

NEWSLETTER

Society of Crystallographers in Australia and New Zealand

FROM THE PREZ



It is a great privilege to start as President of SCANZ following the extremely enjoyable and educational meeting in Adelaide, and leading into the International Year of Crystallography (IYCr) in 2014. Ray Withers will be a difficult act to follow; I already realize I cannot possibly substitute in the conference dinner entertainment role, and I am already twisting Ray's arm to stay as active as possible in his new Past President role!

During the Adelaide conference, a new SCANZ Executive has been elected. Special welcome to the new people on the committees: Chris Ling as the new Secretary, Peter Czabotar as the new Newsletter Editor, and Jo Etheridge as the new Council member.

The most important upcoming matter for our community is clearly the upcoming IYCr. We as the crystallographic community should try to take the best advantage of the IYCr to promote what we do, and this will require some planning and hopefully some of us investing some time into associated activities. A number of suggestions have already been discussed about possible things to do. In particular, we need to think about how to capture school-



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

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FROM THE PREZ



children and the general public. Some possibilities in no particular order and not necessarily separate:

- Exhibitions with posters and other displays on crystallography, particularly at places like the Australian Synchrotron, ANSTO, Questacon, Science Centres
- Featuring crystallography on the web and through social media (Facebook, Twitter)
- Programs featuring crystallography on radio and TV
- Presentation of movies featuring crystallography
- A crystallography roadshow
- Demonstration experiments
- Plans are already underway for Science at the Shine Dome (SATS) featuring crystallography in May, 2015.

Please contact me or any of the SCANZ officials listed above with further suggestions, it probably makes sense to coordinate the various activities through our Society. Perhaps the best way forward is to find volunteers in the community who are willing to take the lead for particular events or activities and organize the rest of us to help out. So if you have an interest in helping out, please let us know!

One of the important SCANZ activities over the last few years has been the support of crystallography schools. The Australian Synchrotron is keen on hosting the next one this year, and there has been lots of discussion in Adelaide and after about changing the current “ad-hoc” approach to organizing these schools wherever and whenever someone was keen to do it, to a more regular event. I believe crystallography education may be the most important mission of SCANZ; all of us are not just “crystallographers” but often primarily something else, and with many crystallographic methods becoming more and more routine and fewer and fewer opportunities existing to learn the fundamentals of crystallography, we need to provide young researchers using crystallographic approaches an opportunity to obtain more than just a surface education on the topic. Perhaps a regular event at an appropriate venue such as the Australian Synchrotron is the way to go, as long as others in the community interested in driving this endeavour continue to be involved.

Finally, just a reminder that the deadline for early bird membership fees is 31 March. We have kept the fees at rock bottom level for many years, and it has never been a better time to join SCANZ, leading up to IYCr in 2014. So please remind your colleagues who have not yet joined SCANZ, and especially students, to do so. To finish with a mention of the upcoming conferences. The next AsCA conference is in Dhaka, Bangladesh, 1 - 4 December, 2013 (<http://www.asca2013.org/>). Our next Crystal conference is planned tentatively in April 2014 at a location currently being discussed.





*Mathieson Medalist,
Darren Goossens with
Mrs Lois Mathieson.*



*Bragg Medalist Peter Colman
with Mrs Patience Thomson.*



*Jose Varghese
Chair: International Science Advisory Committee (ISAC) and Science Program.*

MEETING REPORT
ASCA 12 / CRYSTAL 28
ADELAIDE,
DEC 2-5, 2012

The ISAC together with the SCANZ Council decided on the format of the meeting which was similar to the previous AsCA Meeting. The symposia consisted of three parallel sessions, one relating to biological sciences and two to chemical and physical sciences. Two Chairs, experts in the field for each of the sessions were nominated, one from overseas in the AsCA domain and the other from Australia and New Zealand. Following the acceptance of the Chairs they were given the task of inviting three speakers to their symposium and selecting two speakers from the abstracts with some degree of flexibility. Guidelines for the selection included gender and geographical balance.

