $20 and $5 respectively if payment is made by April 1, 2004. Members who are over 60 years of age at the time subscriptions are due can elect to become Life Members of the *Society* by paying a one-off amount of five times the current (discounted) subscription rate (i.e. $100).

Paul Carr

OBITUARIES

Maurice Hugh Frederick Wilkins (1916-2004)

New Zealand-born Nobel Laureate Maurice Hugh Frederick Wilkins, joint winner with Francis Crick (1916-2004) and James Watson of the Nobel Prize for Physiology and Medicine in 1962 for his role in the discovery of the double helix structure of DNA, died on October 5 2004. Wilkins was still a member of the staff of Kings College London, which he had joined in 1946, and took an active part in the celebrations at King's surrounding the fiftieth anniversary in 2003 of the elucidation of the structure of DNA.

The son of a doctor, Wilkins was born on 15 December 1916 in Pongaroa, where a monument to his achievements stands today. Although he was taken to England at the age of only 6, he stated in a radio interview during a visit to New Zealand in 2001 that he and his sister both regarded their early years in New Zealand as "probably the most enjoyable part of our whole lives ... the New Zealand connection is extremely important to me."

He studied physics at St. John's College, Cambridge, then gained his doctorate at the University of Birmingham in 1940 under Dr J. T. Randall on the luminescence of solids. During the Second World War Wilkins worked on the separation of uranium isotopes at Berkeley, California, under Marcus Oliphant as part of the Manhattan Project. When the war ended, Wilkins became a lecturer in physics at St.Andrews University, and then moved with Randall's group to the Medical Research Council Biophysics Unit at King's College London. Wilkins became assistant director of the Medical Research Council Unit in 1950 and deputy director in 1955.

Maurice Wilkins with one of the cameras he developed specially for X-ray diffraction studies.

Ray Gosling, professor emeritus at the University of London, met Wilkins in 1949 when he joined the Biophysics Unit, headed by Sir J.T. Randall. He recalled that he and Wilkins shared a "eureka moment" when they found that if they added water to the asbestos-like mass of DNA, it turned into a gel, out of which they could pull fibres, which gave complex X-ray diffraction patterns. By this time, the importance of DNA as the stuff of genes was becoming clear. Everyone in biophysics, including Linus Pauling, realised that elucidation of the structure of DNA would lead to new, crucial insights into the biochemistry of replication and the underlying coding and function of genetic material in living things, an aspect of biology hitherto shrouded in mystery.

The history of science is full of quirky minor accidents with major consequences. In 1951, Wilkins's boss, Professor Randall, was invited to a conference on macromolecules in Naples. At short notice he asked Wilkins to take his place and, in doing so, precipitated a meeting of incalculable importance. Wilkins went to Naples armed with the best X-ray picture of DNA that he had so far taken. Dr James Watson, at this time touring European laboratories to find the best place to settle to study the biology of genes, was also at the meeting. Expecting Randall to be talking, Watson was, however, immediately and permanently fired by Wilkins's talk on the investigation of DNA structure and by the beautiful X-ray diffraction pattern revealed by his

single slide. Watson said later that this contribution "stood out from the rest like a beacon." Watson, a biologist, ended up at Cambridge, beginning a collaboration with Francis Crick that, with the crucial, but not always open, exchange of ideas and information between the Cambridge group and Maurice Wilkins and Rosalind Franklin in the MRC unit at King's College, led to their postulated double-helical structure for DNA.

Gosling noted that when Watson and Crick built the model of the double helix, they offered a co-authorship to Wilkins, who declined, because he had not helped build the actual model. However, Wilkins and Franklin in papers immediately following Watson's and Crick's landmark paper in the April 25th 1953 issue of Nature provided key semi-quantitative interpretations of the diffraction data in support of the Watson-Crick model (Wilkins, M. H. F., Stokes, A. R., and Wilson, H. R. *Molecular structure of deoxypentose nucleic acids*, Nature 171, 738-740; and Franklin, Rosalind E. and Gosling, R. G. *Molecular configuration in sodium thymonucleate*, Nature 171, 740-741).

In the following decades this work served as the springboard for a vast worldwide expansion of research into molecular genetics. Wilkins went on to study the structure of various forms of RNA, a genetic material in its own right as well as an information messenger within cells, and a wide range of genetic problems, such as those of ageing, of genetic diseases and of obesity. His contributions to science extend far beyond the work that won him a Nobel Prize.

Wilkins's post-war transition into biology was accompanied by an increasing concern about matters of humanity and scholarship, about the problem of distortion of science by political and financial pressures, concerns shared by many other prominent scientists of the time, and he became actively involved in the activities of organisations concerned with justice and with peace. Maurice Wilkins was an intensely private and self-effacing man who was much loved by colleagues and students. He hated pomposity and was particularly proud of his involvement with the Campaign for Nuclear Disarmament.

