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NZIC

Chemistry

IN NEW ZEALAND

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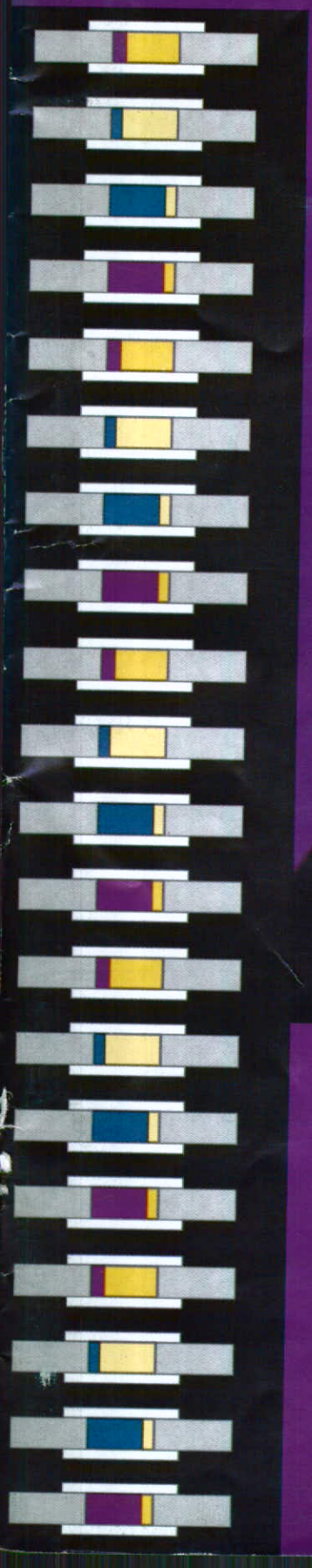
Focus on Forensics, Toxicology, Chemical Pathology, Clinical Chemistry



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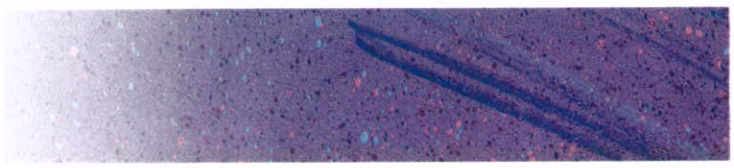

Firsts in FT-IR Spectroscopy from Perkin-Elmer

Perkin-Elmer continues to define confidence in the quality of Fourier transform infrared (FT-IR) spectroscopy analyses and results with two industry firsts: validated FT-IR software and interactive multimedia FT-IR. Using experience as the industry leader in quality assurance/quality control (QA/AC) and method development, Perkin-Elmer developed Spectrum™ for Windows™ software - the world's first validated FT-IR software designed to help users comply with Good Laboratory Practice (GLP) requirements. The new i-Series FT-IR Microscope with IMAGE (Infrared Microspectroscopy Automated Graphical Environment) software provides users with the potential to change the way they perform FT-IR microspectroscopy.

Validated FT-IR Software:

Spectrum for Windows software is validated for each data processing routine against strictly defined rules formulated to check the qualitative and quantitative accuracy of spectra. It is the first software to be validated in this way for both FT-IR instrumentation and processing.
Spectrum for Windows software controls Perkin-Elmer's Automated Precision Validation (APV) accessory. The software automatically generates validation reports, eliminating the need for manual checking procedures. It offers four automatic instrument validation tests: abscissa, ordinate, noise, and ASTMO, the standard procedure established by the American Society for Testing and Materials (ASTM) for measuring the performance of FT-IR spectrometers.

Spectrum for Windows software includes an interactive tutorial with example spectra and worked examples for each data command. Together with the on-line help, this tutorial reduces training time for inexperienced or occasional users. In addition to these features, Perkin-Elmer's own IR Tutor software, which can be run from the Spectrum for Windows package, offers instruction in IR spectroscopy and an introduction to the interpretation of spectra.
Spectrum for Windows software's user interface is easy to use and can be customized for individual applications, allowing users to log in to only those commands they need for performing specific tasks. Additionally, the Spectrum OBEY option enables users to write their own methods and create Standard Operating Procedures (SOP's) to suit individual laboratory requirements.

Interactive Multimedia FT-IR:

Representing the latest in interactive multimedia technology, Perkin-Elmer's new i-Series FT-IR Microspectroscopy System combines superior image quality, breakthrough microspectroscopy data handling and unmatched IR performance. The system comprises the new i-Series FT-IR Microscope, the new IMAGE data handling system, and a Perkin-Elmer FT-IR Spectrometer to provide users with state-of-the-art optical design and high-quality IR analysis. Designed for maximum versatility, the system is also ideal for QA testing and a host of additional applications, including biochemistry, forensics, pharmaceutical, inorganics, plastics and more.

The i-Series FT-IR Microspectroscopy System's IMAGE software system is based on easy-to-use Windows multimedia technology to control a motorised microscope stage, allowing users to interact directly with a video image of the sample on the PC screen. It provides complete control of data collection from Perkin-Elmer FT-IR spectrometers and a range of IR profiling, imaging and surface projection tools, all designed to help isolate and identify areas of chemical difference in microscopic samples.
By marking the visible image the system can be programmed to scan a series of sample points or to produce a complete IR image. The display includes real-time updates of spectra and progress across the sample. IR image types include total absorbance, single wavenumber, absorbance band ratio and ChemiMap functional group images. The open throat design permits access from three sides and the cassegrain optics provide a working distance of more than 20mm.
New facilities include a visible image survey mode, which allows the user to view the sample at high and low magnification simultaneously. In addition, a new multifunctional objective option allows reflection, transmission and ATR measurements to be made without changing the objective.

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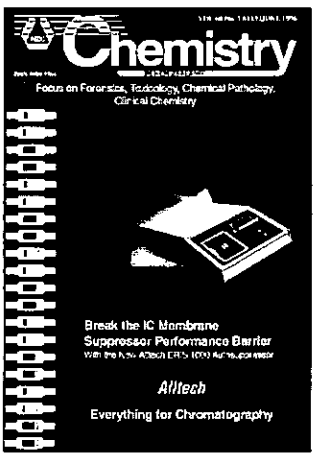
UP FRONT ...

Alltech supply the Odyssey range of Ion Chromatography Systems. The newest development from Alltech's laboratories is the ERIS Autosuppressor pictured on the cover breaking through a barrier representing the performance limitations of membrane-based suppression systems previously available.



For further details see the cover story on page 3

NZIC Chemistry IN NEW ZEALAND

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IN THIS ISSUE ...

COMING UP ...

July 1996 - Focus on Forestry, Timber Treatment, Pulp and Paper

September 1996 - Focus on Education and Training

Deadline for material:
5th of the month of publication

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Editorial

"Why Do I Get Two Copies of *Chemistry in New Zealand*?, and Marketing? and Other Issues?"

It is now three full years since my company Ancat Holdings Limited took over the publishing of *Chemistry in New Zealand*. During this time I have not been tempted to put pen to paper with editorial ramblings; there has always been other material more worthy of publication and of appeal to a wider audience.

Positive comments are continually received on the appearance and content of *Chemistry in New Zealand* and encourage the editorial board to continue development of the publication to provide a better voice for the NZIC and chemists in general to a wider audience. We have been approached by an overseas corporation with respect to electronic publishing of *Chemistry in New Zealand* on the Internet and we are actively investigating this and other initiatives.

In recent months, however, and particularly following the March 1996 issue, some NZIC members have contacted me to ask the question: **"Why do I get two copies of the journal?"**

Each issue of *Chemistry in New Zealand* is distributed using two mailing lists. The main list comprising the members of the New Zealand Institute of Chemistry and individuals or organisations who are paid-up subscribers to *Chemistry in New Zealand* is the same for each issue. This list 'belongs' to the NZIC and because it is assembled from the membership records, the database and all records are held by the NZIC Secretariat in Wellington. We as publishers receive a label print-out to distribute each issue of *Chemistry in New Zealand*.

The second list varies with each issue of *Chemistry in New Zealand*, both in numbers and names on the list. This list is the mainstay of Ancat Holdings Limited's marketing plan for *Chemistry in New Zealand*, and the content is directly related to the industry focus of the issue. This 'marketing' list is custom-made for each focus/issue using Ancat Holdings Limited's master list assembled over the last six years for distribution of *LABSPEC* and for use in Techmail, our scientific direct-mail marketing business.

How this works is that every laboratory or individual whose work is associated with the industry focus of a particular issue will receive a complimentary copy of that issue, regardless of whether they have had any contact with *Chemistry in New Zealand* or the NZIC before. The printing costs, mailing costs and all other costs relating to these promotional copies are covered by Ancat Holdings Limited.

The distribution duplications arise because a number of NZIC members are also on Ancat Holdings Limited's list. This means that when we run an industry focus covering their field of work, they will receive two separate copies - one from the NZIC, one from *Chemistry in New Zealand*. An example would be with the food and dairy industry focuses where a number of the staff of New Zealand Dairy Research Institute who are NZIC members should receive two copies of these issues.

Generating advertising sales and maintaining them and ensuring the future of *Chemistry in New Zealand* or indeed any publication is a numbers game - it's all about circulation. Our circulation varies between 2100 and 2400 copies, depending on the industry focus. This is significantly higher than any other similar competitive commercial science publication in New Zealand. As a comparison, *Chemistry in Australia* has a circulation of around 8000 copies, only 3.5 times that of *Chemistry in New Zealand*, but RACI has some 9500 members (10 times that of the NZIC).

Sure, the (relatively few) duplications are an extra cost to us as publishers, but the Privacy Act (1993) prevents us from merging the NZIC's (smaller) membership list with our large mailing list to remove duplicates electronically. The cost in time/labour to remove them manually far outweighs the printing and postage costs. We are, however, working with the NZIC Secretariat to determine ways to minimise duplications.

My advice is, if you do receive two copies, do us all a favour (the NZIC, *Chemistry in New Zealand*, our advertisers and me!) and give the extra copy to a fellow chemist or scientist who doesn't get *Chemistry in New Zealand*, and let them see what they're missing!

NZIC members may be pleasantly surprised to learn that the 'extra' copies distributed through our marketing program regularly generate two or three enquiries per issue regarding membership of the NZIC.

Robert B Lyon
Managing Editor

COVER STORY

ELECTROCHEMICALLY REGENERATED ION SUPPRESSION (ERIS™) IMPROVES AND SIMPLIFIES SUPPRESSOR-BASED ION CHROMATOGRAPHY

Abstract

A new suppression technique called Electrochemically Regenerated Ion Suppression (ERIS™) is described (patent pending). A solid-phase chemical suppressor is regenerated via an electrochemical process for continuous, reagent-free operation. This technique provides the convenience and performance of self-regenerating membrane suppressors, with the improved reliability and durability of packed-bed suppressors.

Introduction

Suppressor-based conductivity detection is one of the most popular detection methods for low-level ion analysis. The suppressor improves the detection sensitivity by reducing the background conductivity of the eluant, while enhancing the analyte's signal. Table 1 summarizes the chemical reactions that take place in the suppressor.

Various suppressor devices have been used for ion chromatography. These include packed-bed suppressors and membrane-based suppressors. One main disadvantage of membrane-based suppressors is poor reliability. Rupture is likely when downstream back-pressure increases. Organic compounds present in the sample can irreversibly adsorb onto the membrane, reducing its suppression capacity, necessitating extensive cleaning or replacement. Membranes are typically replaced every three to twelve months depending on application conditions[1]. Packed-bed suppressors are more rugged and reliable [2].

Experimental

The ion chromatograph was an Alltech (Deerfield, IL, USA) Ion Chromatography System. It consists of the Alltech Model 526 HPLC Pump, Alltech ERIS 1000 Autosuppressor, Model 330 Column Heater, and Model 350 Conductivity Detector. Sample introduction was performed with the Model 570 Autosampler.

Anion separations were carried out using Alltech Anion HC (150 x 4.6 mm), and Sarasep ANI (250 x 4.6 mm) Anion Columns. Cation separation was carried out using the Alltech Universal Cation (100 x 4.6 mm) column. Anion and cation standards were prepared by diluting 1000 ppm Certified IC Standards (Alltech). All eluants were prepared using Alltech's EZ-LUTE® Buffer Concentrates. Deionized water was used for preparing all solutions.

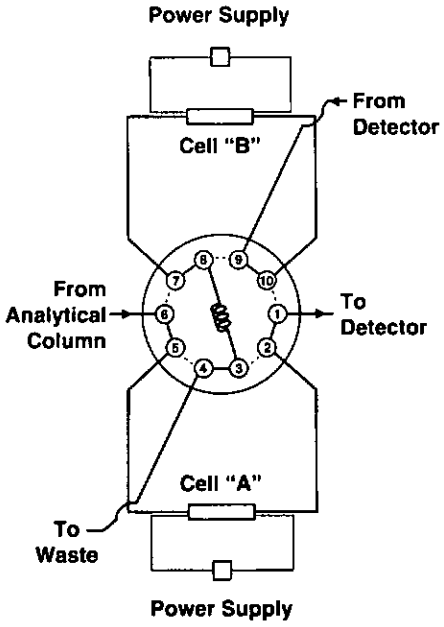
Results and Discussion

Alltech ERIS-1000 Autosuppressor

The Alltech ERIS 1000 Autosuppressor consists of a 10-port valve, two electrochemical cells packed with either cation (for anion analysis) or anion (for cation analysis) exchange resins, and a constant-current power supply. The 10-port valve is used to direct the eluant flow (*Figure 1*). The eluant from the analytical column flows through one cell at a time. While one cell is being used to suppress the column effluent, the detector effluent is recycled back through the second cell where electrochemical regeneration takes place.

Table 1: Chemical Reactions in Anion and Cation Suppressors

ANION SUPPRESSOR
Eluant: $NaOH + Resin\text{-}SO_3^-H^+ \rightarrow Resin\text{-}SO_3^-Na^+ + H_2O$ Analyte: $NaX + Resin\text{-}SO_3^-H^+ \rightarrow Resin\text{-}SO_3^-Na^+ + HX$ where X^- = anions (Cl^-, NO_2^-, Br^-, etc.)
In the suppressor, the eluants' background conductivity is reduced by converting them to a less conductive medium - water. Simultaneously, the analytes' conductivity is increased by converting them to a more conductive form - anions are converted into their acid forms; cations are converted into their hydroxide forms. These reactions result in higher signal-to-noise ratios, and significantly improving baseline stability and detection limits.
CATION SUPPRESSOR
Eluant: $HCl + Resin\text{-}NR_3^+OH^- \rightarrow Resin\text{-}NR_3^+Cl^- + H_2O$ Analyte: $MCl + Resin\text{-}NR_3^+OH^- \rightarrow Resin\text{-}NR_3^+Cl^- + MOH$ where M^+ = cations (Na^+, K^+, Mg^{2+}, etc.)



The valve switches between cell A and cell B at every injection. While one cell is being used to suppress the eluant, the other is being regenerated and equilibrated. This arrangement allows endless cycling between two electrochemical suppressor cells for continuous instrument operation without interruption or suppressor replacement.

Figure 1

Electrochemical Regeneration Process

The suppressor cells are equipped with two electrodes. The cation and anion exchange resins are sandwiched between these two electrodes. The detector effluent (typically water or carbonic acid) that is passed through the cell will undergo electolysis when current is applied across the cell. The electrolysis products regenerate the anion and cation suppressor cells.

Two electrolysis reactions take place at anode and cathode:

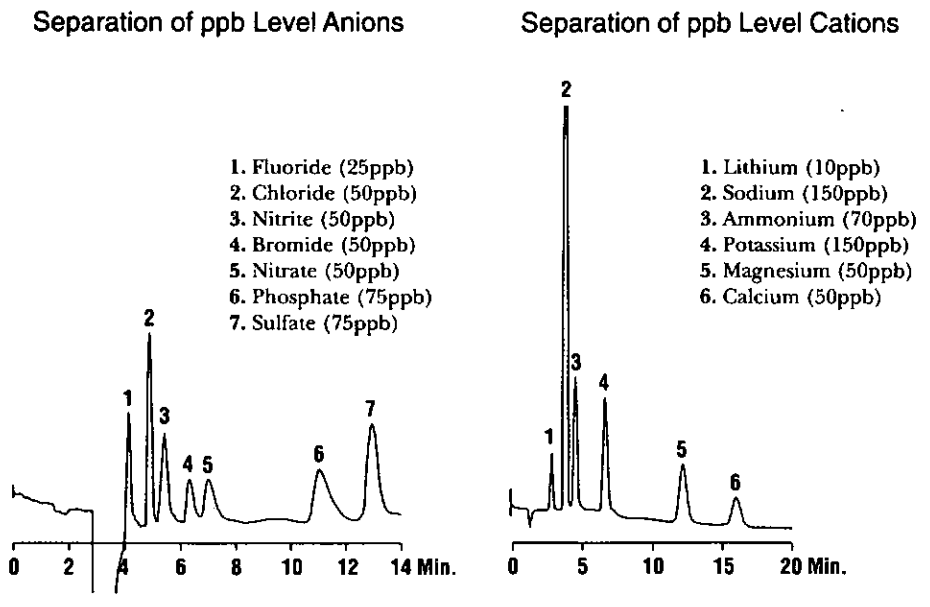
Anode:	$2H_2O \rightarrow 4H^+ + O_2 + 4e^-$
Cathode:	$2H_2O + 2e^- \rightarrow H_2 + 2OH^-$

For anion analysis, the anode is connected to the inlet side of the detector effluent. Hydrogen ions and oxygen gas are generated at the anode. Since the detector effluent is flowing from the anode side to the cathode side of the cell, the released hydrogen ions are carried by this flow across the sodium form resin (exhausted portion of the suppressor) converting it back to the hydrogen form by ion-exchange according to the following reactions:

$$Resin\text{-}SO_3^-Na^+ + H^+ \rightarrow Resin\text{-}SO_3^-H^+ + Na^+$$

The released oxygen gas, hydrogen gas, and sodium hydroxide are delivered to waste.

If the polarity of the cell is reversed and the cation exchange material is replaced with anion exchange material, the same configuration may be used as a cation suppressor.



Column: Sarasep ANI, 250 x 4.6 mm
Eluant: 1.7 mM $NaHCO_3$/1.8 mM Na_2CO_3
Flowrate: 1.0 mL/min
Detection: Suppressed Conductivity

Column: Universal Cation, 100 x 4.6 mm
Eluant: 3 mM Methane Sulfonic Acid
Flowrate: 1.0 mL/min
Detection: Suppressed Conductivity

Analyse ppb level anions and cations easily without preconcentration

Figure 2

Separation of Anions and Oxyhalides
(EPA Method 300.0, part B)

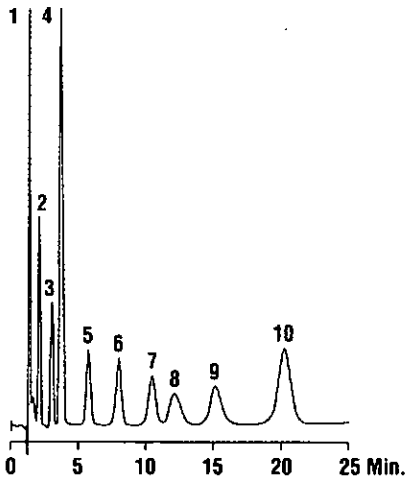


Figure 3: ERIS operates reliably with organic containing eluant

1. Fluoride (1 ppm)
2. Chlorite (5 ppm)
3. Bromate (5 ppm)
4. Chloride (2 ppm)
5. Nitrite (2 ppm)
6. Phosphate (3 ppm)
7. Bromide (2 ppm)
8. Chlorate (5 ppm)
9. Nitrate (2 ppm)
10. Sulphate (3 ppm)

Column: Anion HC, 150 x 4.6 mm
Eluant: 2.8 mM $NaHCO_3$/2.2 mM Na_2CO_3 in 10% methanol
Flowrate: 1.4 mL/min
Detection: Suppressed Conductivity

For fast visual verification of the suppressor operation, the resin used in the ERIS™ cell is coated with an inert dye. For anion analysis, the colour changes from gold to magenta as the hydrogen ions are being replaced by the sodium ions from the eluant. The colour change can be monitored easily through the transparent suppressor cell housing. For cation analysis, the colour changes from blue to beige as the hydroxide ions are being replaced by chloride (or methane sulfonate) ions from the eluant.

Applications

Figure 2 shows the separation of part-per-billion (ppb) level anions and cations using this system. Since the ERIS 1000 enhances detection sensitivity, ppb level anions and cations are easily analyzed. The detection limits for anions and cations are in the 1-30 ppb range and are comparable to the values reported in US EPA Method 33.0.[3]

This system meets the demanding US EPA requirements for monitoring inorganic anions in water per method 300.0. *Figure 3* shows the separation of the seven anions plus oxyhalides (EPA Method 300.0, part B) using an eluant containing 10% methanol. One disadvantage of the self-regenerating membrane suppressor is that it is not compatible with eluants containing organic solvents[4]. The Alltech ERIS 1000 Autosuppressor is compatible with organic containing eluants such as methanol and acetonitrile. ERIS 1000 is also compatible with gradient analysis.

The packed-column suppressor introduced originally by Small *et al*[5] suffered from several drawbacks such as retention time shifts, band broadening, and poor peak area reproducibility for the nitrite ions. These problems are eliminated with ERIS 1000. The dimensions of the ERIS 1000 suppressor cell are very small (7 x 7.5 mm and 14 x 7.4 mm), eliminating band broadening. Since the cell is always completely regenerated when an injection is made, no Donnann dialysis effect[6] occurs and reproducible retention times and peak areas are achieved from run to run.

Conclusion

This system provides the convenience and performance of self-regenerating membrane suppressors, with the improved reliability and durability of packed-bed suppressors. No regenerant reagents or pumps are required and no chemical waste (other than the detector effluent generated on any IC system) is generated. The device uses no fragile membranes and will tolerate high back-pressures for greater reliability than membrane-based devices. Since the regeneration is automatic, its operation does not require operator involvement. This is particularly important in applications requiring simple, unattended operation, such as monitoring ions in process control and quality control laboratories.