Two plenary speakers were selected by the SCANZ council by offering Maslen Fellowships. Initial choice of Dame Louise Johnson had to be altered due to her illness, and Prof. Wayne Hendrickson and Prof. Xiao-Ming Chen were selected as Maslen Fellows. Wayne who played a key part in the development of protein crystallography talked about the development of methods of phase determination by anomalous scattering (SAD phasing) and also presented a talk in the membrane proteins session, and Xiao-Ming presented some amazing data on metallo-organic lattices that have been engineered to selectively absorb compounds and gases with small volumetric differences. Prof. Henry Chapman was also nominated as a third plenary lecturer and presented the latest results from Free

Electron Laser experiments on protein crystals. Three keynote speakers, Prof. Ringer, Prof. Welberry and Prof. Cole, addressed the state of the art in optoelectronics, diffuse scattering and solid solutions, and Dr. Vivian presented a structural study of recognition of self and non-self by cells.

Some 460 delegates attended the meeting and a major proportion of them representing Asian countries like Japan, China and India. There were a large number of students from Asia and Australia, and student scholarships were provided by the IUCr and AsCA for Asian students as well as Maslen studentships for Australian and New Zealand students. The sessions ran smoothly and were well attended. The talks were of a very high standard, equal or better than other international meetings of this kind. Feedback from attendees indicate that everyone thought that this was an exceptional meeting and very much enjoyed the scientific program, the location and the entertainment. The only problem encountered was the AsCA rising stars symposium which needed a better process for the selection of candidates. It was felt in Adelaide that the process was too ad hoc and was inadequate in the ability to select candidates with due process.

I would like to thank the Chairs of the Micro Symposia for the success of this meeting, and the efforts of Prof. Ray Withers and the SCANZ Council and ISAC in advertising the meeting and persuading most of leading crystallography laboratories in Australasia to send delegates to this meeting. The LOC lead by Prof. Carver should be also thanked for arranging the venue and ensuring the planning and logistics ran smoothly.

**BRAGG CENTENNIAL
SYMPOSIUM
ADELAIDE
DEC 6, 2012**



A one-day symposium was held in Adelaide immediately following the AsCA 12/CRYSTAL 28 conference to pay tribute to Lawrence Bragg and his father William Henry Bragg who made pioneering and far reaching contributions to the development of X-ray crystallography and who spent important periods of their lives in Adelaide. The specific event being commemorated was the presentation to the Cambridge Philosophical Society on 11 November 1912, by W.L. (Lawrence) Bragg, of a paper entitled "The Diffraction of Short Electromagnetic Waves by a Crystal", which shortly after appeared in the Society's Proceedings. In this paper he outlined what we now call Bragg's Law and also presented the first correct indexing of a diffraction pattern, namely that for zinc blende.

The symposium included a very distinguished list of speakers who covered many aspects of the Bragg's life and work, especially that of Lawrence. A copy of the Program is available at

http://sapmea.asn.au/conventions/crystal2012/downloads/Bragg_Symposium_Program.pdf

Six members of the Bragg family specially made the journey from the UK to Australia for the symposium, including Mrs Patience Thomson, younger daughter of Sir Lawrence Bragg. Patience gave a wonderful talk recounting her fond memories of her father and also quelled a few popular myths about him. Her talk was followed by an outline of the relative roles of WH and WL Bragg in the development of X-ray crystallography. Brian Matthews spoke about the early days of biomolecular crystallography and some memories of the role of Lawrence Bragg. Anders Liljas spoke about the background to the award of the Nobel Prizes in 1915 to the Braggs referring to internal correspondence and records of the Nobel Committee. Anthony Kelly spoke about the early days of metal physics in the Cavendish and the influence of Lawrence on the development of this field as well as that of X-ray and electron microdiffraction. Other speakers covered the birth of neutron diffraction (Thom Mason), the role of Bragg's law in electron diffraction (Colin Humphreys), the evolution of microdiffraction from simple lab-based set-ups to XFEL-based studies (John Spence). Tony Cheetham gave an impressive overview talk on the impact of crystallography in various frontier areas of materials science. Many Bragg related papers by speakers at the Symposium have been published in the special Bragg Centennial issue of Acta Cryst A, see

<http://journals.iucr.org/a/issues/2013/01/00/issconts.html>

Towards the conclusion of the Symposium, Jenny Martin gave a very personal tribute to Dame Louise Johnson who died a few months before the Bragg Symposium. Jenny is a former PhD student of Louise. Louise had been invited to be a speaker at the Symposium and had worked under Lawrence Bragg at the Royal Institution on the structure of lysozyme. However, this unfortunately was not to be.