He is survived by his wife, Patricia Ann, two sons and two daughters. His autobiography, "The Third Man Of The Double Helix," was published last year. More on his life can be found at www.rsnz.org/topics/biol/dna50 and www.kcl.ac.uk/depsta/iss/archives//dna/

Carl-Ivar Brändén (1934-2004)

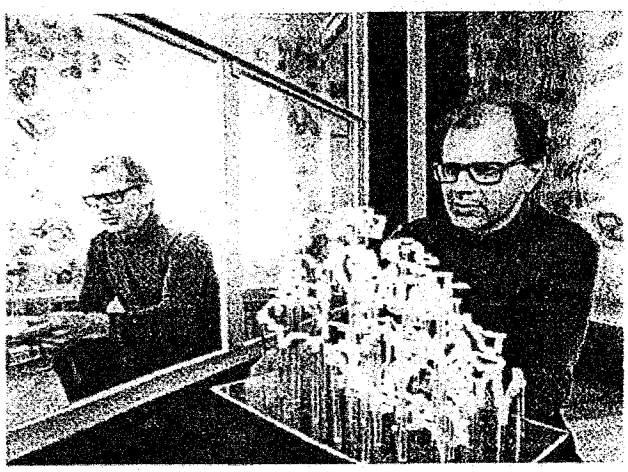
Carl-Ivar Brändén of the Karolinska Institute, Sweden, died on April 28, 2004. He was born in a tiny village in Lappland in the far north of Sweden, where his father was the local schoolteacher. Carl left home at the age of 13 with the intent of becoming a school teacher. He won a scholarship to study mathematics and chemistry at Uppsala University, completing a PhD under the supervision of Ingvar Lindqvist on X-ray crystallography of small inorganic complexes.

In the early 1960's, Brändén made seminal contributions to the development of computer programs for small-molecule crystallography during his PhD and, following a course in Biochemistry, for protein crystallography during a post-doctoral fellowship with Sir John Kendrew in the MRC Laboratory for Molecular Biology (LMB), headed by Max Perutz, in Cambridge, UK.

After returning to Uppsala in 1963, Carl formed a long-time collaboration with Hugo Theorell and Åke Åkesson of the Karolinska Institute, who were biochemistry experts on alcohol dehydrogenase (ADH). Awaiting lab facilities, Eila Cedergren-Zeppezauer, Carl's first graduate student, obtained the ADH crystals in her kitchen refrigerator. In 1969, at a meeting in Konstanz, Germany, Michael Rossmann compared his structure of LDH with Brändén's ADH. To their delight they showed that even when there is no significant sequence identity, there could be a similar structural fold. In the late 1970's Carl took on an ambitious project to solve the crystal structure of Rubisco, an enzyme that catalyzes the initial carbon dioxide fixation in bacteria and plants. In 1986 his group published the X-ray structure of this bacterial enzyme.

In the mid 1980s, he and John Tooze co-authored *Introduction to Protein Structure*, a textbook, which in its first edition had. elegant hand-drawn (rather than computer-generated) illustrations. Its astonishing clarity has had a tremendous impact on several generations of molecular and structural biologists, especially graduate students.

Carl spent five years as research director at the European Synchrotron Radiation Facility in Grenoble, France, establishing facilities for chemistry, biology and medicine, as well as for structural biology. In the late 1990s he participated in designing the ultimate tool for structural biology, a free-electron laser with femtosecond-pulse diffraction combined with three-dimensional holographic instant data collection.



Through the work of his wife, Dr. Malin Åkerblom, on science in the third world, he met a number of bright and devoted scientists from developing countries, who struggle against difficult odds, and developed a deep insight into the problems that face science in these countries, remarking that "From a global perspective of science policy it is a dreadful waste of human resources that the industrialized world supports mediocre scientists in large numbers while many bright young people in the Third World are deprived of the possibility to make their impact on the development of science."

He was one of five members of the Nobel Committee for the Chemistry Prize, a chairman for three years of the EMBO fund committee for postdoctoral fellowships in molecular biology, a chairman of the Chemistry Committee of the Swedish Natural Science Research Council, a board

member of a large consortium for functional genomics, a member of advisory committees for synchrotron sources worldwide, and, with Wayne Hendrickson, a founding editor of the journal *Structure* (launched in 1993).

He was to have received an honorary doctoral degree from the Karolinska Institute on May 14, also his 70th birthday, honoring him for his lifetime achievement, but died on April 28. Brändén's passion for science, wisdom, friendship and scholarship will be missed by a wide community for years to come.

(Abridged from an obituary in *Nature Structural and Molecular Biology* by Shuguang Zhang, Alexander Rich, Joel L Sussman and Allan R Fersht, in turn based based on Carl Brändén's autobiography, *My Own Obituary, My Life in Science: from Reindeers to Synchrotrons.* in *Comprehensive Biochemistry 43: A History of Biochemistry - Selected Topics in the History of Biochemistry. Personal Recollections VIII* (ed. Semenza, G., Elsevier, Amsterdam, 2004). ISBN: 0444517227.

FROM THE NEWSLETTER EDITOR

The Editor has been overwhelmed by the number of responses (zero) to the item flown in the last newsletter that it is probably time to consider distribution of the newsletter by electronic means -- this would allow colour to be used. Extreme responses in favour or against this idea could be communicated to the Editor.

The Editor would also like to use the newsletter to highlight papers and results from the membership. We are a diverse group and this newsletter offers a way, between SCANZ meetings, to profile research across the disciplines in Australia and New Zealand.

As this is your newsletter, please send any items of news or commentary to the Newsletter Editor.