References

[1] Noble, D, *Anal. Chem.*, (1995), **67** (5): 205A
[2] Saari-Nordhaus, R and Anderson Jr., J M, (1994), *Am. Lab.* January:28C.
[3] Test Method 300.0. "Determination of Inorganic Anions by Ion Chromatography". U.S. EPA, August 1993.
[4] Rabin, S; Stillian, J; Barreto, V; Friedman, K and Toofan, M, (1993), *J. Chromatogr.*; **640**:97.
[5] Small, H; Stevens, T S; Bauman, W C, (1975), *Anal. Chem.*; **47**: 1801.
[6] Haddad, P R; Jackson, P E. Ion Chromatography Principles and Applications. Amsterdam: Elsevier, 1990: 262-3.

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LOCAL NEWS

A.i. SCIENTIFIC (NZ) MOVES TO LARGER OFFICE

Due to increased business demands, A.i. Scientific (NZ) has moved to larger premises and also has a new phone number. The new premises will enable a higher level of stock to be stored and provides a suitable area for pre-delivery checks and support activities.

Street address:	Unit A, 46 Constellation Drive Mairangi Bay Auckland
Postal address:	P O Box 35579 Browns Bay Auckland
New phone number:	(09) 478 1351
Fax remains unchanged:	(021) 788 940

TENDERING FOR PGSF RESEARCH

A corollary of the two-year cycle for the PGSF is a process for allocating funding in the off-year that is efficient and does not create a lot of overhead in the system. The Foundation's Board has decided to adopt a tendering process that will have the added advantage of enhancing the Foundation's ability to fulfill the goals of the Government's Statement of Science Priorities and to implement the Research Strategies.

The process will operate as an adjunct to the current mechanism of allocation via the Advisory Committees, who make funding recommendations to the Board. During the main two-yearly funding round, Advisory Committees will be asked to identify research gaps in the portfolio of applications available for funding in each Output. Research gaps may be areas for which there are no applications, or applications of insufficient merit or relevance. The Committees may also identify a gap when the work offered to the Foundation is not focused in a way likely to make real progress toward the research goals of an area, or where the proposal lacks appropriate collaboration or links with users. Once a gap is identified, funding will be held back for later allocation by tender.

Following the main PGSF allocation round, the research to be tendered will be specified further using Advisory Committee members or, where necessary, additional experts in the field or even a special review team. It will thus largely take place during the off-year of the two-year funding cycle.

Once research needs are specified, the Foundation will advertise for brief expressions of interest for each research gap, and will select only a few applicants for consideration of full proposals in each case.

ROLES OF AND INTERACTION BETWEEN MoRST AND FRST

(Reprinted from *SCI-TECH* 7(2) 1996, the newsletter of the Ministry of Research, Science and Technology)

Following recent apparent confusion in the science sector about the respective roles of the Ministry of Research, Science and Technology (MoRST) and the Foundation for Research, Science and Technology (FRST) and the interactions between the two agencies, it was decided to outline the respective roles in a recent Science Provider Forum hosted by MoRST.

The confusion is most evident at working scientist level, and much less so at management level. Confusion often leads to unreasonable expectations which can be frustrating to both MoRST and FRST.

A paper presented at the forum sets out a few simple benchmarks. Following are extracts of the paper prepared by Dr Basil Walker, Chief Executive of MoRST:

MoRST is a department and is therefore a part of the Crown. The department (through the Chief Executive) is directly and solely accountable to the Minister. MoRST has an advisory role primarily, but also acts on behalf of the Crown in supplying specified services. MoRST's core business is the provision of policy advice.

FRST is a statutory agency which is formally accountable to Parliament rather than to the Minister. However FRST is statutorily required to act in accordance with certain types of instructions issued by the Minister (priority statements, Ministerial instructions). FRST also has a contractual relationship with the Minister through the annual purchase agreement. FRST is an executive agency. Its core business is the allocation of science funding. However, it also has the function of providing independent policy advice.

It is stressed that MoRST's role is essentially advisory. The key executive agents in the system are:

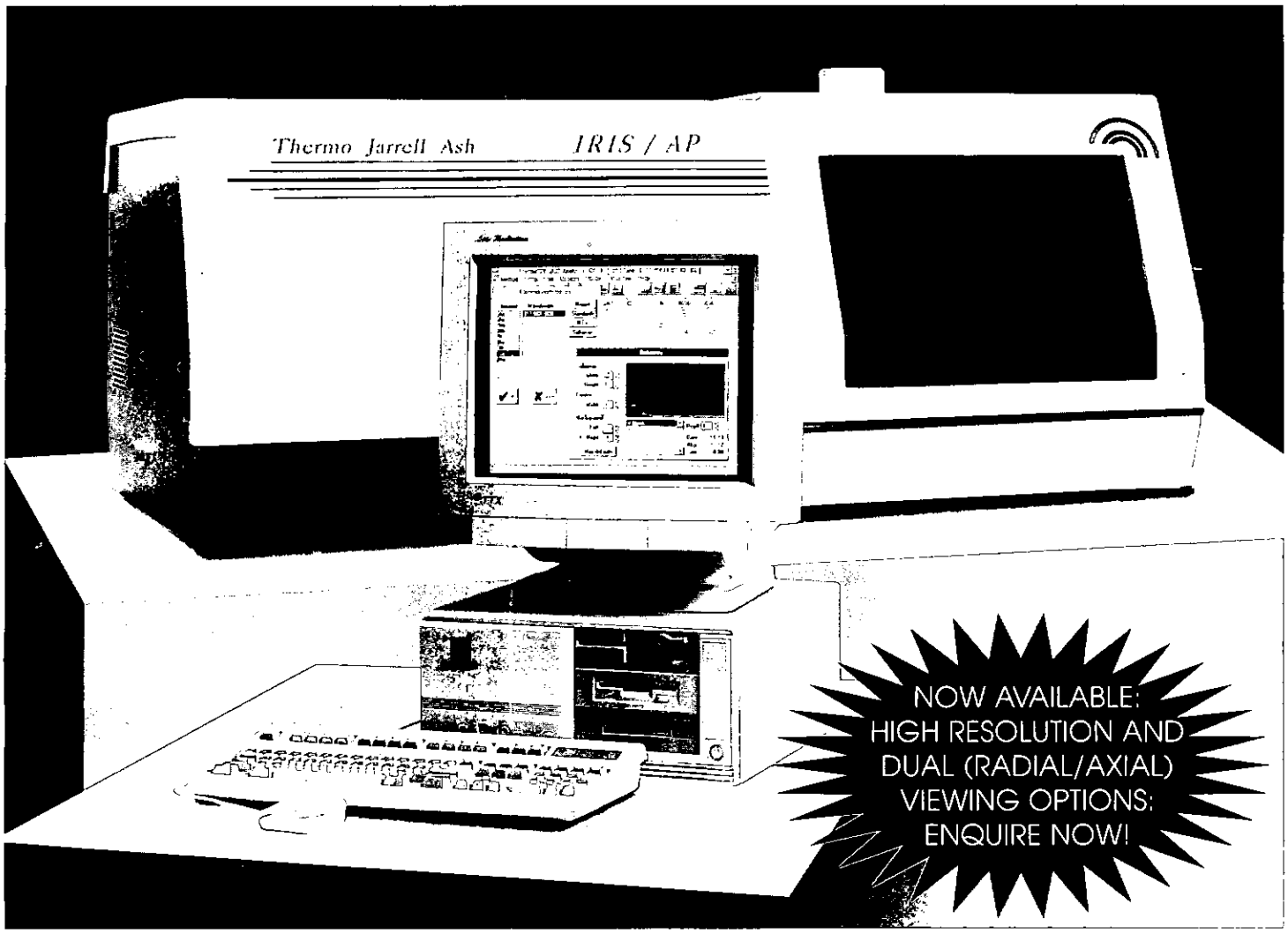
- The Minister (who determines policy and especially policy relating to the allocation of funding);

- FRST (which determines how and to whom funding should be allocated in accordance with policy, and manages resulting contracts).

A particular role of MoRST is that of monitoring purchase agencies such as FRST. However this function is carried out as an agent of the Minister. The current protocol in place is that MoRST's monitoring role is restricted to the critiquing of reports provided by FRST. The Minister decides what action if any should be taken in regard to the performance of FRST, having read both the reports and the critiques.

Some confusion is apparently caused by the fact that both FRST and MoRST have roles in the provision of policy advice.

Another Innovation from
Thermo Jarrell Ash ...



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However, the roles are quite distinct and should not be seen as an integrated continuum. Thus:

Policy advice is MoRST's core business; it is a peripheral function of FRST.

FRST's policy advice is supposed be independent - that can be taken to mean independent of the Government. But it is also supposed to take account of consultation with the communities with which FRST deals.

While in practice FRST and MoRST usually work closely together on policy projects (current work on technology policy is a good example) the two policy programmes remain distinct from each other. This is partly to preserve FRST's independence, but also reflects some conflict of interest with the monitoring role of MoRST. There are some obvious difficulties in too obviously "running with the hare and hunting with the hounds".

Interactions between MoRST and FRST are frequent and occur in both structured and *ad hoc* format.

1996 SCIENCE FAIR

The National Science Fair is to change its name and be held later in the year. The 1996 fair, which usually brings together the best of exhibits from regional fairs, is to be called the ECNZ National Science and Technology Fair. It will be held in early December in Christchurch. Richard Meylan, the Royal Society's Science Fair Manager, said that holding the national fair later in the year will give regions greater flexibility for timing of their own fairs, and will allow students to use investigations they may have carried out at school during the year. He said the introduction of technology into the name would celebrate the innovation of technologists as well as the research capabilities of scientists. It would also reflect the introduction of the new technology curriculum into schools. The fair is designed to be an entertaining and educational way of provoking a greater awareness of the impact of science and technology on our lives, both now and in the future. It will involve a wide range of activities for the general public as well as school programmes.

POWERFUL COMPUTER FOR AUCKLAND

A supercomputer, thought to be 10 times bigger than any other in New Zealand, is to be commissioned by the University of Auckland in May. The Silicon Graphics Power Challenge computer is about half way up the ratings list of the world's top 500 supercomputers. The computer cost less than $2 million and is about the size of two large fridges. Associate Professor Peter Hunter from the University's Department of Engineering Science says the computer is expected to provide significant benefits for New Zealand research. It will be able to process billions of computations per second and help scientific researchers who had been held back by the lack of access to high computational performance.

MARSDEN RESEARCH PROPOSALS

Over 600 preliminary research proposals from scientists have been received by the Marsden Fund, the Government's fund to support "blue skies" research, now administered by the Royal Society. This is some 400 fewer initial proposals than were received last year, the first year of the fund. In 1995 approximately 120 applicants were invited to submit full proposals. Invitations for submissions of full proposals were this year made in early April. Final announcement of successful proposals will be made in September. New funding for this year's round totals $5.5 million which is in addition to the multi-year funded grants made for 1995-96 of about $5.5 million. The Government has forecast spending on the fund will be lifted to $22 million in 1997-98.

NATIONAL SCIENCE AND TECHNOLOGY CERTIFICATE PROPOSED

Two national certificates, one in the sciences and one in the arts have been proposed as part of the national qualifications system to replace the Sixth Form Certificate. The proposed national certificate in science and technology and a national certificate in arts and humanities will each take two year's full-time study to complete. Qualifications Authority chief executive, Dr David Hood said the certificates would bridge the gap between school, employment and further training. School Certificate remains but it might move to the fourth form later. Bursary also stays. Seventh formers next year will do units towards one of the new national certificates as well as Bursary. Units towards the certificates will be a prerequisite for sitting Bursary exams. The Bursary will remain the main route to university but the national certificates will also act as entrance qualifications though the details of how that will work have not been finalised. The new certificates will be internally assessed. If students do not complete a certificate at school, they can continue at other educational institutions or credit the units to other polytechnic or training qualifications.

AUCKLAND UNIVERSITY ABANDONS OPEN ENTRY FOR SCIENCE

The University of Auckland is abandoning open entry for high school graduates and of its biggest degree courses, the sciences and the arts, to make way for more post-graduate students. The change, outlined in the university's new mission statement, means a school leaver with a bursary will no longer have automatic entry into a BA or BSc course. Within a few years the number of students in each faculty will be limited, on top of the present limits on numbers in each paper. The Vice-Chancellor, Professor Kit Carson, said the University of Auckland aimed to re-position itself at the "top of the market" by increasing the proportion of post-graduate students from 16 to 25% by early next century. He said the policy change would stop runaway growth in student numbers. Students who missed selection because of low marks would not be neglected. In Auckland there were now plenty of other degree courses to choose from. Arts and sciences are the last two faculties at the University of Auckland open to any student with bursary passes. Enrolment figures from 1994 show 7446 arts students and 4460 science students. The university roll is now about 25,000 students and could reach 30,000 by 2001 without restrictions.

MARSDEN FUND APPOINTS SIX GROUP PANELS

The Marsden Fund has appointed six specialist assessment panels to recommend research projects to the Marsden Fund committee for the 1996-97 funding round. The panels are all

chaired by Marsden Fund committee members, who are: Sir Ian Axford (chairperson), Professor Carolyn Burns (vice-chairperson), Dr Garth Carnaby, Professor Marston Conder, Dr Janet Davidson, Dr Margaret Lawton, Professor Bob Park, Professor George Petersen and Dr Roger Slack. The panels are:

Physical Science and Engineering: Dr Carnaby (Wool Research Organisation) chairperson; Sir Ian Axford; Professor Park (Engineering, University of Canterbury); Professor Petersen (Biochemistry, University of Otago); Professor Warren Roper (Chemistry, University of Auckland); Professor Paul Callaghan (Physics, Massey University).

Maths and Information Science: Professor Conder (Mathematics, University of Auckland) chairperson; Sir Ian Axford; Professor John Butcher (Mathematics, University of Auckland); Professor Rob Goldblatt (Mathematics, Victoria University); Professor Ian Witten (Mathematics and Computing, University of Waikato); Professor Brian Manly (Mathematics, University of Otago).

Social Sciences: Dr Davidson (Museum of New Zealand) chairperson; Professor Geoff White (Psychology, University of Otago); Professor Gary Hawke (Policy Studies, Victoria University); Professor Warren Moran (Dean of Arts, University of Auckland); Dr Robin Hooper (English, University of Auckland).

Agricultural and Life Sciences: Professor Burns (Zoology, University of Otago) chairperson; Dr Lawton (Manaaki Whenua-Landcare Research); Professor Petersen; Dr Slack (Crop and Food Research, Palmerston North); Dr David Penny (Plant Biology and Biotechnology, Massey University); Professor John Montgomery (Biological Sciences, University of Auckland); Dr Charles Daugherty (Biological Sciences, Victoria University), Dr Peter Wardle; Dr Tricia Harris (AgResearch).

Biochemical and Biomedical: Dr Lawton and Professor Petersen, joint chairpersons; Professor Christine Winterbourn (Pathology, Christchurch School of Medicine); Dr Geoffrey Krissansen (Molecular Medicine, University of Auckland); Professor David Lambert (Ecology, Massey University); Professor Sir John Scott (Medicine and Health Science, University of Auckland); Dr Peter Thorne (Medicine and Health Science, University of Auckland); Professor Bruce Baguley (Cancer Research, University of Auckland).

Earth Sciences and Astronomy: Professor Park, chairperson; Sir Ian Axford; Professor Cam Nelson (Earth Sciences, University of Waikato); Professor Vernon Squire (Mathematics, University of Otago); Dr John Haines (Institute of Geological and Nuclear Sciences, Wellington).

NEW MANAGER FOR FUND APPOINTED

Michael Prebble, a senior policy analyst with the Ministry for the Environment, has taken up a position with the Royal Society as the Manager of the Marsden Fund. Mr Prebble has a background in education, has five times visited the Antarctic, and was officer in charge of Scott Base in the winter of 1966 and in 1979-80. He is a graduate of Victoria University with a degree in physical geography. Mr Prebble first went to the Antarctic in 1960 as a field assistant. After carrying out studies on the cavernous weathering of rock in the Dry Valleys he went to Cambridge University, to the Scott Polar Research Institute in 1968-69 to write up this work. Mr Prebble became a secondary school teacher and taught at Nelson College between 1974 and 1987. There he was head of outdoor education, senior master and deputy principal. In 1988 he took a position with the Department of Education as officer in charge of environmental and outdoor education. He joined the Ministry for the Environment in 1990. Among a number of tasks he undertook as senior policy analyst were the reform of hazardous substances and new organisms legislation and climate change work. He was also coordinator for the ministry's research needs for policy advice. Mr Prebble says the Marsden Fund is an exciting development, providing an avenue of funding to develop excellence in both research and in research skills.

POLYTECH PLAN FOR NEW ZEALAND UNIVERSITY OF TECHNOLOGY

Moves by some polytechnics to become universities have led the President of the Association of Polytechnics, John Scott, to propose the establishment of a New Zealand University of Technology. The new body would be an umbrella for most of New Zealand's polytechnics. Each would offer the degree courses it chose, to be conferred by the combined university. The courses would be up to doctorate level. Mr Scott, the director of the Christchurch Polytechnic, told his polytechnic council recently that the concept of the new university had received strong support. The idea had come from a meeting of polytechnic directors and council chairpersons late last year. Smaller polytechnics had become "agitated" about the prospect of bigger ones becoming universities. They feared a domino effect resulting in them being seen as inferior. They foresaw the country asking why polytechnics were needed. "The sector is in significant turmoil," Mr Scott said. The international market demanded university qualifications. Mr Scott had drawn up a proposal for the new system and sent it to all 25 polytechnics. Of the 22 which had responded, 19 had given the proposal their full support. The Auckland Institute of Technology had decided to apply on its own for university standing, though it supported the combined university concept for other polytechnics.

* * * * *

INFRARED MICROSCOPY - A FORENSIC SCIENTIST'S VIEW

Harry van Enckevort, ESR:Forensic, P O Box 30-547, Lower Hutt

Introduction

Scientific analysis for criminal investigations is provided in New Zealand for the New Zealand Police by The Institute of Environmental Science and Research Ltd (ESR). ESR:Forensic provides analytical functions in forensic biology (the examination of body fluids and DNA), controlled substances (typically illicit drugs and pharmaceuticals), toxicology, and criminalistics (physical evidence such as glass, paints and fibres).

Forensic scientists examine items to determine whether or not a link exists between a suspect and a crime. The variety of items examined is limitless and they range in size from large to very small.

For the criminalist, the examinations may involve direct comparisons but typically also involve the identification of materials. Identification can be very important in helping the scientist come to an assessment of the value of evidence and in answering questions such as "How common is this material or item in the community?" and "How does the material behave while an offence is being committed and after the crime?"

Simple visual observations provide a wealth of information for the forensic scientist. If the use of only a single instrument was permitted to assist in analyses, that instrument must be the microscope. Chemical analyses are also invaluable and infrared (IR) spectroscopy is a powerful technique for the chemical characterisation, identification and comparison of materials. If a criminalist could choose a second instrument, the choice must be the IR microscope.

These two instruments together provide the forensic scientist with information on visual and physical attributes, as well as chemical information on microscopic sized particles. Samples as small as those with micrometre diameters and picogram weights can be examined and analysed.

It is my intention in this article to describe IR microscopes, their scope, limitations and some practical aspects, particularly those that relate to forensic science. I will begin with an introduction to IR spectroscopy and the developments in this field that lead to the introduction of practical IR microscopes. IR spectroscopy is described in many standard analytical texts and it is not my intention to describe the technique in detail.

IR Spectroscopy

IR spectroscopy describes the interaction between matter and infrared radiation. IR spectrometers characterise the absorption and transmission of IR radiation by the material under analysis. The spectrum obtained contains a great deal of diagnostic information which can be used to characterise chemical structure. There is much literature in which the frequencies at which particular groups of atoms absorb IR radiation is reported. Also, handbooks which report the spectra of numerous materials and chemicals have also been published.

The detail present in a spectrum can be interpreted to provide direct evidence of the functional groups and nature of the compound(s) present. Detail which is absent can also be used as this allows the elimination of some compounds. It is also possible to make comparisons with standard or reference spectra to determine identity.

IR spectra are often described as "chemical fingerprints" but this is not a good analogy in forensic science. Spectra are not necessarily unique to a particular material. For example, the spectra of members of the same class of compounds, or polymers which vary only in length of the monomer chain, can have very little difference between them. Sample preparation can also affect the spectrum obtained.

Other limitations include sensitivity and problems associated with the analysis of mixtures. Some classes of compounds provide only limited information. Ionic salts, for example, may not give any absorption in the frequency range investigated. But this observation has then immediately eliminated millions of compounds. IR is not always sensitive to minor components in mixtures. The concentration of a particular component might vary anywhere from 5% - 30% before it is registered in the spectrum.

Also, forensic scientists frequently only have small and limited amounts of material to work with. Small amounts of material typically result in a small response from the traditional dispersive IR spectrometers and very sensitive instruments are required.

Over time, a wide variety of sample preparation techniques and instrument modifications or accessories have been developed for use with dispersive IR spectrometers, particularly for small and otherwise intractable samples. Accessories and modifications for dispersive instruments included, for example, beam condensers, high pressure diamond anvil cells, and specular reflectance, multiple internal reflectance and attenuated total reflection accessories.

Even so, many of these accessories were difficult to use and their usefulness in forensic science doubtful. For example, small samples might be dealt with by combining a number of particles for analysis and forming micro discs, or solvent casting or pressing to form films which occupy a greater area of the IR beam. To combine samples, however, makes an assumption that they are identical. Casting and pressing can modify sample structure and the sample might be more fragile than before any preparation.

Small samples could also be dealt with by mounting over very small pinholes and then brought into the focus of a beam condenser. This was a time consuming process, benefiting greatly from skilful operators, and hopefully not resulting in the loss of the evidence!

IR microscopes were produced by Perkin-Elmer in the early 1950s but did not inspire the world of IR spectroscopy. The lengthy time taken to accumulate spectra on dispersive instruments remained a disincentive to their use. Filter-type IR spectrometers allowed shorter measurement times but the technique still did not attain a large following.