**BRAGG CENTENNIAL
SYMPOSIUM
ADELAIDE, DEC 6 2012**

The Symposium Dinner for speakers and special guests was held in the former home of the Braggs, now operated as the Public Schools Club. The menu consisted of favourite dishes of Lawrence Bragg. Grandchildren Clare and Nick Heath gave short vignettes on their memories of their grandfather. A special Bragg-labelled wine was served at the Dinner.

Other special events in the AsCA/ Bragg week were a Civic Reception at the Adelaide Town Hall held in honour of the Bragg family and an unveiling of a statue of Lawrence Bragg in a prominent place on North Terrace in front of Government House.

It was a very full week and one that will linger in the minds of those who were present for a long time to come. We were extremely fortunate that we had people present who could still speak with firsthand knowledge about Sir Lawrence Bragg.

Steve Wilkins



Bragg Symposium Speakers



Front row (l to r):, Prof. John Spence, Prof. Anthony Kelly, Mrs Patience Thomson, Dr Steve Wilkins, Prof Brian Matthews.

Second row: Prof. Gautam Desiraju, Dr John Jenkins, Prof. Anthony Klein, Prof Peter Colman, Mr David Thomson.

Back row: Sir Colin Humphreys, Prof Tony Cheetham, Prof Anders Liljas, Prof. Wayne Hendrickson.

ASCA 12/CRYSTAL 28, MASLEN SCHOLARSHIP REPORTS

November 2012 marks the centenary of the founding of X-ray crystallography by Lawrence Bragg. He and his father William were awarded Nobel Prize in 1915 for their contribution to this field. To celebrate this important anniversary, a combined scientific conference of the Asian Crystallography Association (AsCA) and the Society of Crystallographers in Australia and New Zealand (SCANZ) was held in Adelaide, a city where William worked and Lawrence was born and educated. Following the AsCA and SCANZ conference, is the Bragg Symposium, which explored more of the historical and personal context of Braggs' work. Thanks to the Maslen scholarship from SCANZ, I was able to attend both the conference and symposium, which has been a valuable experience for me as a junior PhD student of X-ray crystallography.

The conference was well organized to cover a wide range of topics related to X-ray crystallography. Those topics were classified into various sessions and explored deeply from basic biophysical theory (diffraction physics and structural chemistry) to new techniques (synchrotron, neutron sources, instrumentation and Phaser workshop) and applications (drug discovery and enzyme study), as well as some exciting breakthrough of the field (hot structures and membrane proteins). There were too

many great talks to mention. My personal highlight would be Prof Wayne Hendrickson's plenary lecture about multi-crystal native SAD analysis of macromolecular structure. Another exciting talk is from Zygmunt Derewenda about engineering proteins and complexes to enhance crystallizability. I was also given the opportunity to present my research at the poster session.

The conference offered both academic and social ways for communicating with "comrades" from all over the world. One amazing example is the conference dinner held in National Wine Center. In the dinner, we saw our talent expanded far beyond growing crystals or solving structures. We enjoyed a wine tasting trip, a concert putting together songs from different cultures, and even a magic show contributed by Japanese scientists.

I sincerely thank the conference organizers and chairs for putting together such an inspiring and exciting conference. And all of us are looking forward to the next SCANZ meeting. I also thank SCANZ again for supporting me with the Maslen award.

Xiaoxiao Zhang

University of Queensland

The Maslen scholarship gave me the opportunity to attend the AsCA12/ CRYSTAL 28 conference and Bragg symposium in Adelaide. The conference was a success in more ways than one. It was a wonderful conference by delivering a broad knowledge in crystallography and other protein structure tools. This knowledge was presented by a

bunch of talented people from all over the world especially expertise from the Asian countries and Australia.

Personal highlights of the conference included the structural biology on nuclear hormone receptor lecture by Prof. Eric Xu from Van Andel Research Institute in Michigan, USA, and Dr. Andrew Whitten's excellent lecture about the regulatory role

of Munc18 proteins in SNARE mediated membrane fusion, a study which involved the use of small angle light

scattering. The conference also involved poster presentations from researchers with various levels of expertise, the one I found most interesting was of the structure of a protein-lipid complex by Grant Mills from La Trobe University.

I presented a poster about my PhD project at the conference and got good feedback. The conference gave me new ideas to put into my project, developed my network of contacts, and provided me knowledge about future funding and employment opportunities.





I would like to mention the last day of the trip, which was the Bragg symposium. This meeting was remarkable in knowing the story of those talented scientists; Lawrence Bragg and Bragg the father. It was interesting to know how they used the old tools to study x-ray crystallography and how this field has dramatically developed. Finally, I would like to thank SCANZ for the organization of this conference and for providing me with a Maslen scholarship to be able to attend.

Mohammed Alaidarous
University of Queensland

It was a great honor for me to be awarded a Maslen scholarship from SCANZ, which allowed me to attend the AsCA 12/CRYSTAL 28 and Bragg Centennial Symposium held in Adelaide, Australia. The city has strong historical links with joint Nobel Prize winners, William and Lawrence Bragg, who made remarkable contributions to the early development of x-ray crystallography. The AsCA 12 conference covered a variety of scientific topics, from macromolecular structures in biology to nano-crystallography with x-ray laser pulses, given by local and international speakers. As a beginner in this specialized field, I was surprised how diversified applications of x-ray crystallography are and was excited to meet many senior and young scientists dedicating their effort on improving our understanding of science. The conference was followed by the Bragg Centennial Symposium, a series of talks which gave an excellent introduction to the lifetime of William and Lawrence Bragg and the great scientific and social impact they made.

Apart from science, the conference had a great finish with the conference dinner held in the Australian national wine center. It was a great experience for me to taste different wines with an expert's introduction on tasting wines. Also, another great highlight of the dinner was the singing performance brought by delegates from different countries and the magic show by a funny Japanese delegate. Certainly, they had made this event so wonderful and memorable for me.

I sincerely thank the conference organisers and directors for putting together a successful conference and a warm symposium. I also thank SCANZ for supporting my attendance with the Maslen scholarship.

Chiungwen Chang
University of Queensland



Personally, the impressive talks for me from the conference and symposium were the special plenary lecture on native SAD analysis of macromolecular structure given by Prof.

Wayne Hendrickson and the talk he gave on crystallography in the Bragg symposium. His words really inspired me to go further and feel grateful in this field. Additionally, the tribute given by Prof. Jenny Martin to Prof. Dame Louise Johnson touched and impressed me, what a great success she achieved as a female scientist and as a person.



Special thanks to Bill Duax for photos of ASCA12/Crystal28 and the Bragg Symposium.

IUCR 2011, MASLEN SCHOLARSHIP REPORT

The XX11 Congress and General Assembly of the International Union of Crystallography was held in Madrid in August 2011. Australia and New Zealand were well represented among the thousands of attendees from across the globe. Thanks to SCANZ scholarships, several grateful PhD students made it as well, myself included.

The lead up to the conference began with an XAFS workshop. This was the first IUCR congress to include a commission on XAFS, a micro-symposium on XAFS, and an XAFS workshop. Needless to say this is exciting news for XAFS researchers.

There were many excellent crystallography presentations. It was interesting to see how crystallography is used by researchers with a very different background to my own.

Ross Piltz's talk gave a very interesting account of the accurate treatment of image plate diffraction data, amongst other things. Christina Hoffmann's talk similarly described a very thorough analysis of neutron data. The microsymbosia "Atomic Dynamics Using X-ray and Neutrons" was very interesting, and Garry McIntyre gave an excellent overview in "Phonons observed by Laue diffraction on a continuous neutron source".

Some applications of crystallography were presented in the microsymbosia titled "Crystallography in Industrial process control". I enjoyed hearing about the importance of calibration in Juergen Neubauer's talk, and especially the importance of having accurate x-ray mass attenuation coefficients! Ray Withers' talk was booming with enthusiasm and very entertaining. My colleague Jay Bourke and supervisor Chris Chantler also gave excellent presentations.

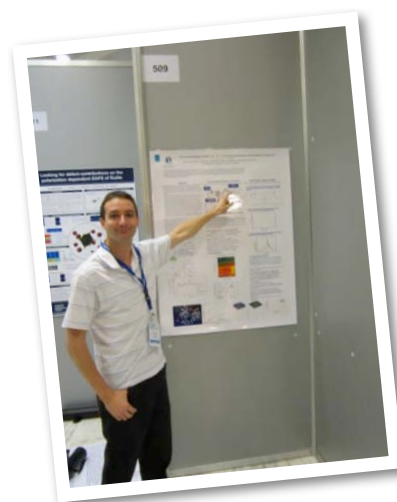
Following Francesco Grazi's "Japanese sword metallurgy", the inevitable question was asked (not by me) "which sword would win in a fight between a samurai blade and a Toledo blade"! Apparently you'd be better off with a samurai sword in such an unfortunate scenario.