The introduction of Fourier Transform Infrared (FTIR) instrumentation in the late 1970s was a major leap forward in IR technology. Fourier transform instruments allowed more simple sample preparation and presentation methods to be used and many of the accessories available for dispersive instruments became redundant. They led to a general resurgence in the use of IR techniques.

More importantly for the forensic scientist, FTIR instrumentation was a major advance for IR microscopy. Very small samples could be analysed on a "what you see is what you get" basis. If a sample could be seen under the ordinary bench microscope, a spectrum could be obtained. The minimum sample size tended to be limited only by what could be handled. Preparation and presentation techniques were simplified still further.

I do not intend to compare the workings of fourier transform instruments with dispersive spectrometers in any detail but will provide a brief comment. I will also provide a brief description of the workings of an IR microscope.

FTIR Spectroscopy

Dispersive instruments measure the interaction between the sample at specific frequencies of IR radiation, one at a time and record this directly.

Fourier transform instruments examine the whole spectrum at once as a multiplex signal. After mathematical analysis, the spectrum, in the form that we are familiar with, is produced. They provide higher frequency precision, photometric accuracy, radiation throughput and signal-to-noise ratios. And all in a few seconds! The fast measuring time allows kinetic data to be obtained on changing samples and "on-the-fly" sampling in combined techniques with gas chromatography (GC-FTIR) and pyrolysis gas chromatography (PGC-FTIR).

An FTIR spectrometer might be simply described as an IR optical box connected to a computer producing digitised spectra. The better signal-to-noise ratio is simply provided by scanning the sample repeatedly and averaging the response. The digitising of spectra also allows the production of many applications programs for spectral manipulation, enhancement, storage, plotting, comparisons and library building. High speed computers and digitised databases and reference libraries make spectral searching very easy.

Although there are difficulties associated with data manipulation in forensic areas, such an approach can be useful for spectral library searching. The recent development of validated software that tracks and records any manipulation may help counter courtroom accusations of deception.

There are now many different spectral libraries available to the chemist and forensic scientist. These include those of gases and vapours, inorganic materials, pollutants, solvents, pharmaceuticals, commonly abused drugs and polymers, plasticisers, adhesives, paints and other materials which might be related to crime laboratories.

IR Microscopes

Schematic representations of the optical and IR pathways of an IR microscope are presented in Figure 1. Moving mirrors allow optical examination and setup of the sample, and then IR analysis. Many models also allow the collection of spectra in transmission and reflection modes.

Metallic reflecting optics, called Cassegrainian objectives, are used, as lenses made of glass are IR absorbing, and alkali halides are hygroscopic. Also, IR radiation refracts more than white light when it passes through a lens. These objectives allow a sample to be brought into focus by eye and also be in focus to the spectrometer.

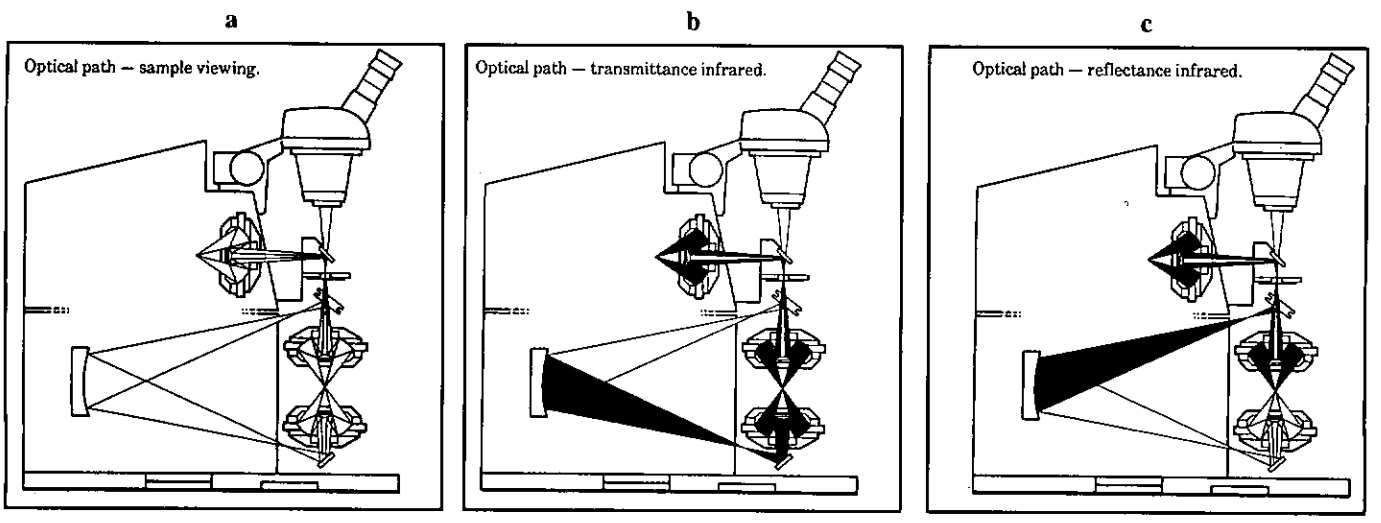

Figure 1: Schematic representations of the optical pathways through an infrared microscope: (a) Sample viewing; (b) Transmission; (c) Reflectance. (Reprinted courtesy of Perkin-Elmer.)

The detector is very close to the sample and this provides higher sensitivity. It also allows the size of the detector to be matched to the optics and the field of view of the microscope. As the IR beam is comparable in size to the detector element, it is less likely to pick up excess noise such as can occur with a large detector and poorly positioned beam condenser.

High sensitivity mercury cadmium telluride (MCT) detectors are used, rather than triglycine sulfate (TGS) detectors. They have a faster response and are some 40x more sensitive. They are also operated at liquid nitrogen temperatures and therefore provide less electronic and thermal noise.

The essentials of an IR microscope are an eyepiece to view the sample, a moveable stage so that the area of interest in a sample can be examined, and a mask to define the specific area of analysis. The mask may be of fixed aperture size, for example a circular pin hole, or it may be an adjustable iris or slit with four, independently operated, knife-edge blades.

The IR microscope is the ultimate beam condenser. It still allows large amounts of radiation to be presented to the sample, even when reduced by the optics of the microscope and the sample mask. Higher magnifications than could be obtained with the traditional beam condenser can therefore be used and sample alignment with the IR beam and detector is easily established. The optical microscope used to view samples can have fixed or variable magnification but this does not affect the IR throughput.

The FTIR microscope instrument is a single beam instrument and a spectrum of the material to be analysed is obtained in the same manner as for any single beam instrument. Initially, a sample is set up for analysis under the microscope. A background spectrum is obtained under the conditions to be used for analysis of the sample. The spectrum for the sample is then measured and the background and sample spectra ratioed to obtain the spectrum for the sample alone. Should repositioning of the sample stage and realignment of the sample be a particular problem after accumulation of the background spectrum, software facilities can allow the sample spectrum to be obtained first and then corrected for background.

Sample preparation is generally simple and a stereo zoom microscope and steady hand provide highly effective, general purpose tools for many different types of materials.

Sample preparation is important for IR microscopy, however, as a number of factors can affect spectra significantly. The conditions under which spectra are obtained are also important. Peak absorbancies can otherwise be distorted and any attempts at quantitation or comparisons on the basis of peak absorbance made meaningless. It could be possible to determine samples were indistinguishable when in fact they had different chemical compositions; or, to conclude they were different when in fact they cannot be distinguished by IR spectroscopy. False exclusions and matches are always to be avoided in forensic science.

The majority of the interactions of IR with materials result in a collection of narrow, smooth, bell-shaped curves originating from a flat baseline. Deviations from this may or may not be artefacts and spectral appraisal is an important skill in the IR spectroscopist's repertoire.

I will therefore describe some of factors that should be considered in sample preparation and analysis in IR microscopy. Some of these are common to any area of IR spectroscopy, others more peculiar to IR microscopy.

Factors Affecting IR Spectra

Sample thickness, or concentration effects are problems in any area of IR spectroscopy. Thick samples absorb too much radiation and give rise to distorted peaks which are broad, blunt or flat-topped. Samples that are too thin give spectra which show little sample response, or are noisy.

If a sample is too thick, it may be possible to reduce its size. If the sample is too thin, spectra can be improved by decreasing the resolution and/or increasing the number of scans.

Decreasing the instrument resolution by half, for example from 4 cm^{-1} to 8 cm^{-1}, increases the signal-to-noise ratio by a factor of 2. Increasing the number of scans is a simple matter with fourier transform spectrometers. For example, in the typical 10 minute scan time of a dispersive spectrometer, it is possible through the microscope and MCT detector to accumulate about 1000 scans. However, the signal-to-noise ratio is proportional to the square root of the number of spectra and accumulating more and more spectra becomes a problem of diminishing return.

Sloping baselines are also commonly encountered in IR spectroscopy. This might be caused, for example, by coarse or granular particles and particles which are IR opaque or reflecting and therefore scatter the IR beam. A mathematical correction may be available in IR software for baseline correction and the correction of peak intensity errors caused by scattering. Although altering the nature of the spectrum, this can assist in database searches in the first instance.

For forensic scientists, scattering can be a particular problem with some rubber, paint and fibre samples, where these contain high proportions of filler, metallic particles, pigment or delustrant. With the IR microscope, however, it can be possible to analyse areas in some samples, for example metallic paints, where there are comparatively few or no metallic flakes.

And for some heavily filled polymers, even as small samples, it is possible by the careful application of heat to initiate pyrolysis of the sample and condense pyrolysate material on a cool surface. The condensate can then be sampled and readily analysed to identify the type of polymer used.

Interference effects are also well known to the IR spectroscopist. This phenomenon becomes apparent whenever radiation travels through thin uniform films, and is seen to the eye in such examples as the rainbow colours in oil films. In IR spectra it produces a uniform pattern of small peaks as a sinusoidal modulation in the spectrum.

Interference patterns can occur when the sample itself is a thin film, or the IR beam travels through the air space between two IR windows which are to be used to hold a sample for analysis. In this latter case, background spectra obtained by using a small amount of KBr between the windows, or using only one of the windows, also alleviates the problem.

Detector saturation is possible with IR microscopes. Although the field of view in the microscope is small, the sample can still be much smaller. This allows high radiation levels and stray radiation to reach the detector unless masks are used.

Sample masks are also used to define the area to be analysed, particularly in samples such as paint flakes with multiple layers and composite plastics, or where a smaller area of a larger sample is to be analysed.

Diffraction effects occur when radiation passes an edge or through a mask such as a slit or aperture. Diffraction dilutes the intensity of the absorption bands and can allow the inclusion of radiation from neighbouring areas of a sample.

Variations in sample thickness, irregular surfaces and geometric shapes can also be a problem to the IR microscopist. The sample and any support can act as a lens and irregularly shaped samples can cause significant amounts of scattering. Parallel upper and lower faces are desirable.

Diagrammatic representations of these effects are shown in Figure 2. Defocussing and aberration of the IR beam by the sample and support can be compensated for by the controls available on the microscope itself.

Diffraction effects can also be minimised. Diffraction is a function of frequency, and high frequencies (shorter wavelengths) are diffracted less. In our view of the world in visible light, diffraction effects are very small and our eyes are not able to resolve the blurring. In IR microscopy, diffraction effects can be problematic in the analysis of very small samples. This is most noticeable when the wavelength of the IR approaches the dimensions of the sample or slit.

Diffraction effects can also mean that the IR radiation passing through the area of interest is diluted by radiation from neighbouring areas of a sample or passing by the sample. Increasing the surface area of very small samples, by pressing or flattening, and limiting the slit size to a maximum of about 70% of the width of the sample are useful techniques in this respect. In this case, high quality spectra to approximately 1000 cm^{-1} can be obtained if the sample size is limited to a minimum of some 15 mm.

As the slit size increases, diffraction becomes less of a problem. The running of background spectra helps cancel out diffraction effects and multiple apertures, one before and one after the sample, can be useful. However, extraneous spectral contributions from adjacent material have been known to occur from as far away as 40 mm from the aperture edge, even when double apertures are used.

Consistency of preparation is important, particularly when comparing samples whose IR spectra show characteristics that reflect secondary structure such as crystallinity or molecular orientation effects. The effective use of computerised libraries to assist in identification is also assisted by consistent sample preparation techniques.

The importance of secondary structure is common in some areas of polymer identification and discrimination, for example in the identification of nylon. Both nylon 6 and nylon 6.6 are commonly encountered as plastic films, threads and fibres. In preparation for analysis, the over-zealous flattening of a nylon sample can destroy the feature which would otherwise allow them to be distinguished easily by IR spectroscopy. Spectra of nylon 6 and nylon 6.6 fibres are shown in Figure 3.

Contaminants can be accentuated in spectra. They may either be present on or in sample supports, or within the sample itself. Their presence may be the object interest, for example in the analysis of inclusions in paints, plastics and papers, and an IR microscope is particularly useful in their analysis. However, I can recall an excellent spectrum of a cellulose fibre in my early days of IR microscopy when a spectrum of some very small particles embedded in KBr was intended!

Despite the pitfalls which might befall the IR spectroscopist and IR microscope user, IR microscopes offer unparalleled sample handling convenience. Films, powders, liquids can all be analysed in transmission and produce excellent spectra with minimal sample preparation. Some microscopes also offer analyses by reflectance techniques.

Spectra obtained by transmission are favoured for ease of interpretation, better reproducibility, fewer spectral artefacts and more accurate library searches. The majority of samples

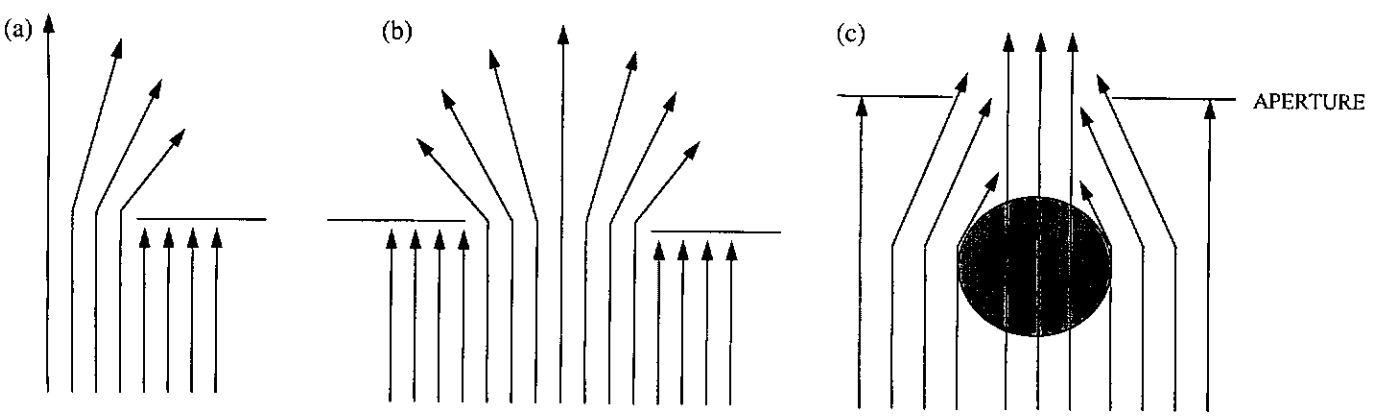

***Figure 2**: Diagrammatic representations of diffraction patterns that can occur as IR radiation passes: (a) an edge; (b) through an aperture; (c) past a sample.*

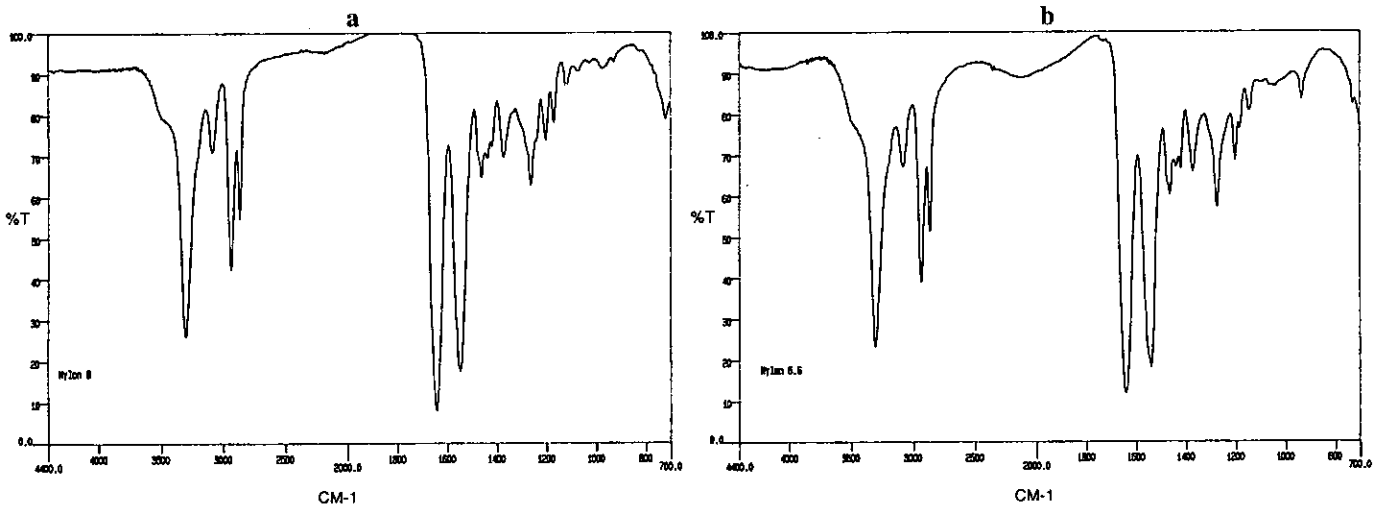

Figure 3: Spectra of: (a) nylon 6; and, (b) nylon 6.6, obtained by miniature diamond cell.

encountered can be handled and prepared for transmission spectroscopy. However, microreflectance techniques offer the opportunity for analyses which provide information or identification with even less effort.

Some of the commonly used techniques in sample preparation for IR microscopy are as follows. Whereas few accessories might be used, examples of imaginative sampling techniques always appear to be in evidence in IR spectroscopy.

Sampling Techniques, Sample Preparation and Sample Presentation

Transmission

Powders, thin films and liquid samples can all be presented for transmission. Materials that appear quite hard on the macro scale can be quite ductile or malleable on the micro scale. Thin slices of solid materials can be cut with a scalpel or microtome and the hardest substances scored to produce a powder. There is therefore much that can be done with a steady hand and a scalpel.

Sufficiently "large" samples can be suspended across a conveniently sized aperture for presentation to the microscope. Small particles can be laid down on IR windows such as 13 mm diameter KBr plates. They can also, with a little more effort, be embedded directly in KBr using the IR press. This latter technique has the advantage that it can provide an easier handle on a particle, facilitate archival and still allow easy recovery of the particle if required.

For transmission spectroscopy, sample thicknesses of 2 mm - 5 mm are preferred. Solid samples generally require flattening by pressing or rolling. This can be achieved by using a roller ball, a diamond anvil cell (DAC), a press, or even the end of a probe.

The DAC provides a means of flattening samples as well as maintaining compression on elastic materials and particularly elastomers. There are two types of DAC - the high pressure and the low pressure cell. The low pressure cell is also known as the miniature diamond (anvil) cell as it uses thinner diamonds.

Diamond absorbs IR radiation in the 2400 cm^{-1} - 1800 cm^{-1} range. However, the diamonds of the miniature DACs are sufficiently thin so differentiation of compounds on the basis of nitrile and isocyanate groups, which show absorption in this frequency range, is still possible. The thinner diamonds absorb less radiation and, with the improved signal-to-noise ratios available on FTIR spectrometers, can still distinguish between, for example, polystyrene and acrylonitrile-butadiene-styrene polymers or between different acrylic fibres.

Although the DAC can be used to apply and maintain compression on the sample, it can also be used without pressure. Samples can be presented to the microscope between both halves of the cell, or presented sitting on the face of one of the diamonds. This makes the sample easier to view and set up, suffers from half the attenuation, and minimises optical interference.

The diamond anvils in the miniature diamond cell are of different sizes to facilitate alignment, the smaller being about 0.5 mm - 1 mm diameter. This size therefore becomes the effective aperture of the cell.

Liquid samples can be applied as very small droplets on the surface of KBr windows or discs or to a diamond face in the DAC. If retention or spreading of the sample becomes a problem, the liquid can be placed in small wells made in the surface of a KBr plate, or, after scratching the surface, be absorbed into the powdered area.

The simplicity of use and versatility of the miniature diamond cell means it has become the method of choice in our laboratory for sample flattening and sample presentation to the microscope. Locating samples on or in a 13 mm diameter IR window at high magnifications can be difficult, particularly for liquids or samples which do not contrast with the background!

And although the electrostatic charge build up on a DAC can be devastating for the forensic scientist, this is easily discharged using carbon fibre brushes of the type used for LP records.

Reflectance

Three types of reflectance techniques are available for use with the IR microscope. These are specular, diffuse and reflection-absorption reflectance.

Specular reflectance occurs off smooth, glossy surfaces which are optically flat; diffuse reflectance off coarse, grainy textured

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materials with good scattering properties; and, reflection-absorption when the IR radiation passes through a thin film on an IR reflecting surface and is then reflected back through the film. These are illustrated schematically in Figure 4.

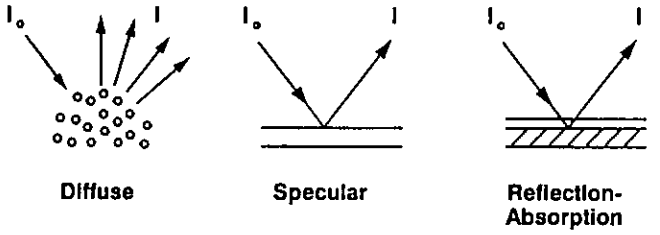

Figure 4: Types of reflectance measurements available with IR microscopes. (Reprinted courtesy of Perkin-Elmer.)