In addition to the oral and poster presentations there were many meetings, software installation sessions and industry stalls. I enjoyed a lunch time presentation of the new Dectris detectors. Hopefully someone will let me play with one...

Along with my supervisor, Prof. Chris Chantler, I presented my work on the X-ray mass attenuation coefficients of zinc, selenium and zinc selenide: XAFS, XANES, Bijvoet ratios, and related quantities. My poster session was exciting, but alas, I didn't manage to win the coveted student poster prize for best physics poster!

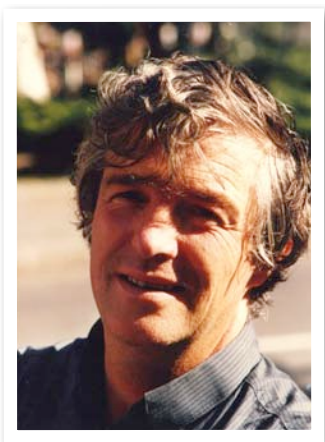
Nicholas A Rae

The University of Melbourne



OBITUARY

Remembering Guy Dodson (1937-2012)



One of the most beloved and influential figures in the development of protein crystallography, Guy Dodson passed away peacefully on Christmas Eve, aged 75, with his wife Eleanor and other family members at his side. Guy was an inspirational scientist whose engaging personality and passion for science have enriched the lives of many people round the world. Although almost all his career was made in the UK, he had deep personal connections with Australia and New Zealand and will be dearly remembered.

Guy was born in Palmerston North, New Zealand, which he liked to describe affectionately as “the centre of the universe.” He received his secondary and tertiary education in Auckland, and it was at the then Auckland University College that his love of crystallography and the concept of “seeing molecules” were developed. His first choice on entering university was to enroll in history but when faced with a late enrolment fee of £10 he chose chemistry instead. His career shows how fortunate that choice was, although he remained passionate about history; his Churchillian orations are legendary! Luckily, he found in Auckland an excellent crystallography research group, and undertook the X-ray analysis of a plant alkaloid as his PhD topic. He remained very grateful for the freedom given by his tolerant supervisor, David Hall, who provided guidance, support and crystallographic training while turning a blind eye to the impromptu cricket, water fights, fire extinguisher episodes etc. that punctuated lab activities.

Guy’s move to Oxford in 1962, when he went to work with Dorothy Hodgkin on what was originally expected to be only a short-term postdoctoral position,

transformed his life. The revolution in the development of protein crystallography was gathering pace, and he became Dorothy’s right-hand person in the successful solution of the structure of insulin, achieved in 1969. He also met and married Eleanor, a mathematics graduate from Melbourne, who had also been absorbed into Dorothy’s group.

I came to Oxford in 1967, barely knowing what a protein was and somewhat overawed (should I wear a tie to the lab?). Guy’s reaction was typical, warm and welcoming – definitely no ties! My initial brief was to develop data collection strategies on the new 4-circle diffractometer, but I became absorbed into the insulin team, socially and scientifically. Heather, too, became involved as Dorothy was keen that she “keep her hand in” after our first child was born. Dorothy’s philosophy of helping to build the careers and talents of others was one that Guy and Eleanor took on wholeheartedly. In turn it enabled Heather and I to go back to New Zealand full of confidence.

Guy remained in Oxford until 1976 when Dorothy retired. These were exciting days as the biology of insulin began to be teased out. It was already apparent that the hexameric 2-Zn structure did not give all the answers, but many insulin biologists and clinicians came through the lab, and there were many “aha!” moments when visitors would suddenly see the structural basis for some aspect of insulin behaviour.

Guy was sometimes asked “What will you do next?” His answer was “I haven’t finished with insulin yet – there are so many interesting variations to

OBITUARY

*Remembering
Guy Dodson
(1937-2012)*

explore". This determination to understand insulin's conformational flexibility and complex biology has been richly vindicated: several billion-dollar drugs in the form of both rapid-acting and long-lasting insulin derivatives, developed by Novo Nordisk in collaboration with Guy's group; and most recently a Nature paper on the insulin:insulin receptor structure. Guy had encouraged Marek Brzozowski, who had sustained the York insulin work, to collaborate with Colin Ward and Mike Lawrence in Australia. It made a very nice link back into this part of the world, and the paper, accepted just before Guy's death, brought enormous and very fitting satisfaction.

In 1976 Guy and Eleanor moved to York (where Maurice, Guy's twin brother, was already a lecturer in Mathematics) to set up a new lab in the Chemistry Department. The move surprised many, as they could have stayed in Oxford, but it was to bring the full flowering of both their talents. Their warmth of personality and large network of friends brought a steady stream of visitors, many of whom found a place in their cavernous home at 101 East Parade. You never knew who would appear for breakfast.

When I arrived with my wife Heather and our family to spend a year (1977-78) in York, the lab was very small, just 3 people. My experience, however, illustrates Guy's ability to seed and build new research initiatives. In New Zealand I had solved the structure of a cysteine protease, actinidin. Guy's structural and crystallographic instincts suggested this as a perfect vehicle for attempting to refine a protein structure from scratch by least squares. Eleanor's genius for crystallographic methods, which led to her later becoming the central figure in the CCP4 initiative, made it possible, and I was the

beneficiary – it was a turning point in my career. I remember vividly the Saturday when we realized the refinement was working, sitting in York Minster listening to Handel's Messiah and thinking about the R-factor dropping 10%.

Towards the end of our year, Guy was invited to Lodz, in Poland, to visit a group of young researchers wishing to establish research in protein crystallography there. He suggested I go, given my experience of doing the same in New Zealand. Ultimately this brought a series of talented Polish researchers to York, who enriched the York lab and expanded the Dodson "family". Guy's enthusiasm and openness, his generosity of spirit, and his willingness to devote his time to assisting and advising others, similarly attracted many more researchers to the York lab, making it a powerhouse in structural biology. Some stayed, to establish their own research programs, others moved on and made outstanding careers elsewhere. Thinking about how the York lab grew, it is clear that Guy was ambitious for good science, but not necessarily to do it all himself; he was very happy to enjoy the efforts of others.

As Dorothy Hodgkin had also done, Guy established effective collaborations with industry, on protein engineering, insulin derivatives and industrially useful enzymes. In 1993, Guy was persuaded to also lead a Division at the National Institute of Medical Research (NIMR) in Mill Hill, where his energies established yet another internationally leading research group, bringing structural insights to biomedical research. In taking this position, he could not resist the lures of the biological research being undertaken at NIMR, and went on to play a major role in research projects dealing with malaria, TB and the structure of prions.



Guy and Eleanor, 1977, at time of starting the York lab.

OBITUARY

*Remembering
Guy Dodson
(1937-2012)*

*Guy at Downe House
(Charles Darwin in the
background)*

Guy had a broad vision. In addition to his insulin work, he conducted insightful studies of the mechanisms of action of haemoglobin and a variety of hydrolytic enzymes: penicillin acylases, amylases and lipases. His greatest delight came as he explored the exquisite beauty of catalytic sites, perfectly oriented hydrogen bonds and strategically placed water molecules. He was a tireless advocate for pursuing protein structures at the highest possible resolution, believing that key details of their chemistry would be revealed, but he also came strongly to the view that other approaches would provide complementary information, most notably molecular calculations.

Although he avoided the formalities of administration and undergraduate teaching as much as he could – in the process generating some legendary stories – he committed his full reserves of energy and persuasion into matters he thought were important for the community at large. As Chair of the IUCr Commission on Biological Molecules he led the way in establishing criteria for the deposition and release of both the data and the coordinates for biological structures, driven by the belief that they should be available to all. He campaigned tirelessly on issues such as the location of the Diamond Synchrotron and the NIMR. His wisdom and lack of

personal agendas saw him widely sought as a reviewer and a PhD examiner. He had very high standards, but he understood human fallibilities.

Guy liked to say that he had never grown up, and there is some truth in this. He retained a boyish enthusiasm, and his love of life was infectious. He could be describing the exquisite beauty of the catalytic triad in serine hydrolases one moment and be bowling tricky leg-spinners down the lab corridor the next. A typical comment from a young researcher in my lab sums up his personal legacy: “Though I met him only a few times I was always struck by his passion for both life in general and science in particular, as well as what I saw as a mischievous twinkle in his eye and his approachableness. I always came away from talking to him with renewed enthusiasm.”

Guy always saw the best in people, and as a result he got the best from them. Today, researchers all round the world, from the UK and Europe, to North America, Cuba, India, China, Australia and New Zealand carry the benefits of their associations with Guy and an abiding and affectionate love for him.

Ted Baker