Raw specular reflection spectra show absorption bands that are inverted and distorted compared with transmission spectra. This occurs because of the rapid change in refractive index which causes bands to take on a derivative shape. This can be corrected with the Kramers-Kronig (K-K) transformation to produce a spectrum of 'normal' appearance. The K-K transformation does not always produce a fully transformed spectrum because of dispersion and diffuse reflectance effects due to the refractive index changes.

With diffuse reflection, the IR radiation does not necessarily follow the simple laws of reflection - the angle of reflection does not always equal the angle of incidence. Consequently, there are also inherent differences between transmission and diffuse reflectance spectra. These include the intensification of weaker bands and frequency shifts. These effects are predicted by Kubelka-Monk theory. The Kubelka-Monk correction is applied to diffuse reflection data to produce transmission-like spectra.

In practice, surfaces often do not show pure specular or pure diffuse reflections. Also, reflection spectra may have contributions from underlying material as the IR radiation penetrates the surface to a distance comparable to its wavelength. These factors combine to give spectra which are often more difficult to interpret than transmission spectra.

Techniques are available to reduce these effects. For example, a surface showing some specular reflection can be scuffed using silicon carbide paper to improve the diffuse reflectance. If 1200 grit paper is used, the material retained on the paper can itself be analysed *in situ* by diffuse reflectance.

Powders can be analysed by diffuse reflectance after containment in suitable sample cups, by placement on KBr disc or sprinkled on a mirror. Dilution of the sample by powdered KBr assists in removing the any specular reflection component from the sample. Suitable sample cups are easily made, for example, by lining a small depression such as the cap of a vial with aluminium foil.

Reflection-absorption generally provides better spectra and these also correlate well with transmission spectra. It is a useful technique if the sample is not too opaque or thick.

Although reflectance spectroscopy offers opportunities for analysis with minimal or no sample preparation, it is used with caution in forensic science. There is an ever-present possibility that alternative reflection modes may complicate data and make interpretations and comparisons suspect. It remains a useful technique in the IR microscopists and forensic scientists repertoire, however. It can provide analyses of some types of coatings, surface treatments, contaminants, oxidation layers etc., where a sample might otherwise not be obtainable for examination in transmission.

Attenuated total reflectance (ATR) objectives for IR microscopes have recently been developed and are now available with some instruments. ATR is based on the total reflection of radiation in an internal reflection element. The objective is placed down on the surface of the sample in intimate physical contact, and a spectrum obtained from areas of 100 mm^2 or larger. The ATR objective is not useful for samples which are porous as it is not possible to form an intimate contact. It is also not useful with materials which have a refractive index higher than the internal reflection crystal within the objective itself.

Initial evaluations of the ATR objective show it to be an extremely useful and important approach to the forensic examination of some types of physical evidence. It will be of particular value for IR opaque materials and those where secondary structure and molecular orientation effects which might be altered by sample preparation techniques are important. Additional evaluations are being undertaken to determine the evidential value of the spectra obtained from some materials.

The potential of IR microscopy should now be evident. Clearly, the ease of use of IR microscopes makes almost any sample that could be analysed by IR more easily examined by IR microscopy. The problem tends not to be that the sample is too small, rather that it is too big.

My commentary so far has only made fleeting reference to particular applications in forensic science. There have been many applications of IR microscopy demonstrated by forensic scientists. The criminalist, in particular, encounters an endless variety of materials which can have evidential value. I will describe some of those that are more commonly encountered in our laboratory and with which we have greatest experience.

Common Applications of IR Microscopy in Forensic Science

Polymers

Synthetic polymers are ubiquitous in our environment and commonly encountered at crime scenes or in crime samples. Fibres, paints, plastics, foams, rubbers and adhesive tapes are typical samples that require examinations, comparisons and identification. They are encountered in traffic accidents, robberies, thefts, assaults, homicides, kidnappings, explosions etc.

Fibres

There are many types of fibre, for example nylons, polyesters, acrylics, acetates and viscoses. Some could originally be characterised to a high degree of certainty by light microscopy on the basis of physical appearance and birefringence. Advances in fibre technology have ensured that this is no longer so.

In particular, many fibre types have a number of different subclasses. And preliminary investigations show there can also be differences in secondary structure between fibres which are otherwise indistinguishable. To ignore these differences not only opens the possibility of false matches but also underestimates the value of any evidence. Acrylic and polyester fibres are particularly notable in this respect.

IR spectroscopy readily distinguishes and identifies the different classes, and can also distinguish between many of the fibres within a particular subclass. In some cases it appears to be possible to distinguish between the manufacturers of different fibres of the same subclass.

IR microscopy allows single fibre analyses and virtually all types of fibre can be analysed. Although some flattening of a very small length of the fibre is typically required, the technique is essentially nondestructive. The fibre may be retained for archival or other analyses such as instrumental colour comparisons and dye extractions.

A number of fibres are produced as side-by-side or sheath-and-core bicomponent structures. The microscope allows the analysis of individual lobes. In the case of the sheath-and-core structure, the sheath can be analysed by sampling near the edge after a fibre has been flattened. The core can be identified by sampling at the centre and subtracting the spectrum of the sheath material.

With fabrics where the fibres are bonded to a surface, rather than knitted or woven, it is possible to obtain spectra of the adhesive *in situ* on the fibre. Similarly, the pigment dyes on fabrics which have a printed pattern can also be sampled *in situ* on a fibre.

Paints

Paints and other surface coatings are a common item in forensic investigations. The modern paint industry uses many of the organic polymers introduced in past years, and there are now many different types of paint. Examples include alkyds, acrylics, PVAs, epoxies, urethanes and the various modifications. Paints are found on all vehicles and buildings, typically in multiple layers, and are also encountered on other property.

Generally, colour, layer sequence, and texture provide information of high evidential value in determining whether or not paint samples have a common origin. This is particularly true for those samples comprising multiple layers and which provide evidence of reprintings or repairs. However, paint samples which have only one or a few layers are also commonly encountered. Information on the chemical composition of these samples provides greater discrimination and higher evidential value when apparent matches are found.

IR spectroscopy can provide information on the polymers and inorganic materials such as pigments and extenders used in the formulations. It is a powerful technique for the generic typing and comparison of paints.

With IR microscopy, it is now possible for even small samples to combine information on the organic components with that of the inorganic components (which was obtained by energy dispersive X-ray analysis in a scanning electron microscope).

The individual layers in a multi-layered sample can be examined by producing a thin cross section, either by hand or microtoming. If the layers are particularly thin, oblique sectioning effectively increases the width of the layers. The individual aerosols produced during the use of spray paints, typically less than 40 μm diameter, are also readily analysed.

IR is less useful for determining subtle differences in the polymers of non-transparent paints than is the case for fibres. In the composite spectrum of a paint, subtle differences in the polymers, film modifiers, plasticisers and other ingredients used can be masked.

Clear, acrylic top coats which do not suffer from the IR masking effects of inorganic materials are often used on the paintwork of vehicles. Differentiation by the specific acrylic polymer used is possible, as noted for fibres, and this can be extended to the identification of the aromatics and other modifiers/plasticisers used.

There is a greater diversity in the polymer binders of other automobile and architectural paints, as well as material of evidential value that can be obtained from the various pigments and extenders used.

Thin coatings on metal substrates can be examined directly on the metal using reflection-absorption techniques.

Other Polymers

Plastics, rubbers, tapes and adhesives are also common forensic samples. Their analysis is similar to that described for fibres and paints in many respects and it is possible to discriminate different low density polyethylene plastics, cling films, shoe soles, insulation, plastic glitters used in cosmetics and hair gels and automobile plastics.

Plastic and rubber samples are particularly of interest in hit-and-run accidents. Automobile manufacturers place increasing emphasis on polymeric components for weight reduction and non-corroding parts. The techniques of analysis of plastics are conducted along similar lines to those mentioned for fibres and paints. With IR microscopy it is now possible to analyse the very small fragments and smears that are often found as evidence in such accidents.

The analysis of rubber is generally more difficult due to its elasticity and the high concentrations of filler present in some samples that can make samples opaque to IR radiation. Analysis by the DAC is useful for those rubbers in which the concentration of filler is not too high, for example the soles of some types of footwear. It will, otherwise, often defy useful IR analysis and other analytical techniques such as PGC might be resorted to if sufficient sample was available.

I have previously described the use of a pyrolysis technique which can be useful for such samples. Samples can be placed in small tubes for heating and the small amount of condensate sampled by IR microscopy. The spectrum of the condensed pyrolysate of a styrene/butadiene rubber obtained in this manner is shown in Figure 5. Care is required in the heating to avoid alterations in the spectra due to oxidation effects.

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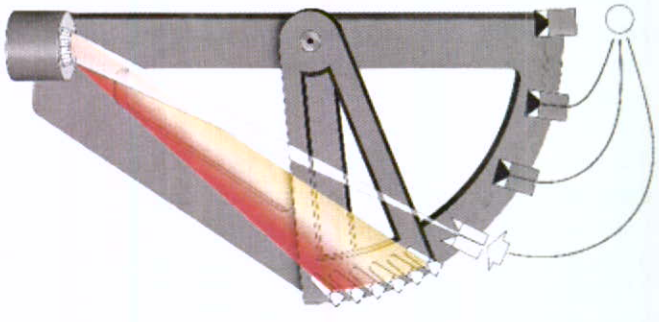

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Element	Wavelength	Std. Plasma	Axial Plasma
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Pb	168.215	20 µg/litre	3.0 µg/litre
P	178.287	12 µg/litre	3.0 µg/litre
K	766.490	60 µg/litre	4.0 µg/litre

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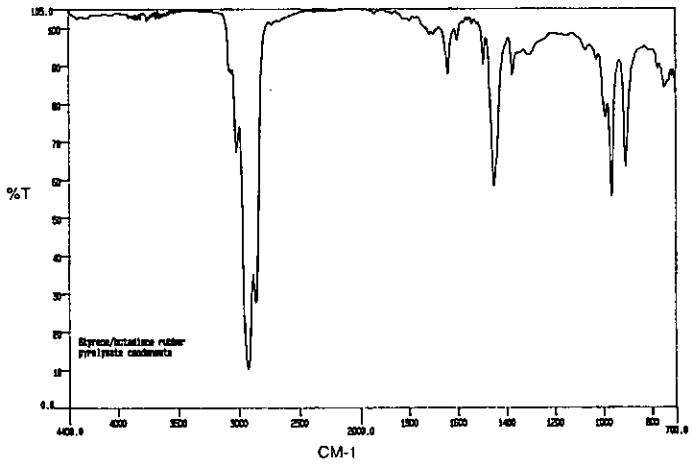

Figure 5: Spectrum of pyrolysate condensate obtained from styrene/butadiene rubber.

The ATR objective has also been reported to provide high quality spectra and has the advantage that it is a non-destructive technique. These objectives therefore appear to be the way of the future.

Controlled Substances

Drug samples and other controlled substances are available in many different forms e.g. free base/free acid/salts. They may be "cut" with a variety of substances and more than one type of drug may be present. It can be necessary to specify explicitly which form is present when statutes governing these substances distinguish between different forms, and quantitative information can be useful for drugs intelligence.

IR spectroscopy can be invaluable for screening, determining the general form of a drug, the specific anions associated and different crystal forms, and can also sometimes distinguish between an optical isomer and its racemic mixture.

IR reflectance microscopy is useful in the screening of drugs and pharmaceuticals in tablet form. These can be analysed by diffuse reflectance after lightly sanding their surface.

With IR microscopy it is also possible to analyse individual crystals in mixed drug samples where different crystal types can be separated under the stereo microscope by crystal morphology and texture. An example of the separation of heroin hydrochloride powder from glucose crystals is shown in Figure 6.

Previously, such samples might be analysed by pressing into KBr discs and, in an attempt to isolate a spectrum of a known drug, the spectra of known components removed by traditional absorbance subtraction techniques. Liquid extraction and recrystallisation from solvents might also be used, although somewhat time consuming and tedious. Direct analyses of individual crystals avoids any recrystallisation problems, polymorphism, hydration, stability and ion exchange effects which might occur in such a procedure.

Explosives

The ingredients of explosive, pyrotechnic and incendiary devices comprise a wide variety of organic materials, polymers and inorganic salts. Dynamite, black powder, smokeless powder, military explosives such as C-4, and various inorganic salts such as nitrates, sulfates and perchlorates are all used. IR spectroscopy is useful in identifying these materials and unusual or unexpected substances found in association with such devices.

IR microscopy is particularly useful in the analysis of residues and traces of unexploded chemical which might be found. Clearly, the ease or lack of sample preparation required for reflectance techniques is invaluable for pressure sensitive materials, and, single crystal analyses for contact sensitive explosives!

Conclusion

IR spectroscopy is a widely applicable and versatile analysis technique, particularly as the modern FTIR instrument is dependable, easy to operate and of modest cost. When combined with an IR microscope, it has the ability to analyse samples quickly, and provide a great deal of information at high sensitivity.

IR microscopy is applicable to macro as well as micro samples, to very small regions of larger samples, and to otherwise difficult and intractable samples. Sample preparation and presentation methods are simplified and the sample can typically be retrieved for further analysis or storage.

IR microscopy consequently has wide application in forensic sciences. The size of sample that can be analysed is so small that it can be invisible to the naked eye and remain hidden from

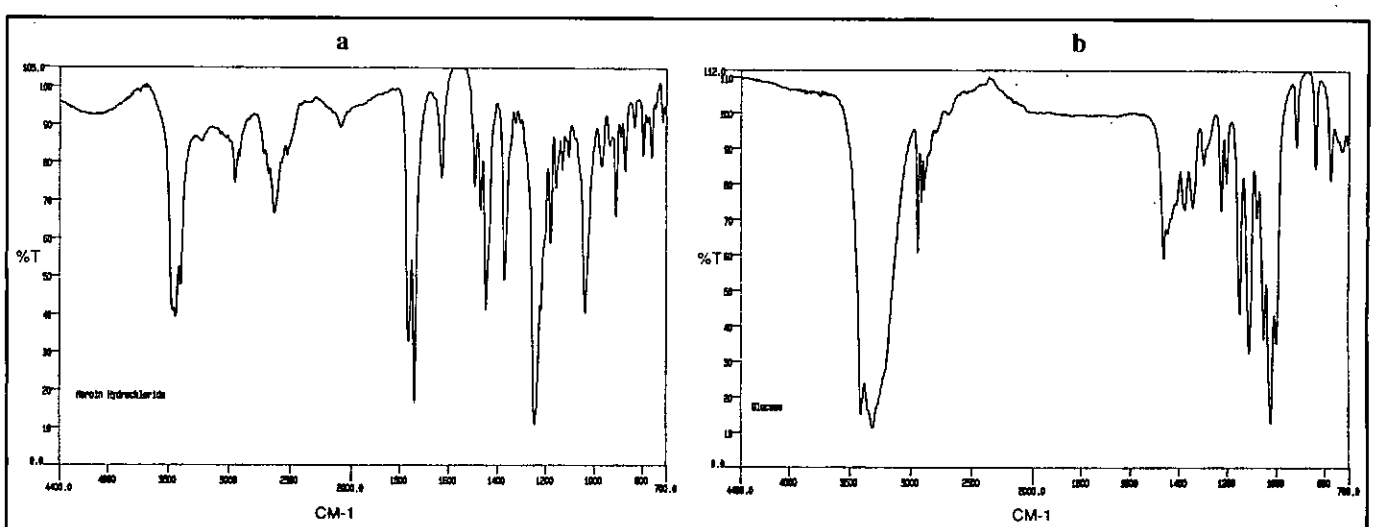

Figure 6: Spectra of: (a) heroin hydrochloride powder; and, (b) glucose crystals, as separated under stereo microscopy.

attempts to cover up crime. And material of evidential value within a larger sample can be analysed.

In our laboratory we use the IR microscope more than any other IR optics or accessory in the examinations. This is true for both the analyses we undertake in forensic casework and those from other areas of science or industry. The advantages of IR microscopes for forensic scientists can also apply, for example, to analytical and research chemists, spectroscopists, polymer chemists, mineralogists, semiconductor process engineers, QA and QC analysts, environmental scientists, materials scientists, microscopists and those involved in the restoration and conservation of artistic and historical artefacts, paintings, writing and art objects.

New developments in IR microscopy such as IR dichroism studies being undertaken and the development of ATR objectives increase the capabilities of IR spectroscopy in forensic science and other fields. Multi-mode objectives which provide viewing, transmission, reflection and ATR analysis from a single objective, motorised stages, and interactive multimedia, software packages which allow "point-and-click" operation, line scanning and mapping further increase the power of IR microscopy and simplify its use. The future of IR microscopy is assured and its reputation as an invaluable and essential tool in many laboratories and disciplines can only be enhanced.

* * * * *

"Perspectives in Marine Natural Products 1996"

11-12 July 1996

Venue: Conference Centre
University of Auckland

This is a two-day symposium organised by the Department of Chemisty, University of Auckland and sponsored by the Auckland Branch, and the Fats and Oils Group, of the NZIC. It aims to promote interest in marine natural products and to show the importance of chemistry in this sphere. It follows similar successful symposia held in Auckland in 1982, 1987 and 1991.

PROGRAMME

THURSDAY, 11 JULY

8.00 am-9.00 am	Registration
9.00 am-9.05 am	Opening Remarks *Professor Con Cambie, Convenor*
9.05 am-10.00 am	Trawling for Treasure and Pleasure: Southern Australian Marine Natural Products Chemistry *Dr Rob Capon* School of Chemistry University of Melbourne, Australia
10.00 am-10.30 am	***MORNING TEA***
10.30 am-11.10 am	Bioactive Compounds from New Zealand Marine Organisms *John W Blunt* Department of Chemistry University of Canterbury
11.10 am-11.30 am	Potential Ecological Roles and Pharmacological Uses of Marine Alkaloids: Ascididemin *Dr Brent Copp* Department of Chemistry University of Auckland
11.30 am-11.50 am	Marine Natural Products: Chemical Investigations of Southern Australian Marine Organisms *Ms Simone Rochfort* School of Chemistry University of Melbourne, Australia
11.50 am-12.10 pm	Structural Studies on Pateamine, a Cytotoxic Metabolite from a New Zealand Marine Sponge *Mr David Stirling* Department of Chemistry University of Canterbury
12.10 pm-1.15 pm	***SEAFOOD LUNCH*** Senior Common Room Old Government House
1.15 pm-2.15 pm	The Chemistry of Some Sponges and Their Symbionts *Professor John Faulkner* Scripps Institute, La Jolla, USA
2.15 pm-2.55 pm	Bryozoans - the Scum of the Sea? *Dr Michele Prinsep* Department of Chemisty Waikato University
2.55 pm-3.15 pm	Chemical Modifications of the Halichondrins

	Miss Rachael Lill Department of Chemistry University of Canterbury
3.15 pm-3.40 pm	***AFTERNOON TEA***
3.40 pm-4.00 pm	Cytotoxic Metabolites from New Zealand Deep Water Sponges *Dr Eric J Dumdei* Department of Chemistry University of Canterbury
4.00 pm-5.00 pm	Some Structural and Synthetic Aspects of Marine Natural Products *Dr Ted Molinski* Department of Chemistry University of California, Davis, USA
5.00 pm-7.00 pm	***DINNER BREAK***
7.00 pm-7.40 pm	Marine Biotoxin Research in New Zealand Since 1993 *Dr Don Hannah* ESR - Environmental, Wellington
7.40 pm-8.00 pm	Healthcare Ingredients from Fish Waste? *Dr Selwyn Yorke* New Zealand Pharmaceuticals Ltd Palmerston North
8.00 pm-8.20 pm	Recent Ecological and Biotechnological Work on Sponges *Dr Chris Battershill* NIWA Marine, Lower Hutt
8.20 pm-8.40 pm	Unusual Sulfated Galactans - An Ignored Resource *Dr Ian Miller* Carina Chemical Laboratories Lower Hutt
8.40 pm	***REFRESHMENTS*** Courtesy of NZIC

FRIDAY, 12 JULY

9.00 am-10.00 am	The Morning After - Hair of the Dog, or Something Entirely Different *Professor John Coll, Pro-Vice Chancellor (Academic)* Australian Catholic University Sydney, Australia
10.00 am-10.30 am	***MORNING TEA***
10.30 am-11.30 am	Anti-tumor Agents from Marine Organisms: a Mechanism-Based Approach *Professor Chris Ireland* College of Pharmacy University of Utah, USA
11.30 am-11.50 am	Novel Biologically-Active Agents from Southern Australian Marine Sponges *Mr Simon Ovenden* School of Chemistry University of Melbourne, Australia
11.50 am-12.10 pm	Structural Studies on a Peptide Lactone From a New Zealand Deep Water Sponge *Mr Li Shangxaio* Department of Chemistry University of Canterbury
12.10 pm-1.10 pm	***LUNCH***
1.10 pm-1.50 pm	Seas, The Opportunities, Big and Small *Dr Peter Murphy* Australian Institute for Marine Science Townsville, Australia
1.50 pm-2.10 pm	Biotoxins From New Zealand Shellfish *Mr Michael Stewart* Department of Chemistry University of Canterbury, NZ
2.10 pm-3.10 pm	Aspects of Research in Chemical Ecology and Pharmacologically-Active Marine Natural Products *Dr Bruce Bowden* James Cook University Townsville, Australia
3.10 pm-3.40 pm	***AFTERNOON TEA***
3.40 pm-4.00 pm	*Thorecta aotearoica* - the Sponge of the Long White Cloud *Mr Keri Wellington* Department of Chemistry University of Auckland
4.00 pm-5.00 pm	Marine Biodiversity: Conservation and Development *Dr Mary Garson* Department of Chemistry University of Queensland, Australia
5.00 pm-6.00 pm	**HAPPY HOUR** Common Room, Sixth Floor Department of Chemistry

The social programme includes a seafood lunch on 11 July and a happy hour on 12 July at the end of the symposium. Visitors from out of town can be accommodated at O'Rorke Hall on request to the Convenor, and parking in the lower car park can be arranged for a minimal fee.

As a consequence of a generous sponsorship, the registration fee has been set at only $100 and in order to encourage as many students as possible to attend, a fee of $50 has been set for *bona fide* student. Registration forms are available from the Convenor:

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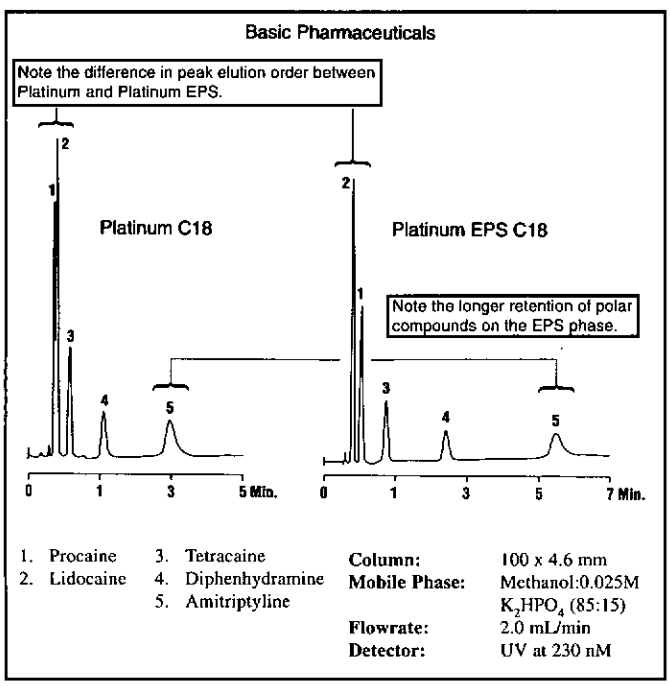

Platinum columns provide an alternative selectivity to other base-deactivated columns and offer a selectivity choice between the two Platinum C_{18} phases.

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SFE ELIMINATES CLEANUP AND ANALYTICAL INTERFERENCES!

Solve your sample preparation problems with SFE! Other automated sample preparation technologies promise fast turnaround and reduced labour. Only SFE gives you these additional time- and money-saving advantages.

- the inherent selectivity of SFE helps you eliminate the messy clean-up steps required by Method 3545, microwave, and traditional extraction techniques.
- SFE helps you avoid ruining your expensive chromatographic columns with dirty extracts.
- SFE reduces solvent costs and hazards by extracting with safe, inexpensive carbon dioxide.

Let us show you how the speed, safety and selectivity of SFE can be put to use in your application.

Contact: Clare Hodgson, Shimadzu New Zealand
P O Box 45-077, Auckland 1230
Ph: 0800 735725, Fax: (09) 8360668
circle number 32 on the reader reply card

REVOLUTIONARY COLUMN CONNECTOR SIMPLIFIES GC COLUMN INSTALLATION!

The biggest revolution in GC technology is now available. Connex - "*The Quick Column Connector*" - is a new technology that significantly reduces column installation time. Superior to metal, fused silica and glass connectors, Connex capillary column connectors provide a leak-free, inert, reusable connection that can be connected or disconnected instantly.

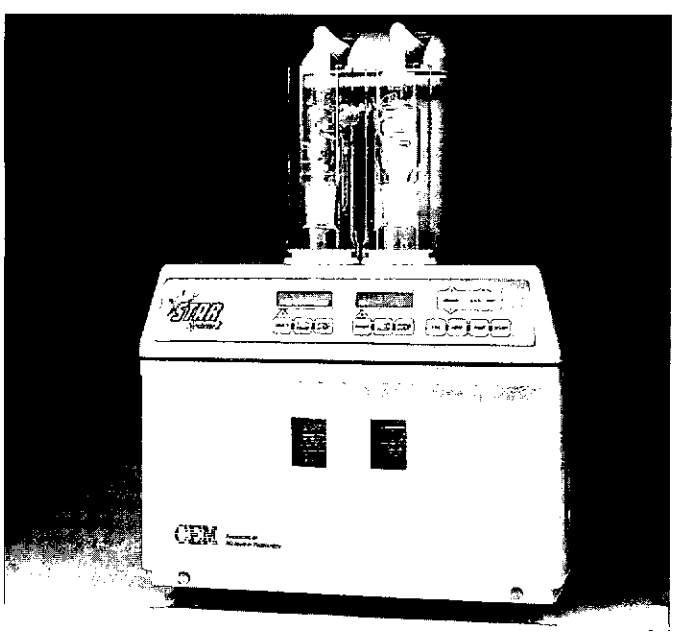
No time-consuming measuring. No messy gluing. Just quick, reliable connection. It will change the way you think about column installation forever.

For more information on this historic new product or any other products from J & W Scientific, *the low bleed leader*:

Contact: Clare Hodgson, Shimadzu New Zealand
P O Box 45-077, Auckland 1230
Ph: 0800 735725, Fax: (09) 8360668
circle number 33 on the reader reply card

MICROWAVE SPEED FOR "SAMPLES ON DEMAND" DIGESTION

A.i. Scientific announces the release of the revolutionary STAR Digestion System from CEM Corporation, the pioneer in microwave technology for laboratory applications. The STAR (Simultaneous Temperature Accelerated Reactions) System brings microwave speed to open-cavity digestions to produce samples on demand and is designed for large sample sizes and/or hard to digest samples.



Special features include: independent position vessels that let each vessel (up to six) run a separate digestion method, staggered start times so the STAR System's individual positions can fit into the laboratory workflow, optional program-controlled reagent addition during digestion and individual temperature feedback control for highly reproducible results. The control software is easy to learn and the system is extremely reliable. Patents pending.

Contact: Kevin Moloney, A.i. Scientific
P O Box 35579, Browns Bay, Auckland
Ph: (09) 4781351, Fax: (021) 788940
circle number 34 on the reader reply card

THE NEW DL50 FAMILY FROM METTLER TOLEDO

From their outward appearance alone, the new METTLER TOLEDO titrators leave you with the impression that titrating has again become simpler, more dependable and more flexible.

One innovative feature is the possibility to insert memory cards in a slot below the control panel as a handy storage medium in credit card format. With the new DL55 titrator, which can be expanded to 2 burettes, and the new DL53 model, they increase data security and greatly simplify method transfer between instruments. The memory cards not only store new methods developed by the user in the smallest possible space, but also facilitate the backup and archiving of setup data. The third member of the new family, the DL50, is primarily designed for routine determinations and has no memory card.

Visually supported operation and analysis

The realisation that visual elements can be understood much more quickly and clearly than words has been incorporated in the operating philosophy of the new METTLER TOLEDO titrators. The multi-line display of the DL53 and DL55 models even has graphics capability, and shows the progress of the titration on-line. The keys for frequently used auxiliary functions such as pH measurement, burette filling and stirring are marked by pictograms on all three models. Soft keys show only those functions which are currently available. Should words be required instead of symbols, they appear in the display in clear text and in one of five selectable languages.

Time tested quality improved yet again

The features which distinguish other titrators from METTLER TOLEDO are also offered by the new DL50 family. For instance, the simple start of the titration with a Run key and the learn titration for method development. Naturally, all determinations are recorded according to the rules of "Good Laboratory Practice". Thanks to the interfaces built in as standard, not only a printer but also a balance, barcode reader, sample changer and sensors from the extensive range offered by the same manufacturer can be attached.

Contact: Watson Victor Ltd
P O Box 1180 Wellington
Ph: (04) 3857699, Fax: (04) 3844651
circle number 35 on the reader reply card

NEW PRODUCTS

CONTROL RETURNS TO BD20/40 DIGESTION BLOCKS

The new BD28/50 microprocessor controller from A.i. Scientific enables owners of BD20/40 Block Digestors to replace their faulty or inaccurate control boxes.

With the discontinuation of the BD20/40 controllers it has not always been possible to replace old and failing controllers. The BD28/50 digestion controller is compatible with Technicon and Tecator 20- and 40-place digestion blocks.

There are two available models; a single method model with up to 40 steps and a nine method model which allows you to programme and store up to nine methods for instant recall. By enabling the storage and recording of the steps, ramps and hold periods of the digestion method, results are consistent from technician to technician.

The BD28/50 microprocessor controller is able to increase the heat with as little as 1 °C increments as opposed to the 5 or 10 °C increments of the earlier model. The BD28/50 is compact, with a footprint of 272 mm by 225 mm and stands at a height of 100 mm.

Contact: Kevin Moloney, A.i. Scientific
P O Box 35579, Browns Bay, Auckland
Ph: (09) 4781351, Fax: (021) 788940
circle number 36 on the reader reply card

REUSABLE PASSIVE SAMPLER FOR MERCURY

Medtec Products announces from SKC an accurate, lightweight, low cost passive sampler to sample for mercury vapours in the workplace. The 520 Series reusable Mercury Passive Sampler gives exact worker exposure as a time-weighted average (TWA). The sampler permits the positive analysis for mercury, at, above, or below the NIOSH/OSHA level of 0.05 mg/m^3.

Mercury vapours enter the sampler by positive controlled diffusion so that a known volume is taken for a given period of time. The mercury is completely absorbed on a solid sorbent. The sorbent capsule is then taken to a qualified laboratory for analysis where the sorbent is dissolved in acid and analysed by flameless atomic absorption spectroscopy.

The OSHA Laboratory in Salt Lake City, UT, USA, conducted an evaluation of SKC's 520 Series Passive Sampler over a broad range of mercury concentrations and sampling times. This evaluation demonstrated excellent accuracy and precision with no interference from chlorine and moisture. The method of reference for this evaluation is OSHA ID 140.

Contact: Wayne Sprosen, Medtec Products Ltd
P O Box 38-543 Wellington
Ph: (04) 5670011, Fax: (04) 5672821
circle number 37 on the reader reply card

CONNEX™ THE QUICK COLUMN CONNECTOR

J&W Connex is a quick column connector that can be connected or disconnected instantly! Leak-free and inert Connex is better because it is reusable. It will change the way you think about column installation forever. No time-consuming measuring. No messy gluing. Just a quick reliable connection, every time.

Connex quick column connector was voted one of the Best New Products at Pittcon '96 Annual Editors Awards. Connex is now available from ALLTECH for use with Hewlett Packard GC and GC/MS systems. Kits for Varian, Perkin-Elmer and Shimadzu will soon follow. For information on the release of the Connex quick column connector for your GC:

Contact: Alltech Associates Inc.
P O Box 100-352, North Shore Mail Centre, Auckland
Ph: (09) 4443230, Fax: (09) 4442399, Freephone: 0800 652766
circle number 38 on the reader reply card

J&W 24 HOUR GC TECHNICAL SUPPORT

J&W Scientific sets itself apart from standard manufacturers of GC capillary columns by leading the industry in technical support. As part of this continuing effort J&W now gives customers worldwide access to emergency technical support 24 hours a day. Call 001-916-731-3316 to contact a skilled applications scientist who will provide free analytical consulting and technical assistance, whether or not you are using a J&W product! For GC technical support in New Zealand,

Contact: Alltech Associates Inc.
P O Box 100-352, North Shore Mail Centre, Auckland
Ph: (09) 4443230, Fax: (09) 4442399, Freephone: 0800 652766
circle number 39 on the reader reply card

J&W OPENS NEW WORLD WIDE WEB SITE

ALLTECH are pleased to announce that J&W Scientific have opened a WWW site: http://wwwjandw.com containing over 250 pages of GC, SPE, and CE data, including a library of over 1,000 chromatograms cross-linked by search capabilities to over 12,000 compounds. The 1996/97 J&W Catalog is also on-line as well as e-mail access to technical support, custom column ordering information and literature requests. A "What's New" feature will be updated quarterly.

For more current information, J&W stockist ALLTECH offer a TOLL FREE Chromatography Help Desk.

Contact: Alltech Associates Inc.
P O Box 100-352, North Shore Mail Centre, Auckland
Ph: (09) 4443230, Fax: (09) 4442399, Freephone: 0800 652766
circle number 40 on the reader reply card

LOW-COST MULTI-DIMENSIONAL GC FROM SRI

ALLTECH and SRI have lowered the cost of ownership of a dual-oven GC. The SRI 8610C is designed for multi-dimensional GC applications, where heart-cut fractions from one column are shunted onto a second more specific and higher resolving column. With its small footprint, the dual-oven 8610C can provide this advanced capability to small laboratories with small budgets.

A complete range of sampling and detection options means a low cost SRI gas chromatograph is not limited in its applications. If you run a commercial or a research laboratory and are considering GC purchase or upgrade, don't overlook this opportunity to increase the power of your dollar There are already many SRI GC users in New Zealand to attest to the complete functionality of these value packed instruments. ALLTECH has SRI instruments ready to demonstrate.

Contact: Alltech Associates Inc.
P O Box 100-352, North Shore Mail Centre, Auckland
Ph: (09) 4443230, Fax: (09) 4442399, Freephone: 0800 652766
circle number 41 on the reader reply card

POLYMER DEFORMULATION SERVICE

Are you curious about why a previously reliable plastic product failed, or what gives your competitors' plastic products their winning qualities? We can supply the answers through Jordi Associates, an ALLTECH agency, specialising in Contract Polymer Characterisation Laboratory Services, and also in LC and GPC Columns. Polymer Deformulation, Additive Analysis and GPC Analysis of difficult to dissolve polymers, are all areas where specialised equipment and expertise are almost unavailable in New Zealand. Jordi Associates can demystify this area using GPC, LC, GC, FTIR, UV-VIS, NMR, X-Ray Analysis, AA, DSC, TGA, TMA, Titration, % Volatiles of Solids, Intrinsic Viscosity, and Melt Flow Indexing.

Contact: Alltech Associates Inc.
P O Box 100-352, North Shore Mail Centre, Auckland
Ph: (09) 4443230, Fax: (09) 4442399, Freephone: 0800 652766
circle number 42 on the reader reply card

GAS CHROM NEWSLETTER FROM ALLTECH

ALLTECH announce their *GAS CHROM* Newsletter to keep gas chromatographers current with new product developments and applications. In addition, instructional material for both the novice and experienced user is included in every issue This newsletter can help you improve your GC results and keep you up-to-date on the best new GC products.

If you have purchased GC products from ALLTECH you will automatically receive a free copy of the *GAS CHROM* Newsletter. If you wish to be added to our GC mail list so you too can receive this free source of GC information and product news, we welcome your call.

Contact: Alltech Associates Inc.
P O Box 100-352, North Shore Mail Centre, Auckland
Ph: (09) 4443230, Fax: (09) 4442399, Freephone: 0800 652766
circle number 43 on the reader reply card

CHROMATOGRAPHY FITTING AND TUBING GUIDE

All the information you need to choose the correct fitting for any job is gathered together in one convenient 16 page guidebook by the experts at ALLTECH. In press, your free guide book can be pre-ordered now.

Contact: Alltech Associates Inc.
P O Box 100-352, North Shore Mail Centre, Auckland
Ph: (09) 4443230, Fax: (09) 4442399, Freephone: 0800 652766
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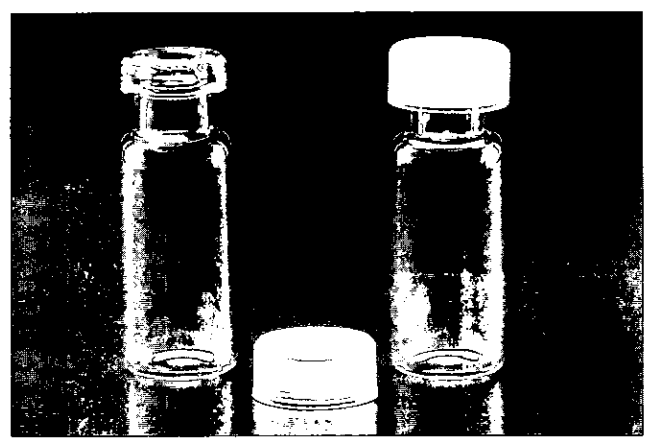
NO MORE CRIMPING! 2 mL CRIMP-TOP VIALS WITH 1-PIECE SNAP-ON CAP/SEPTA



At last! A product that will really change your working practices!

Features:
- The PE closure snaps onto the 2 mL crimp-top vial
- Excellent seal between septum and vial to prevent sample loss
- Coloured caps/septa allows sample coding
- 55% saving on the cost of the traditional crimp-top vial and aluminium cap/septa design
- No time consuming and awkward crimping of the cap/septa onto the vials. The snap-on cap/septa design simply slips onto the vial instantly.

Contact: Alphatech Systems Ltd & Co.
P O Box 37-583, Parnell, Auckland
Tel: (09) 3770392, Fax: (09) 3098514
circle number 45 on the reader reply card

NEW PRODUCTS

SYMMETRY™ - A NEW STANDARD IN VALIDATION AND COMPLIANCE

New Symmetry™ HPLC columns from Waters have been developed with one purpose in mind - to set new standards of performance for the demanding requirements of drug assays. The goals in producing Symmetry columns were to ensure the highest standard of reproducibility for confidence in long term compliance of HPLC methods with unmatched peak symmetry for maximum sensitivity, resolution and accurate quantitation.

Additionally Waters set themselves the challenge of developing a column chemistry that also allows you to optimise your assays for selectivity and retention time, whether at pH 3 or pH 7, whilst still retaining the same superior peak shape for bases, neutrals or acids across the entire pH range.

In creating this new standard Waters had to go back to square one and develop Symmetry silica from first principles. This meant developing a synthesis scheme that begins with absolute purity and composition control of these new silica molecules. From this point every element of the manufacturing process was designed specifically to new high tolerances exceeding Waters' own already exacting requirements, thus minimising variability between batches for unmatched reproducibility.

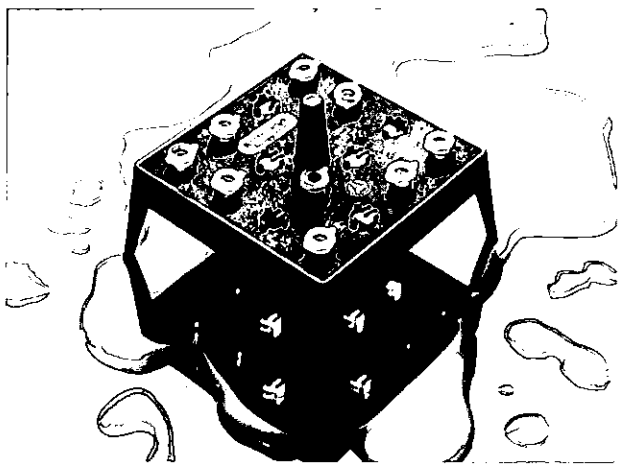
Since Waters control silica synthesis right through to the final bonding chemistry it also makes sense that for ultimate performance this control should pass right through to the finished packed column. Every steel column and its end fittings are precision machined and chemically cleaned prior to being packed, tested and finally shipped all under lot control. Waters cGMP, ISO 9000, FDA registered manufacturing facilities are managed entirely by Waters ensuring absolute quality control of all the above processes.

Accordingly every Symmetry column is shipped with a comprehensive Certificate of Analysis and batch QC test data assuring compliance in your validated method.

Undoubtedly method validation of a new drug assay is tough and time consuming, with faster validation of new products and processes a major requirement in today's regulated and cost-controlled environment. Symmetry has been designed specifically to meet these demands, column after column, year after year. No matter whether your method is used in the laboratory next door or all around the world, the same high standard of reproducibility, robustness and superior peak shape can now be achieved.

Contact: Alphatech Systems Ltd & Co.
P O Box 37-583, Parnell, Auckland
Tel: (09) 3770392, Fax: (09) 3098514
circle number 46 on the reader reply card

FLOATING MICROTUBE RACKS



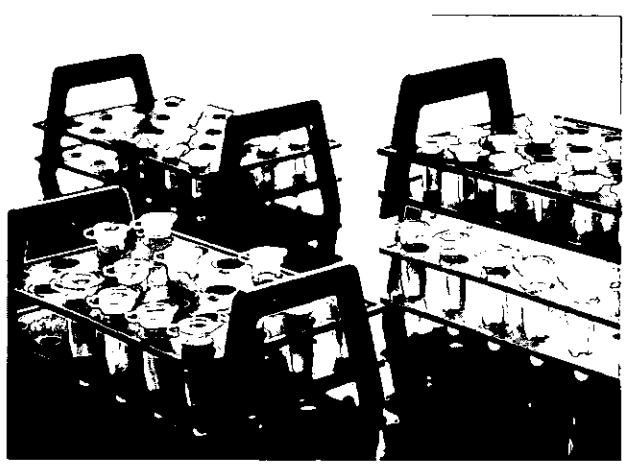
The new size of the NALGENE floating microtube rack holds sixteen filled 0.5 mL Eppendorf tubes in a 4 x 4 array. The rack allows convenient incubation at elevated or reduced temperatures in water or ice baths and is especially useful in gene cloning, microbiology and immunology labs.

The NALGENE floating microtube rack will float with a full load of filed tubes. The tubes are supported below the lips while the conical ends are immersed in water. The rack's legs prevent the bottom of tubes from touching benchtop surfaces.

A molded-in handle allows convenient transport, agitation and removal from a water bath. The floating microtube rack for 0.5 mL tubes is made of black polypropylene which has excellent temperature resistance from -70 °C to 100 °C.

Contact: Grant Washington-Smith
Medic Corporation Ltd
Private Bag, Lower Hutt
Ph: (04) 5770000 , Fax: (04) 5772000 , Freephone: 0800 508070
circle number 47 on the reader reply card

MICROCENTRIFUGE TUBE RACKS



The Nalge Company announces a new size of NALGENE microcentrifuge tube rack that holds 0.5 mL Eppendorf tubes.

A two-tiered design increases visibility of the conical end of the tubes. Holes in both tiers support tubes below the lip and at the conical bottom for easy access and extra stability. The holes are widely spaced to minimize interference from overlapping lips.

The convenient 4 x 6 array is ideal for DNA sequencing. You can place four racks together to hold 96 tubes. The end plates permit carrying and stacking of empty or full racks.

Microcentrifuge tube racks are molded from glass-filled acetal and are available in six colours. They are repeatedly autoclavable.

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circle number 48 on the reader reply card

NALGENE™ BOTTLES FOR HEAVY-DUTY LABORATORY APPLICATIONS

Nalge Company has introduced two new NALGENE™ heavy-duty bottles for applications in biotechnology laboratories. These new 1 and 2 litre thick-walled bottles are molded of rugged polypropylene with a white polypropylene closure and thermoplastic elastomer (TPE) gasket for guaranteed-leakproof service under vacuum. Autoclavable and chemical resistant, the bottles can withstand repeated application of full vacuum for 24-hour periods at room temperature (20 °C). They can be used as waste-aspirator bottles with a NALGENE filling/venting closure or as autoclavable vessels for scale-up activities in cell culture applications. The bottles are manufactured from non-cytotoxic materials which meet the requirements of the CFR 21 section of the Food Additives Amendment of the US Federal Food and Drug Act.

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CELL BIOLOGISTS' - (PC) PERSONAL CENTRIFUGE

Awarded "Most Innovative Instrument" in 1994, by America's *BioConsumer Review*, Denver Instrument's Force 7 personal micro centrifuge sets a new standard for scientists in biotech laboratories, medical research facilities and reference laboratories. *BioConsumer Review* summed it up as: "The Force 7 from Denver Instruments has several features usually found on more costly equipment. This space-age looking microfuge has the greatest tube capacity and speed of any machine in its class".

Medic product manager, Bettina Simpson, points out how the design brief of Denver Instrument's engineers "to keep the user at the forefront" of their priorities was achieved. Extensive use of innovative polymers enables the unit to withstand wipe-downs with solvents and acids, while also providing good thermal tolerance and ease of maintenance.

Sample containment is achieved throughout the Denver range of micro centrifuge models with a unique aerosol seal and individual tube slots in the rotor. Both features assist in the prevention of user contact with samples, cross-contamination and isolation of infectious or radioactive material in cases of accidental spillage.

A rotor snap allows for easy removal and cleaning or disposal of the rotor system. The entire rotor assembly with aerosol guard can be autoclaved at 121 °C.

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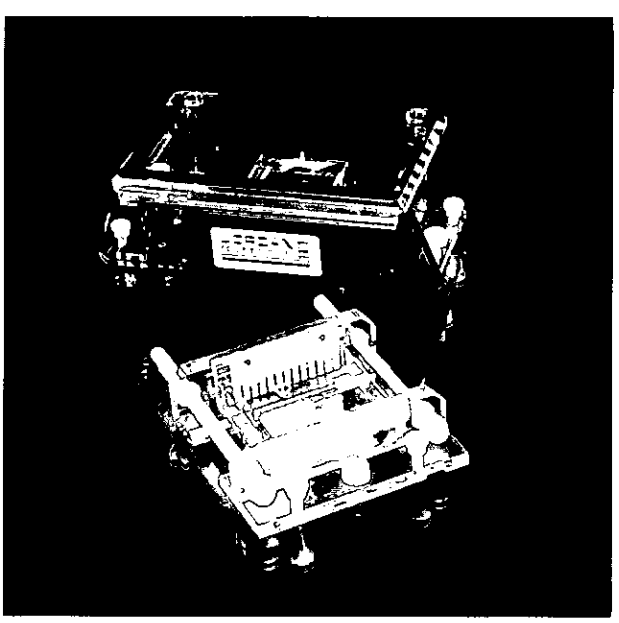
BIO-RESEARCHERS' GEL ELECTROPHORESIS SYSTEM

"Casting gels with the Jordan unit is a breeze"



Available for the first time in New Zealand, Medic Corporation Ltd introduces the award-winning Gel-o-Submarine electrophoresis unit from Jordan Scientific Co., USA.
Awarded the coveted "Editor's Choice" (Vol.2, Issue 1, pp 4-10 (1995)) by America's *BioConsumer Review*, for top performance out of ten US manufacturers of mini submarine electrophoresis systems.

Medic Corporation product manager, Bettina Simpson, points out that the award by *BioConsumer Review* is based upon evaluation of performance primarily from the standpoints of user-friendliness and value. Being able to cast an even and uniform gel is essential if a researcher wishes to reproduce results. Uniform gels also ensure straighter protein runs from end to end. With its unique QuickCast™ clamps and built-in levelling system, Jordan simplifies gel casting and ensures even and uniform gels are made without the need for adhesive tapes to seal edges, Simpson claims.

All of the Jordan Gel-o-Submarine systems are constructed from heavy-duty acrylic, providing years of trouble-free service. Interlocking safety covers and safety-tipped power cords provide complete operator safety. Levelling feet built into the buffer chamber ensure that the buffer covers the gel evenly - preventing the running of artifacts.

Contact: Grant Washington-Smith
Medic Corporation Ltd
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circle number 51 on the reader reply card

ABSOLUTELY, POSITIVELY SAFE CABINETS FOR BIOTECHNOLOGISTS

Biotechnologists can now opt for absolute safety when choosing new Class II laminar flow cabinets.

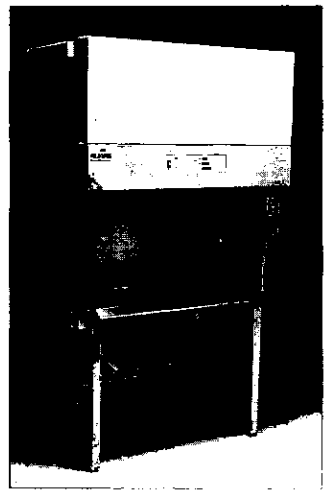
New Zealand laboratory professionals face risks constantly when working with potentially biohazardous materials, but now they have a real choice of cabinets from US manufacturer, Nuaire, that incorporates several advanced technological safety benefits.

Imported by Medic Corporation Ltd, Nuaire's range of laminar flow biological safety cabinets have outstanding monitoring systems which ensure the utmost safety for both scientists and samples.

All industries are becoming more accountable about environments in which staff work and older gear is now being replaced, says Bettina Simpson, of Medic Corporation.

"Managers are now in the personal protection mode, and the biological, laboratory and clinical areas of industry are in a state of rigorous upgrade," she explains.

Staff are more aware of regulations and are less tolerant of putting up with working conditions that may have been acceptable even five years ago. As well as new hazardous biological products, ergonomics is playing a large part in staff well-being, says Ms Simpson.



People in hospitals, research institutions, quality assurance laboratories, pharmaceutical and food and beverage industries are all affected by the new Health and Safety Act. With such legislation in place, managers need to be pro-active and seek ways to ensure work places are up-to-scratch, she explains.

With the new Nuaire cabinets every design detail has been with the end-user in mind. For staff this means even less likelihood of contact with airborne biological or chemical particles because of a new microprocessor control system. The advanced electronic airflow control monitors all cabinet functions. For example, one activates audible and visual alarms when the window is raised above a standard opening height.

The cabinet's newly designed working surface eliminates "dead zones". More tests can be done at any one time, which improves work output and concurrently, lessens the risks of sample contamination. Another planning plus is that cabinets are smaller. They use less room, and fully assembled, they can fit through a standard door.

Considering the amount of time staff spend at these work stations, Ms Simpson says, any feature that provides real benefits to staff safety and comfort, is a good return on investment.

Nuaire's cabinet has several ergonomically designed parts. These include front airfoil; the polished-edge glass window means less eye fatigue and better viewing; there's more leg room and an arm rest is now a standard feature.

Has anyone ever found cleaning cabinets an enjoyable job? Probably not, but the Nuaire cabinet has its service valves staggered on the side walls which makes them easily accessible. Front access to filters means their replacement is quick and easy, because you don't need to remove windows. All controls and adjustments are placed at the front, making calibration and certification trouble-free.

Everyone knows that working in a safe environment has countless benefits for both staff and employers. Staff are happy know-

ing their personal safety is top priority, and managers can abate worry, conscious they're doing everything in their power to ward off clinical mishap.

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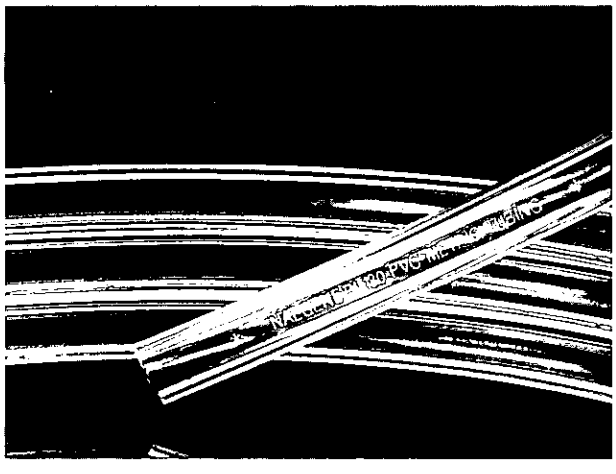
NEW METRIC SIZES OFFERED FOR NALGENE™ 180 CLEAR PLASTIC TUBING

NALGENE 180 PVC (polyvinyl chloride) tubing is now available in pure metric sizes to fit laboratory equipment with metric connections. This eliminates possible leaks when using "close-to-size" English-unit tubing. This autoclavable tubing is made from the highest grade resins and special plasticizers - no fillers or extenders are ever added.



This new metric tubing has a Durometer (Shore S) of 55 and is available in 17 sizes from 1.0 to 20.00 mm, inside diameter. Tubing is labelled "metric" and marked every 10 cm for convenient dispensing and cutting. Fifty-meter tubing coils (10 m for larger sizes) come in specially-designed boxes for cleanliness, easy dispensing and storage.

NALGENE 180 tubing resists a wide range of chemicals, is dimensionally stable and highly resistant to hardening and discoloration. It is made of materials which comply with the Food Additives Amendment of the US Federal Food, Drug and Cosmetic Act of US Pharmacopoeia Class VI Requirements for Plastic Materials.

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circle number 53 on the reader reply card

THE SECRETS BEHIND SPECTRO ANALYTICAL'S SPECTROFLAME MODULA ICP SPECTROMETER

The Spectroflame Modula ICP Spectrometer employs fibre optic technology for light transmission between the plasma and spectrometer. It is possible to measure up to 128 wavelengths simultaneously including the background signals.

The modular system can be equipped with either one or two monochromators to measure any analytical line you desire.

The system is so flexible that up to five complete spectrometers, polychromator(s) and monochromator(s) can be added either during manufacture, or later in the field. This flexible approach results in several benefits for the user ...

- Each spectrometer is optimised for the task in hand.
- The most suitable wavelengths are utilised ... without compromise.
- Ideal light transmission from the plasma through optical fibres. No need for complex optical components.

For measurement in the UV range (wavelength below 200 nm), patented gas-filled spectrometers are used, requiring neither vacuum pumps nor purging gas. With this technique the halogen elements can be measured and more sensitive wavelengths can be utilised for elements such as Pb and Al.

The day-to-day running of the Spectroflame is simplified ...

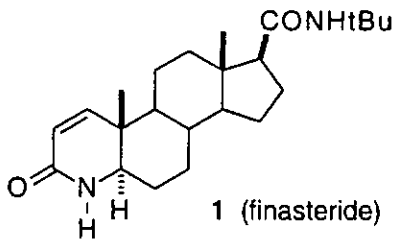
- The complete sample introduction system can easily be removed or replaced on a single plate.
- There is a push-button start and all spectrometer functions are computer controlled.
- MS-Windows™ software gives simple and easy spectrometer control for routine operation and method development.

Contact: David Sidwell, Sidwell Management Systems
P O Box 34789 Birkenhead, Auckland
Ph: (09) 4180275, Fax: (09) 4180275
circle number 54 on the reader reply card

THE INHIBITION OF STEROID 5 α-REDUCTASE

Andrew D Abell* and B R Henderson
Department of Chemistry, University of Canterbury, Private Bag 4800, Christchurch

Approximately 50% of all males will develop, to at least some extent, a non-cancerous enlargement of the prostate by the age of 60 years. This condition, referred to as benign prostatic hyperplasia (BPH), can result in a reduction in the diameter of the urethra, resulting in a decrease in urinary flow with frequent and often sudden and intense urges to pass urine [1,2]. Until recently, the only recognised treatment for this condition was invasive surgery, a trans-urethral resection of the prostate. A pharmaceutical alternative to the traditional surgery has recently been realised for those men whose "torrent has turned to a trickle". Finasteride (**1**)(PROSCAR®) developed and marketed by Merck Sharp and Dohme, has been shown to reduce the size of the enlarged prostate gland, by inhibiting the biosynthesis of dihydrotestosterone (DHT), the causative factor for BPH [3].



1 (finasteride)

An elevated level of DHT is also thought to be responsible for other androgenic-based disorders, including male pattern baldness, acne, female hirsutism and prostatic cancer - a condition commonly treated by castration or chemotherapy [4]. The inhibition of DHT biosynthesis, therefore, offers potential as a treatment or preventative measure for these and other conditions associated with elevated levels of DHT.

DHT is biosynthesised from the major male sex hormone, testosterone (T), in a reaction catalysed by the membrane bound, nicotinamide adenine dinucleotide phosphate (NADPH) dependent enzyme, steroid 5α-reductase (SR, EC 1.3.99.5) [1,2]. The stereospecific reduction of T is thought to proceed via an enolate intermediate as shown in Scheme 1.

The physiological roles of DHT and T have been identified by studying SR and hence DHT deficient, individuals [5]. Those affected possess internal male genitalia, but female external genitalia when born, and are often raised as females. The onset of virilisation (which may be partial or full, depending on the genetic defect) causes maturation of the penis and descendance of the testicles, accompanied by a deepening of the voice and increased muscle mass. The body hair retains a predominantly feminine pattern, and the prostate does not develop normally. The suggested role of DHT in male pattern baldness and acne, stems from the absence of these afflictions in the SR deficient populations. These studies have lead to a differentiation of the functions of T and DHT. Foetal development of the Wolfian duct into seminal vesicles and epididymis is thought to be controlled by T, while the masculinisation of the external genitalia is controlled by DHT. At puberty, however, T can induce the maturation of underdeveloped external genitalia while DHT controls male hair growth and also male pattern baldness.

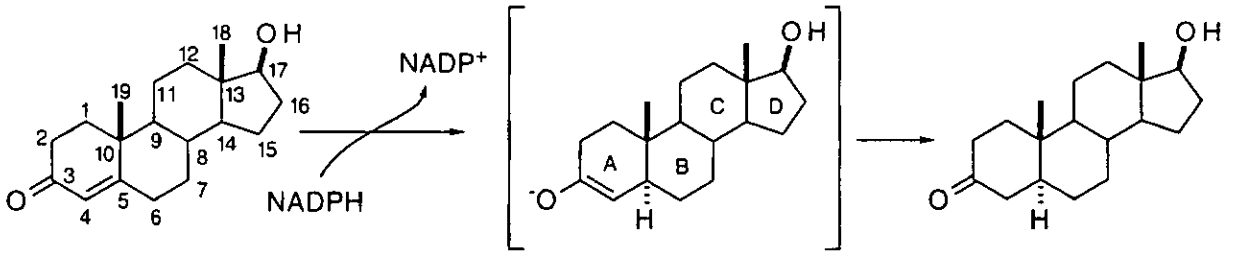
Two isozymes of SR have recently been identified [6]. The type-1 isozyme is predominantly located in non-genital skin and to a lesser extent in the prostate [7]. The type-2 isozyme is predominant in the prostate [8]. The prostate bound type-2 isozyme is thought to control prostate development, and male hair patterns. The role of the type-1 isozyme is less well defined, but its location in non-genital skin implies a role in skin disorders, such as acne and hirsutism [9].

The Inhibition of Steroid 5α- Reductase

Potent inhibitors of SR have been designed as mimics of the proposed enolate intermediate in the biosynthesis of DHT, see structure **2** in Scheme 1. The electrostatic properties and A-ring geometry of these inhibitors mimic those of the enolate **2** [2]. 4-aza steroid-based inhibitors of SR, typified by finasteride (PROSCAR®, **1**) were the first such inhibitors of human SR to be reported [2,10]. Finasteride is now approved for use in the treatment of BPH [3] and shows selectivity for the human type-2 isozyme (type-1 IC_{50} = 500 nM, type-2 IC_{50} = 4.2 nM).†

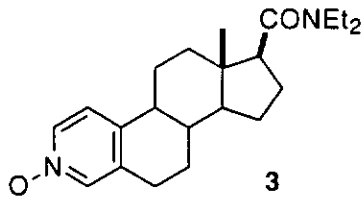
† IC_{50} and $K_{i,app}$ are measures of the level of enzyme inhibition. The lower the number the more potent the inhibitor.

Scheme 1: Steroid 5α-reductase (SR) catalysed formation of dihydrotestosterone



Testosterone (T) Enolate Intermediate **2** Dihydrotestosterone (DHT)

Other steroid-based neutral enolate mimic inhibitors of SR (see **Table 1**) include nitrosteroids [11], e.g. **13**, and 6-aza steroids [12], e.g. **7a** (type-1 $K_{i,app}$ = 190 nM, type-2 $K_{i,app}$ = 0.36 nM).† Extensive structure/activity studies on the 6-aza steroids identified a number of dual types-1 and -2 inhibitors of human SR's, e.g. **7b** (type-1 $K_{i,app}$ = 9 nM, type-2 $K_{i,app}$ = 0.08 nM). A 3-pyridyl-*N*-oxide group has also been incorporated into the A-ring of a steroid nucleus to give potent type-2 SR inhibitors, e.g. **3** (type-1 $K_{i,app}$ = 1500 nM, type-2 $K_{i,app}$ = 31 nM) [13]

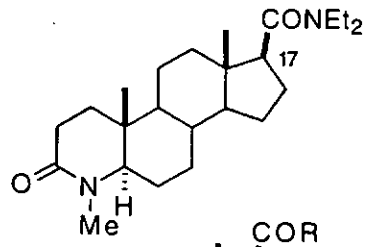
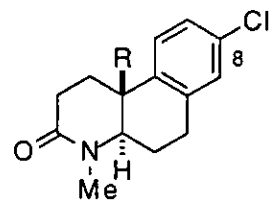
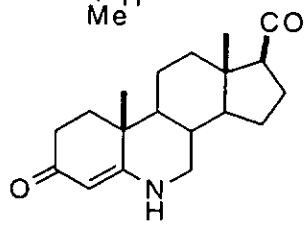
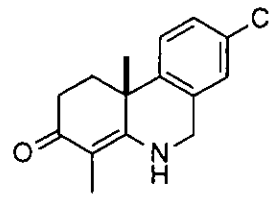
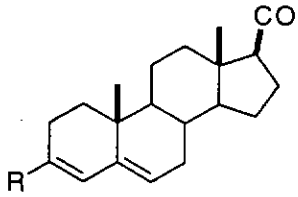
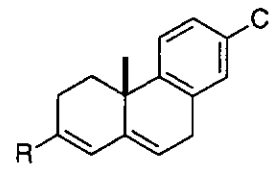
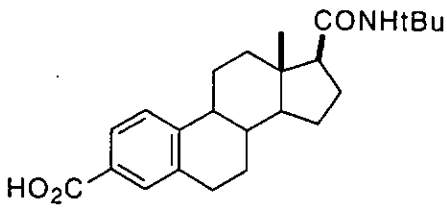
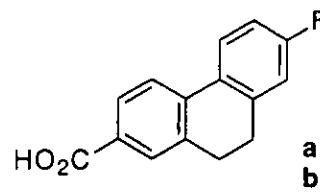
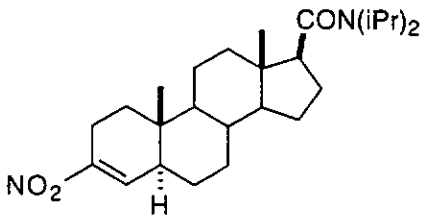
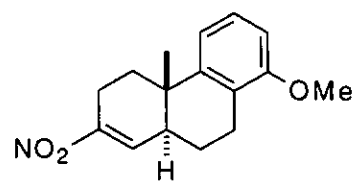


3

Steroid-based transition state mimic inhibitors of SR bearing an acid C-3 group have also been reported (see Table 1). Examples include C-3 carboxylic acids exemplified by the type-2 selective diene acid, epristeride **9a** (type-1 $K_{i,app}$ = 410 nM, type-2 $K_{i,app}$ = 0.2 nM) [14] and the aryl acid **11** [15]. Steroid-based phosphinic (e.g. **9b**), phosphonic and sulfonic acids have also been shown to be excellent inhibitors of human SR [2].

An enormous effort has been made in recent times to develop isozyme selective and dual isozyme inhibitors of SR. These studies have shown that the potency and isozyme selectivity of steroid-based SR inhibitors is influenced by factors including ring substitution (particularly C-17) and the degree and nature of unsaturation of the steroid nucleus. A selective type-1 inhibitor may prove useful in the specific treatment of skin conditions associated with high levels of DHT, e.g. acne, hirsutism, and

Table 1: A comparison of steroid and non-steroid inhibitors of human steroid 5α-reductase

No.	Steroid-based inhibitor	No.	Non-steroid-based inhibitor
4		5[a]	 **a** (+) R =H **b** (-) R = H
		6[a]	**a** (+) R =Me **b** (-) R = Me
7	 **a** R = NHtBu **b** R = iBu	8[b]	
9	 **a** R = CO_2H **b** R = PHO_2H	10[b]	 **a** R = CO_2H **b** R = PHO_2H
11		12	 **a** R = H **b** R = Cl **c** R = Br
13		14[b]	

[a] relative stereochemistry only
[b] racemic compounds

male pattern baldness. A dual type-1 and type-2 SR inhibitor may further reduce serum levels of DHT, as compared to the currently available type-2 selective pharmaceuticals, and therefore offer an improved treatment of BPH.

Our recent efforts in this area have focussed on the identification and development of non-steroidal inhibitors of SR. A non-steroidal inhibitor of SR may provide a pharmaceutical with increased potency and less side effects then the traditional steroid-based systems. There are two basic approaches to obtaining a lead compound for studies of this type. The steroid-based inhibitors of SR discussed above represent an example of using a rational design approach, based on the known chemical and biochemical properties of SR. A second approach involves screening natural products and collections of chemicals for useful activity. Natural products have traditionally been used as a source of novel, often very complex compounds suitable for biological screening. Even though a complex natural product may possess excellent biological properties it may not be a suitable drug candidate due to problems in obtaining sufficient quantities, either by isolation or through organic synthesis, for product development. The chemical collections of the large pharmaceutical companies represent an alternative source of lead compounds. We and others, have used this resource to identify potent, non-steroidal, inhibitors of SR.

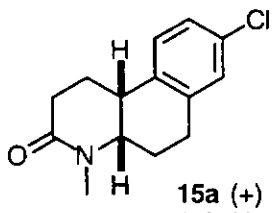
A series of benzoquinolinones has been identified as providing potent type-1, non-steroidal, inhibitors of SR [16]. we successfully prepared and isolated, in >95% ee, the four stereoisomers of the methyl-unsubstituted benzoquinolinones (**5a,b** and **15a,b**) and four stereoisomers of the methyl-substituted benzoquinolinones (**6a,b** and **16a,b**) using a preparative DIACEL CHIRALPAK AS column for the final isomer separation [17]. The angularly unsubstituted *trans* enantiomers, (+)-**5a** and (-)-**5b**, and the angularly substituted *trans* enantiomers, (+)-**6a** and (-)-**6b**, gave very similar and potent inhibition of the type-1 isozyme, $K_{i,app}$ = 6, 4, 9 and 10 nM, respectively. The angularly unsubstituted *cis* enantiomers, (+)-**15a** and (-)-**15b** and compound **17** (a synthetic precursor to **5** and **15**) also demonstrated very potent inhibition of the type-1 isozyme, $K_{i,app}$ = 15, 15 and 17 nM, respectively. By contrast, the angularly substituted *cis* enantiomers, (+)-**16a** and (-)-**16b** and racemic **18** (a synthetic precursor to **6** and **16**) gave a reduced type-1 potency, $K_{i,app}$ = 4000, 7000 and 180 nM, respectively. The *cis*-fused ring junction in compounds **16a, b** and the double bond in the angularly methyl-substituted compounds **18** result in a slightly bowl-shaped structure. This loss of planarity is thought to be responsible for the reduced type-1 activity. Some disruption of planarity can be tolerated without the loss of inhibitory activity as long as the angular position is unsubstituted as in compounds **15** but not **16** or **18**. With the exception of **17**, all compounds displayed poor activity against the type-2 isozyme.

Based on the structural similarity between the 4-aza steroid SR inhibitors, *e.g.* **1** and **4**, and the benzoquinolinones, *e.g.* **5** and **6**, we prepared the non-steroidal diene acids **10a** and **10b** [18] as non-steroidal analogues of the steroid-based diene acid SR inhibitors **9a** and **9b**, respectively (see Table 1). The diene acid **10a** proved to be a selective and potent inhibitor of the type-2 isozyme of SR (type-1 and type-2 isozyme inhibition constants of 1.2 μM and 0.26 μM, respectively). The previously discussed benzoquinolinone non-steroidals, by contrast, are potent inhibitors of the type-1 isozyme. However, in both series, an 8-chloro substituent gave optimum inhibitory activity. The corresponding phosphinic acid **10b** was a modest inhibitor of type-1 and type-2 steroid 5α-reductase.

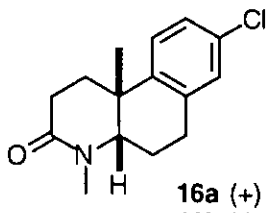
We also recently reported the synthesis and testing of tricyclic aryl acids **12a, b, c** and the tricyclic nitro-alkene **14** as non-steroidal analogs of the steroid-based, type-2 selective, SR inhibitors **11** and **13**, respectively [19] (see Table 1). The tricyclic aryl acids **12a, b, c** were potent and selective inhibitors of the type-1 isozyme of SR. Here, an 8-bromo substituent was favoured for potent inhibition (type-1 isozyme inhibition constants for **12a, b, c** were 315, 320 and 26 nM, respectively). The type-1 selectivity of **12a, b, c** is analogous to that observed for the non-steroidal derivatives **5** and **6** but opposite to that of the diene acids **10**. The nitro-alkene **14** proved to be a weak inhibitor of type-1 SR (inhibition constant of >2500 nM). The analogy between the steroidal and non-steroidal series has been extended with the preparation and testing of **8**, an analog of the 6-aza steroids **7** [20]. Compounds of this type are modest type-1 selective inhibitors of SR.

In summary, five classes of tricyclic non-steroidal inhibitors have been reported, typified by compounds **5**, **6**, **8**, **10**, **12** and **14** (see Table 1). All but the diene acids **10** are selective for the type-1 isozyme of SR. The benzoquinolinone non-steroidal inhibitors **5**, **6** and the aryl acid inhibitors **12** provided the most potent inhibitors of SR. From this work it is clear that potent non-steroidal inhibitors of SR, based on the tricyclic skeleton initially identified in compounds **5** and **6**, are obtained by employing the A-ring groups (4-aza, 6-aza, diene acid, aryl acid and nitro-alkene) found in the more traditional, steroid-based, inhibitors of SR. A halogen substituent at the 8-position is favoured for potent inhibition of SR in all cases studies.

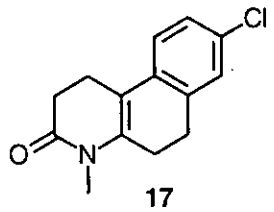
A selected screening of non-steroidal aryl carboxylic acids possessing the A-ring features of the putative enolate transition state species **2** (Scheme 1), identified benzophenone carboxylic acids of the type **19** as potent inhibitors of human type-2 SR (type-2 $K_{i,app}$ = 5 nM) [21]. The subsequent synthesis and testing of a range of compounds of this type established that electron-donating and small lipophilic substituents at the aromatic C-ring enhance inhibitory potency. The related analogs **20** and **21**, which contain a modified A-B ring linker, are also potent and selective inhibitors of type-2 SR (type-2 $K_{i,app}$ = 35 and 60 nM,



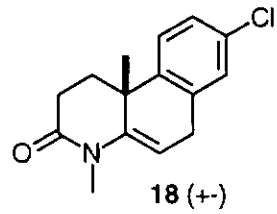
15a (+)
15b (-)



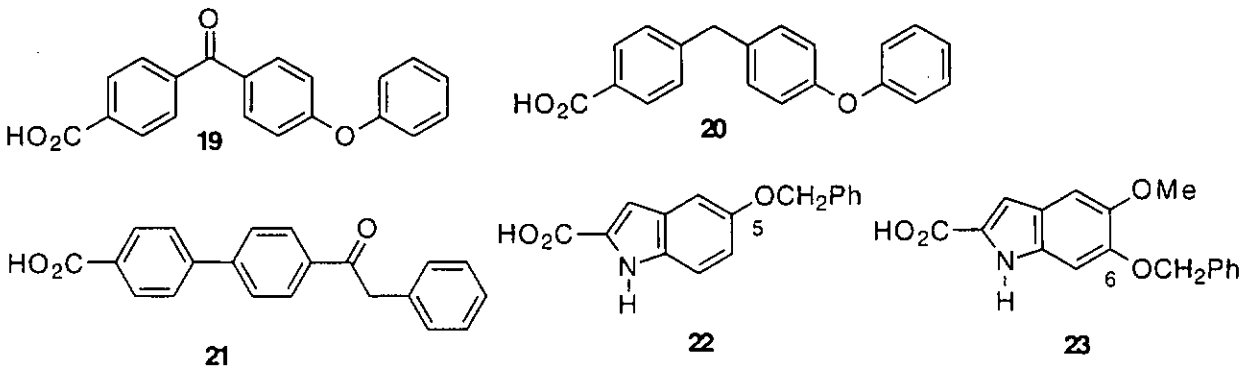
16a (+)
16b (-)



17



18 (+-)



respectively). We have also identified the 5-benzyloxy indole acid **22** as a potent and selective inhibitor of type-2 SR ($K_{i,app}$ = 40 nM) [21]. The introduction of a methoxy group and a change in the position of the benzyloxy group to the 6-position (as in **23**) greatly increased potency for the type-1 isozyme while maintaining type-2 potency, (type-1 and type-2 $K_{i,app}$ = 20-30 and 460 nM, respectively).

The identification of inhibitors of SR is currently a very high profile area of medicinal chemistry with a number of compounds marketed worldwide, or soon to be, for the treatment of BPH. Other potential therapeutic targets for SR inhibitors have been identified including male pattern baldness and prostatic cancer. Time will tell if SR inhibitors are to play an important role in the treatment, or prevention, of these and other important human diseases.

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INDUSTRY APPLICATIONS

THE ROLE OF HPLC AND AUTOMATED SAMPLE PREPARATION IN CLINICAL LABORATORIES

Clinical laboratories have large numbers of samples to process, within a short period of time after samples are received. With the need to reduce costs and minimize exposure of personnel to hazardous materials, many laboratories are now equipped with high-capacity, dedicated auto-analysers employing colourimetric or immunological methodologies with ready-to-use chemistries.

The limitation of auto-analysers is that they are suitable for only a restricted number of specific assays. The HPLC remains the method of choice for more complex analyses (e.g. for catecholamines, amino acids, anti-convulsants, anti-depressants etc.), due to the versatility and accuracy of the technique. However, when HPLC is used the sample throughput required by large clinical laboratories can only be achieved by a high degree of automation: from sample preparation through to data processing.

Gilson autosamplers and sample processors are designed to automate sample pretreatment and clean-up procedures before HPLC.

ONLINE ASTED CLEAN-UP FOR DETERMINATION OF PTERIDINES IN URINE BY HPLC

by Y Sawada, H Shintaku et al. (Juso Citizens' Hospital and Osaka City University Medical School, Japan)

Objectives

Pteridine analysis is essential for the diagnosis and treatment of hyperphenylalaninemia in new-borns. In addition, neopterin and bioterin provide important clinical markers for other diseases such as cancer, kidney dysfunction and rheumatoid arthritis[1,2]. It is unlikely that pteridine analysis will become an increasingly routine laboratory examination.

At present, the most commonly used assay for pteridines is that of Fukushima-Nixon.[3] However, following iodine oxidation of reduced forms of bioterin, an extremely involved sample clean-up step is required prior to HPLC.

The sample clean-up, carried out on a Dowex 50 ion exchange column, takes 4-5 hours.

In this application, ASTED is used to perform on-line sample clean-up within just a few minutes.[4]

Sample pretreatment

Iodine oxidation was performed manually as in the original Fukushima-Nixon method. A 100 µL portion of sample (such as urine, umbilical cord serum or breast milk) was mixed with 20 µL of iodine solution (1.2 N HCl containing 3.6% I_2 and 7.2% KI) and left for one hour. The mixture was then mixed with 14 µL of 2 N NaOH and 10 µL of 10% ascorbic acid in citric acid buffer (pH 6.0), before clean-up using ASTED with on-line HPLC analysis.

ASTED sample preparation

Instrumentation: Gilson ASTED fitted with a flat-bed dialyser (Kel-F™ membrane with 15 kDa MW cut-off; a 100 µL donor cell; 175 µL recipient cell) and a HEMA (ion exchange) trace enrichment cartridge.

Sample preparation was performed using ASTED as follows:

1 LOAD DIALYSER

Sample (75µl) loaded into donor channel of dialyser at 0.75 ml/min (static)

↓

2 ONLINE CLEAN-UP

Recipient channel of dialyser flushed with 1 ml of solvent A = [10 mM K_3PO_4 (pH 6.8) - methanol (99:1)] in pulsed mode at 0.18 ml/min.
Wait time of 20 s.

↓

3 TRACE ENRICHMENT

Dialysate loaded onto trace-enrichment cartridge (TEC) for concentration of analytes.

↓

4 HPLC

Concentrated analytes eluted from TEC with HPLC mobile phase, for online HPLC analysis:
Column: Spherisorb ODS1 5 µm (250 x 4.6 mm).
Mobile phase: 0.1 M potassium phosphate buffer (pH 6.8) containing 0.2 M NaCl - methanol (99:1 v/v)
Flow rate: at 1 ml/min.
Fluorescence detection: at 450 nm (Excitation at 350 nm)

↓

5 REGENERATION

(i) Dialyser donor cell regenerated with aq. 0.01% Triton X-100.
(ii) Dialyser recipient cell and TEC regenerated with solvent A
(iii) TEC re-equilibrated with 2 N HCl

Results and discussion

ASTED was successfully applied in the analysis of neopterin and biopterin in human urine. Following the initial manual oxidation step, the system perfomed on-line clean-up and injection in just eight minutes. Furthermore, concurrent processing of samples with ASTED enabled samples to be

cleaned up during the analysis time of the previous sample. Comparison of chromatographs for the conventional method and that using ASTED, show a good correlation of results (*Figure 1*).

Using ASTED, sample clean-up was achieved in minutes rather than in hours as in the Fukushima-Nixon method. The efficiency of the on-line clean-up also resulted in a longer lifetime of the analytical column, with excellent chromatographic reproducibility.

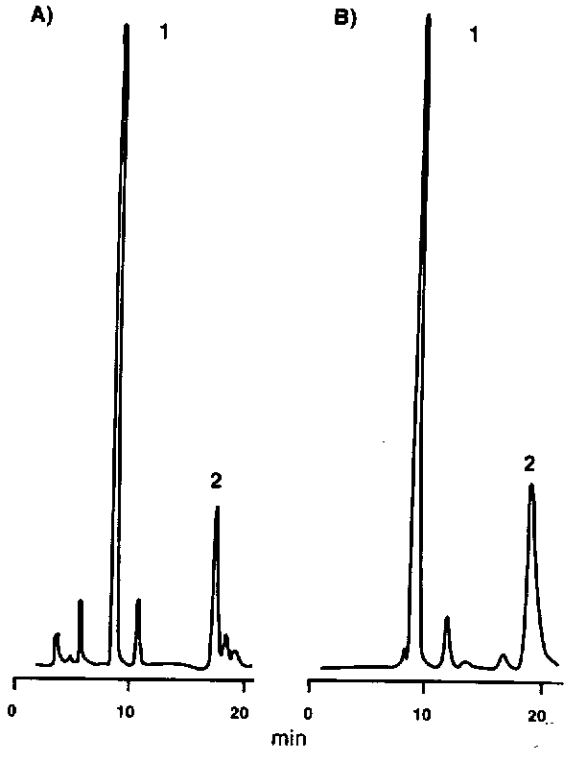

Figure 1: *Chromatogram of human urine containing neopterin (1) and biopterin (2) with sample preparation by: A) Fukushima-Nixon method, and B) ASTED method*

References:

1. B Stea *et al.*, *Cancer Res.* **38** (1978), 2378-2384
2. R J Leeming, *J. Clin Pathol.* **29** (1976), 444-451
3. T Fukushima, J C Nixon, *Anal. Biochem.* **102** (1980), 176-188
4. Y Sawada, H Shintaku; T Nakajima, C Iwamura, Y Tsubakio, M Fujioka, A Nishimura, G Isshiki, T Ohura, M Kawakatsu, T Nakamura, *Pteridines* **3** (1992) 1/2. 87-88

For more information:
Contact: John Morris Scientific Ltd
P O Box 6348 Wellesley Street, Auckland
Ph: (09) 3663999, Fax: 3663060
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OPTIMIZATION OF SOLID-PHASE EXTRACTION IN THE ANALYSIS OF DRUGS

Solid-phase extraction (SPE) methods have become very popular over the past ten years for biological sample clean-up and trace enrichment. Based on adsorption/desorption mechanisms, SPE offers various benefits over other separation techniques (e.g. liquid-liquid extraction, micro-filtration or protein precipitation), such as: low solvent usage, speed and facility of implementation, and compatiblity with a wide range of analytes.

Unfortunately, many SPE methods do not really optimize the chemistry of an extraction and rely on a rather simplified approach to method development. Such protocols typically use conventional C_{18} packings, methanol as a conditioning solvent, water as a washing solvent, acidic or alkali methanol as an eluting solvent, with analysis by HPLC. The importance of the effects of, equilibration times, solvent/sample volumes, load and elute flow rates on analyte-eluent-matrix interactions, are rarely considered.

With the ASPEC™ XL sample preparation system, Gilson automates SPE with fine control of all these liquid handling parameters, permitting an optimization of both the efficiency and reproducibility of a method. Moreover fitted with an injection valve, ASPEC XL offers the advantages of sample preparation coupled directly to an analytical system.

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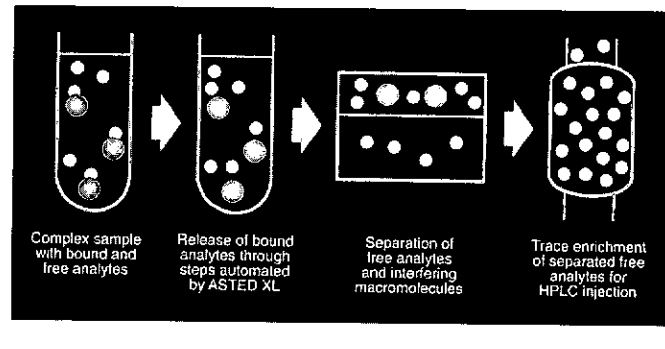
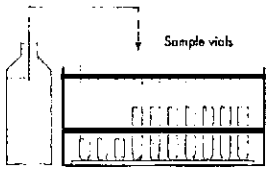
ASTED XL brings a unique, patented technology to complex sample cleanup. ASTED XL's operating principle is unlike that of any alternative cleanup method. The system automatically cleans up and concentrates complex samples in these four steps:



- Bound analytes are released from larger protein molecules
- Analytes of interest are separated from interfering macro-molecules
- Analytes are concentrated for analysis
- System regenerates in preparation for the next sample.

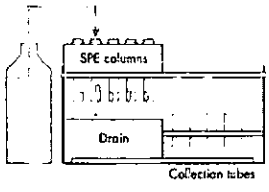
Easy automation of your manual protocol

1 - Sample pretreatment

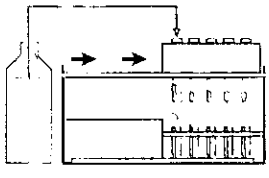


Dilutes
Adds standards
Derivatizes

2 - Automated SPE

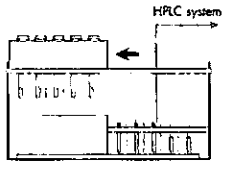


Conditions
Adds sample
Washes



Elutes

3 - Direct HPLC injection



And injects
your cleaned-up
sample

Manual SPE methods are directly transferable to ASPEC XL. Each step is automated - from initial sample dilution ... to solid phase extraction ... right through to direct HPLC injection.

For more information:
Contact: John Morris Scientific Ltd
P O Box 6348 Wellesley Street, Auckland
Ph: (09) 3663999, Fax: 3663060

circle number 56 on the reader reply card

4th Annual RACI Research and Development Topics In Analytical Chemistry Meeting
(9-11 December 1996)
Hosted By: RMIT, Melbourne, Australia

This conference provides a forum for young researchers in the area of analytical chemistry to present their work. We are now calling for expressions of interest from people who wish to be added to our mailing list.

Contact: Marie Bou-Raad
Secretary of the Organising Committee
Tel: (+61-3)-96602557
Fax: (+61-3)-96391321
Email: chem_rd96@bunyip.ph.rmit.edu.au

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  - residue trials for registration of agrichemicals
- Mycotoxins in grains and grain based products
- Persistent contaminants in soil, sediments, biota - organochlorines, PCBs, chlorophenols, PAHs
- Spray drift - hormone herbicides, sulfonylureas, glyphosate
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Colin Malcolm
Laboratory Manager, Ruakura Research Centre, Private Bag 3123, HAMILTON
Tel: 07 856 2835 Fax: 07 838 5085 Email: MalcolmC@hort.cri.nz

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CONFERENCES & SEMINARS

4-5 June 1996

4th New Zealand Symposium on Chemical and Biosensors

Venue: William Sutton Room
The Arts Centre of Christchurch
Christchurch, New Zealand

Contact: Wendy Collier
AgResearch Grasslands
Private Bag 11008
Palmerston North, New Zealand
Tel: (+64-6)-3568019
Fax: (+64-6)-3518032/8042
Email: collierw@agresearch.cri.nz

16-21 June 1996

HPLC'96: 20th International Symposium on High Performance Liquid Phase Separations and Related Techniques

Venue: Marriott, San Francisco, California, USA

Contact: Janet Cunningham
Barr Enterprises
P O Box 279
Walkersville
MD 21793, USA
Tel: (+1-301)-8983772
Fax: (+1-301)-8985596

14-18 June 1996

1st Science Centre World Congress

Venue: Heureka, Vantaa, Finland

Contact: Ms Helena von Troil
Secretary General, Keureka
The Finnish Science Centre
P O Box 166, FIN-01301 Vantaa, Finland

27-28 June 1996

IQT International Quality Techniques

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Venue: Barrycourt Motor Inn
10-20 Gladstone Rd
Parnell, Auckland

Contact: Professional Courses
Centre for Continuing Education
The University of Auckland
Tel: (09)-3737599 ext 7050 or 7619
Fax: (09)-3737419

29 June - 3 July 1996

UIB-GBF-CSIC-TUB Symposium on 'Biodegradation of Organic Pollutants'

Venue: Mallorca, Spain

Contact: Professor K N Timmis
Division of Microbiology
GBF, Mascheroder Wegl
D-38124 Braunschweig, Germany
Fax: (+49-531)-6181411
Email: kti@gbf-braunschweig.de

30 June - 6 July 1996

12th International Symposium on 'Flavins and Flavoproteins'

Venue: Calgary, Canada

Contact: Dr K J Stevenson
Department of Biological Sciences
University of Calgary
Calgary T2N 1N4
Alberta, Canada
Fax: (+1-403)-2844184

7-12 July 1996

Organometallic Chemistry XVII

Venue: Brisbane, Australia

Contact: Eva Comino
Secretariat, International Conference on Organometallic Chemistry
Faculty of Science and Technology
Griffith University
Brisbane, QLD 4111, Australia
Tel: (+61-7)-8757564
Fax: (+61-7)-8755369

8-12 July 1996

International Congress on Clinical Chemistry

Venue: London, England, UK

Contact: Tel: (+44-1280)-860613

9-11 July 1996

Chromatogra

ence for all educational decision makers and those concerned about tertiary education issues.

Contact: Kate Richardson
Auckland Institute of Technology
Private Bag 92 006, Auckland
Tel: (09)-3079871
Fax: (09)-3079792
Email: Kate.Richardson@AIT.ac.nz

11-12 July 1996

Perspectives in Marine Natural Products

Venue: The Conference Centre
University of Auckland, Auckland, New Zealand

Contact: Professor R C Cambie
or Dr B R Copp
Department of Chemistry
University of Auckland
Private Bag 92019, Auckland, New Zealand
Tel: (+64-9)-3737999 ext. 8259 or 8284
Fax: (+64-9)-3737422
Email: c.cambie@auckland.ac.nz

14-18 July 1996

Ribonucleases: Chemistry, Biology and Biotechnology

Venue: Groningen, The Netherlands

Contact: Secretariat, 4th International Meeting on Ribonucleases
Biochemisch Laboratorium
Nijenborgh 4, 9747 AG
Groningen, The Netherlands

CONFERENCES & SEMINARS

14-19 July 1996

RACI/SETAC/ASE International Conference on Environmental Chemistry and Toxicology

Venue: Sydney, NSW, Australia

Contact: Dr Graeme Batley
CSIRO Centre for Advanced Analytical Chemistry
PMB 7, Menai
NSW 2234, Australia
Tel: (+61-2)-7106830
Fax: (+61-2)-7106837

14-19 July 1996

14th International Conference on Chemical Education (14ICCE)

Venue: Brisbane, Queensland, Australia

Contact: Sally Brown
Conference Secretariat
14th ICCE
Continuing Professional Education
The University of Queensland
Brisbane, QLD 4072, Australia
Tel: (+61-7)-3656360
Fax: (+61-7)-3657099
Email: chemed96@ceu.uq.oz.au

29 July - 2 August 1996

Recent Advances in Polymer Synthesis

Venue: University of York, England, UK

Contact: Professor P Hodge
Department of Chemistry
University of Manchester
Oxford Rd, Manchester
M13 9PL, England, UK
Fax: (+44-1)-612754598
Email: philip.hodge@man.ac.uk

4-9 August 1996

IUPAC MACRO '96

Venue: Seoul, Korea

Contact: Dr Kwang Ung Kim
Secretariat IUPAC MACRO SEOUL '96
Division of Polymers, KIOST
P O Box 131, Cheongryang
Seoul 130-650, Korea
Fax: (+1582-2)-9576105
Email: iupac@kistmail.kist.re.kr

4-10 August 1996

VI World Conference on Clinical Pharmacology and Therapeutics

Venue: Buenos Aires, Argentina

Contact: CPT96
Marcelo T de Alvear 1980
1122 Buenos Aires, Argentina
Tel: (+54-1)-8116650
Fax: (+54-1)-8142733

11-16 August 1996

3rd International Hydrocolloids Conference

Venue: Sydney, Australia

This conference will focus on the new industrial opportunities for hydrocolloids in important areas including foods, nutritional products, pharmaceuticals, health and personal care products and agricultural and veterinary products. To meet those challenges, the conference will discuss novel production and processing techniques.

Contact: Gail Hawke, Conference Secretariat
P O Box N399, Grosvener Place
Sydney, NSW 2000, Australia
Tel: (+61-2)-2523388
Fax: (+61-2)-2415282

11-16 August 1996

6th Annual Queenstown Molecular Biology Meeting

Venue: Queenstown, New Zealand

Contact: Dr Martin Kennedy
Cytogenetic and Molecular Oncology Unit
Christchurch School of Medicine
P O Box 151, Christchurch, New Zealand
Fax:(+64-3)-3640750
Tel: (+64-3)-3640880
Email: mkennedy@chmeds.ac.nz

12-16 August 1996

Australasian Association of Clinical Biochemists Annual Scientific Meeting

Venue: Darwin, Australia

Contact: Tel: (+61-9)-3705224

25-30 August 1996

10th International Biotechnology Symposium

Venue: Sydney, Australia

Contact: Symposium Secretariat
G P O Box 128
Sydney, NSW 2001, Australia

1-4 September 1996

Environmental Biotechnology, An International Conference

Venue: Massey University
Palmerston North, New Zealand

Contact: Conference Secretary
Environmental Biotechnology Conference
Process and Environmental Technology Dept.
Massey University
Palmerston North, New Zealand
Tel: (+64-6)-3505351
Fax: (+64-6)-3505654
Email: g.f.withers@massey.ac.nz

10-13 September 1996

NZWWA Annual Conference and Expo

Venue: Quality Hotel Rutherford, Nelson, New Zealand

Contact: NZWWA Annual Conference and Expo
C/- Conferences & Events
P O Box 1254, Nelson, New Zealand
Tel: (+64-3)-5466022
Fax: (+64-3)-5466020

CONFERENCES & SEMINARS

16-18 September 1996
Engineering Crops for Industrial Uses
Venue: Bristol, England, UK
Contact: Professor P. R. Shewry
IACR-Long Ashton
Department of Agricultural Sciences
University of Bristol, Long Ashton
Bristol BSl9 9AF, England, UK
Fax: (+44-1275)-394299

24-26 September 1996
BioInnovations Convention
Venue: Wembley, London, England, UK
Contact: Bob Kyte, Step Exhibitions Ltd
The Studio, Northfields, Speldhurst
Tunbridge Wells, TN3 OPL, England, UK
Tel: (+44-1892)-863986
Fax: (+44-1892)-863464

24-26 September 1996
Science 2000 Conference and Exhibition
Venue: Melbourne, Australia
Contact: Tel: (+61-2)-8716180

29 September - 4 October 1996
The International Meeting and Exhibition of the Australian and New Zealand Societies For Microbiology
Venue: Christchurch, New Zealand
Contact: ASM and NZSM '96 Secretariat
G P O Box 128
Sydney, NSW 2001, Australia
Tel: (+61-2)-2622277
Fax: (+61-2)-2622323
Email: TOURHOSTS@TOURHOSTS.com.au

3-4 October 1996
The Second Australian Molecular Modelling Workshop
(ASBMB/ASPP Satellite Meeting)
Venue: John Curtin School of Medical Research
Australian National University
Canberra, Australia

The Workshop has invited overseas and local speakers presenting review/future directions talks, selected oral papers, posters and software demonstrations. The planned program includes sessions on:

Protein Structure Prediction (1-D to 3-D profiling/threading, sequence analysis, secondary structure prediction, derived 3-D databases and folds, homology building)

Drug Design (molecular similarity, docking, *de novo* ligand design)

Computational Chemistry and Simulations (hybrid quantum and molecular mechanics (qm/MM), conformational searching, protein dynamics, free-energy perturbation/molecular dynamics)

Force Fields and Solvation (force field development, electrostatic potentials, solvation).

Contact: Dr Jill Gready
John Curtin School of Medical Research
Australian National University
Canberra, ACT 0200, Australia
Tel: (+61-6)-2798304
Registration: mmworkshop@jcsmr.anu.edu.au
www: http://biocomp.anu.edu.au/Wkshops/MolMod

6-11 October 1996
Australian Institute of Medical Scientists, National Scientific Meeting
Venue: Adelaide, South Australia
Contact: Tel: (+61-8)-2391515

8-11 October 1996
Hands-On Computer Workshop on Molecular Modelling and Bioinformatics of Protein Structure and Function
(ASBMB/ASPP Satellite Meeting)
Venue: Computational Science and Engineering Laboratory, Australian National University
Canberra, Australia

The Workshop will focus on developing skills in accessing and analysing database information on protein structure (1-D and 3-D) using molecular graphics and other display tools, manipulating protein structure and investigating protein-protein and protein-ligand interactions, undertaking limited computations (molecular mechanics and dynamics), and using protein structure prediction methods (1-D to 2-D and 1-D to 3-D). The format will be mostly structured exercises leading into project work chosen within participants' interests. Exercises will be conducted on SGI workstations using commercial software and with net access to external databases and servers. There will be a minimum of lectures to introduce topics. The main targeted participants are research students and postdoctoral workers in experimental biomolecular science.

Contact: Dr Jill Gready
Computational Molecular Biology and Drug Design Group
Division of Biochemistry and Molecular Biology
John Curtin School of Medical Research
Australian National University
Canberra, ACT 0200, Australia
Tel: (+61-6)-2798304
Fax: (+61-6)-2490415
Email: Jill Gready@anu.edu.au
Registration: mmworkshop@jcsmr.anu.edu.au
www: http://biocomp.anu.edu.au/Wkshops/HandsOn

8-11 October 1996
AUSPLAS '96 (Australian Plastics Conference)
Venue: Melbourne Exhibition Centre
Melbourne, Australia
Contact: John Kelly
Exhibition Management Pty Ltd
Melbourne, Australia
Tel: (+61-3)-96464044
Fax: (+61-3)-96461828

9-11 October 1996
Anti-Cancer Targets and Strategies for the 21st Century
Venue: Castres, France

Contact: Marian Cabailh
Conference Secretariat, CRPF
17 Avenue Jean Moulin
81106 Castres Cedex, France
Tel: (+33-63)-714368
Fax: (+33-63)-714299

22-25 October 1996
19th International Federation of Societies of Cosmetic Chemists Congress
Venue: Darling Harbour, Sydney, Australia
Contact: Secretariat
P O Box 249 Kingsgrove
New South Wales 2208, Australia
Fax: (+61-2)-5543228
or Peter Strasser
Tel: (+61-3)-93875371

23-24 October 1996
Near Infrared Spectroscopy and Imaging of Living Systems - A Royal Society Discussion Meeting
Venue: London, England, UK
Contact: Science Promotion Section
The Royal Society
6 Carlton House Terrace
London SW1Y 5AG, England, UK
Fax: (+44-171)-8392891
Tel: (+44-171)-8395561

23-24 October 1996
Applications of Membrane Technologies - A Short Course
Venue: University of Auckland, Auckland
Contact: Dr Paul Pickering
Natural Products Processing Group
School of Engineering
University of Auckland
Private Bag 92019
Auckland
Tel: (+64-9)-3735799 ext 8112
Fax: (+64-9)-3737463

12-15 November 1996
Pacific Rim Biotechnology Conference
Venue: Seoul, Korea
Contact: Fax: (+82-42)-8604739

19-21 November 1996
Joint ICP and New Zealand Trace Elements Groups Conference
Venue: Le Grand Hotel, Victoria Street, Hamilton, New Zealand
Organisor: Waikato Branch, New Zealand Institute of Chemistry, New Zealand Trace Element Group
Topics to be included:
Trace elements - analysis, importance in agriculture, horticulture, health, and the environment
ICP-MS and ICP-OES - instrumental technique, sample preparation, applications.
The conference will include Plenary Speakers, invited and submitted papers, a trades display and a conference dinner.
Contact: Dr Peter Robinson
R J Hill Laboratories Ltd
P O Box 4048
Hamilton, New Zealand
Ph: (+64-7)-8552266
Fax: (+64-7)-8549886
Email: Peter@rjhill.co.nz

24-27 November 1996
Australian Society for Medical Research, National Scientific Conference
Venue: Gold Coast, Queensland, Australia
Contact: Fax: (+61-7)-38757665

25-29 November 1996
13th International Corrosion Congress
Venue: Carlton Radisson Hotel, Melbourne, Australia
Contact: Conference Secretariat
P O Box 5142, Clayton
Victoria 3168, Australia
Tel: (+61-3)-95440066
Fax: (+61-3)-95435905

2-6 December 1996
NZSBMB/NZIC Joint Conference 1996: "Molecules for the Future"
Venue: University of Otago, Dunedin, New Zealand
Contact: Dr K J F Farnden
Biochemistry Department
University of Otago
P O Box 56
Dunedin, New Zealand
Ph +64-3-4797874
Fax +64-3-4797866
Email:kevinjff@sanger.otago.ac.nz
Confirmed speakers at this time are:

Colloids and Surfaces	- Roger Horne, Adelaide
Chemical Education	- Professor John Emsley, Imperial College London
Cell Walls	- Professor Nick Carpita, Purdue University
Pigments	- Professor Raymond Brouillard, Universite Louis Pasteur, Strasbourg
Analytical Chemistry	- Professor Frank Millero, Rosenstiel School of Marine and Atmospheric Sciences, University of Miami

9-11 December 1996
4th Annual RACI Research and Development Topics In Analytical Chemistry Meeting
Venue: RMIT, Melbourne, Australia
Contact: Marie Bou-Raad
Secretary of the Organising Committee
Tel: (+61-3)-96602557
Fax: (+61-3)-96391321
Email: chem_rd96@bunyip.ph.rmit.edu.au

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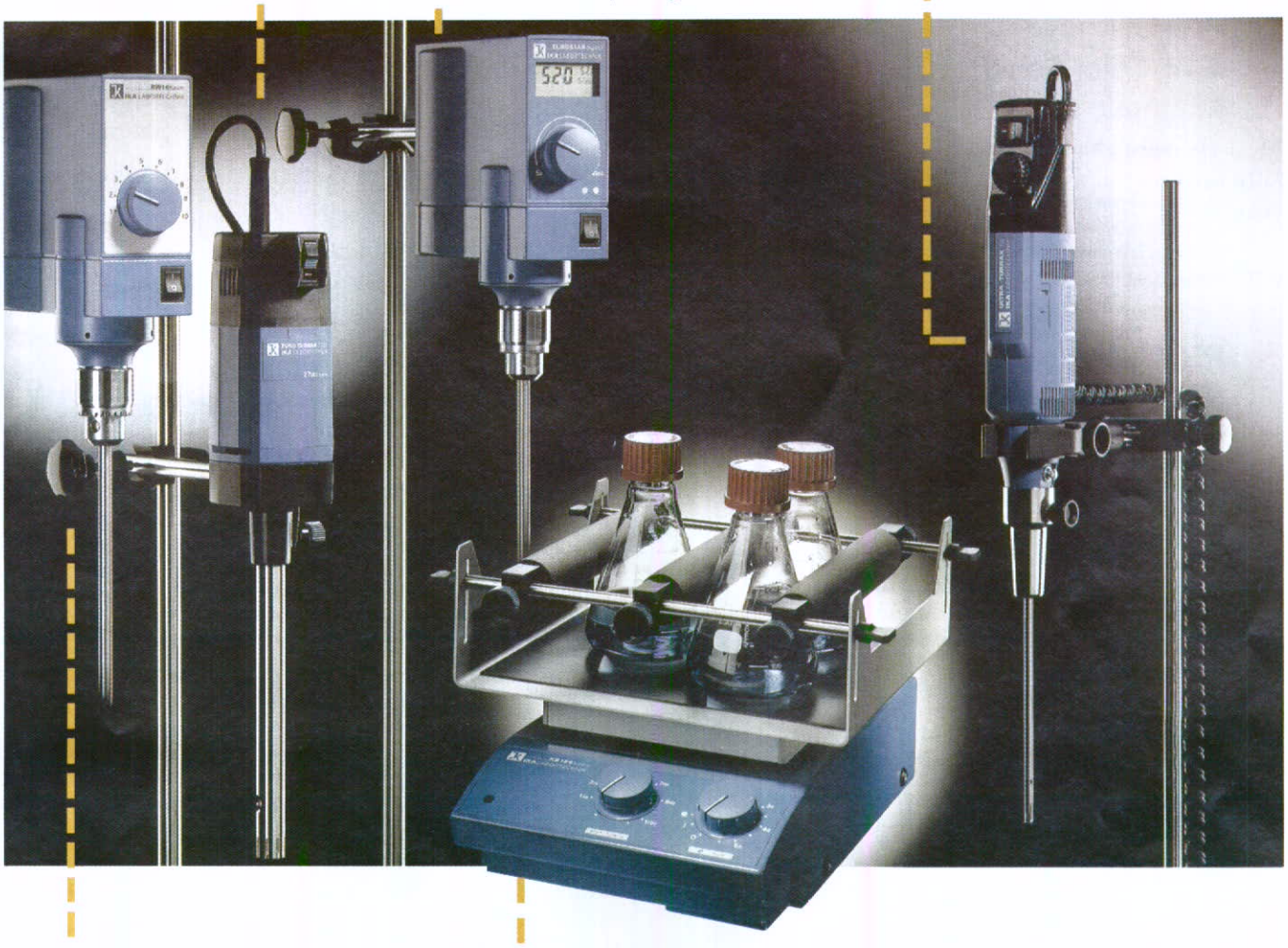

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CONFERENCES & SEMINARS

13-15 December 1996

Second Symposium on Oceanian - Japanese Organic Chemistry Synthesis and Natural Products

Venue: Tokushima Bunri University
Faculty of Pharmaceutical Sciences, Japan

Contact: Associate-Professor Rob A J Smith
Chemistry Department
University of Otago
P O Box 56
Dunedin, New Zealand
Tel: (+64-3)-4797924
Fax: (+64-3)-4797906
Email: rajsmith@alkali.otago.ac.nz

10-14 December 1996

Fifth Eurasia Conference on Chemical Sciences

Venue: Zhongshan (Sun Yatsen) University
Guangzhou (Canton), China

Contact: Professor Liang-Nian Ji
General Secretary, EuAsC_2S-1996
Biotechnology Research Centre
Zhongshan (Sun Yatsen) University
Guangzhou (Canton) 510275, China
Tel: (+86-20)-4185461
or Tel: (+86-20)-4186300-7115
Fax: (+86-20)-4189173 or (+86-20)-4185551
Email: leiy@pebc2ihep.ac.cn
or Professor Charmian O'Connor
Chemistry Department, University of Auckland
Private Bag 92019, Auckland, New Zealand
Tel: (+64-9)-3737999

2-6 February 1997

The Australian and New Zealand Society for Mass Spectrometry 16th Conference (ANZSMS 16)

Venue: University of Tasmania, Tasmania, Australia

Contact: Mures Convention Management
Victoria Dock
Hobart, TAS 7000, Australia
Tel: (+61-002)-312121
Fax: (+61-002)-344464
Email: mures@hba.trumpet.com.au
http://www.cslutas.edu.au/ANZSMS/anzsms16.html

3-7 February 1997

22nd Australasian Polymer Symposium

Venue: Auckland, New Zealand

Contact: Mr N R Edmonds
Faculty of Science and Engineering
Auckland Institute of Technology
Private Bag G P O, Auckland, New Zealand
Tel: (+64-9)-3079999 ext: 8181
Fax: (+64-9)-3079973

9-13 February 1997

1997 Lorne Meeting on Protein Structure and Function

Venue: Lorne, Victoria, Australia

Plans for the meeting will be available on the WWW site: http://grimwade.biochem.unimelb.edu.au.

Contact: lorne_orgs@unimelb.edu.au

10-14 February 1997

Microscopy 97. Microscopy New Zealand Conference.

Venue: Medical School, University of Auckland
Auckland

Contact: Dr Ian Hallett
HortResearch, Private Bag 92169, Auckland
Tel: (09) 8493660
Fax: (09) 8154201
Email: ihallett@hort.cri.nz

16-20 May 1997

Seventh Asian Chemical Congress

Venue: International Conference Center Hiroshima
Hiroshima, Japan

Contact: Mr A Nakanishi
Head, Administration Office of 7ACC'97
Chemical Society of Japan
1-5, Kanda-Surugadai
Chiyoda-ku, Tokyo 101, Japan
Tel: (+81-3)-32926161
Fax: (+81-3)-32926318
Email: 7acc97@chemistry.or.jp
www: http://www.t.soka.ac.jp/chem/csj/7ACC.html

18-22 August 1997

8th European Congress on Biotechnology, 70th Event of The European Federation of Biotechnology

Venue: Budapest, Hungary

Contact: Professor Laszlo Nyeste
Department of Agricultural Chemical Technology
Technical University
Budapest, H-1121 Budapest XI
Hungary
Tel/Fax: (+36-1)-463220

21-26 September 1997

XXX Colloquium Spectroscopicum Internationale

Venue: World Congress Centre
Melbourne, Australia

Contact: The Meeting Planners
108 Church Street
Hawthorn, Victoria 3122
Australia
Tel: (+61-3)-98193700
Fax: (+61-3)-98195978

13-17 July 1998

MACRO '98 - 37th IUPAC International Symposium on Macromolecules

Venue: Gold Coast, Queensland, Australia

Contact: Department of Chemistry
University of Queensland
Queensland 4072, Australia
Tel: (+61-7)-3653511
Fax: (+61-7)-3653628

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Chemie-Tech Ltd, P O Box 51-064 Pakuranga, Auckland

Update

The Select Committee considering the Hazardous Substances and New Organisms Bill reported back to Parliament on 19 December 1995. The Bill underwent it's second reading on the 16 April 1996 and awaits debate by the Committee of the House. This debate is likely to occur late May or early June. The third reading is usually a formality, occurring within a few weeks of the debate. The reported back Bill showing the detailed changes is available from Government Book Shops.

A few of the points raised in our submission (*Chemistry in New Zealand*, May 1995) have been addressed. Many have not but could be addressed in the Regulations. The major changes to the Bill are outlined in a document entitled "Hazardous Substances and New Organisms Bill Report of the Committee on the Bill". Changes on which we commented include:

- A slight strengthening of the "precautionary principle"
- A small increase in the number of Authority members.
- Increase in the magnitude of the fines.
- A co-ordination role for ERMA in enforcement.
- Competency requirements for enforcement officers

Submission on the Ministry for the Environment's (MfE) Discussion Paper "Proposals for Regulations Under the Hazardous Substances and New Organisms Bill" closed officially on 28 March 1996, however, late submissions were accepted up to the middle of April. The comments received are being analysed.

Where to from here?

This year will see a major drive to finalise HSNO Regulations and encourage / guide industry to develop (approved) Codes. Once the analysis of the comments has been completed MfE will be seeking expert groups to assist with specific aspects of the Regulations development.

It is clear that the Regulations are to be performance-based and where possible to be scientifically measurable, rather than descriptive. This requires:

- **The required performance to be elucidated.**
- **Suitable parameters to be chosen as measurements of the required performance.**
- **Values of the chosen parameters to be chosen as either acceptable or not acceptable.**

Specifying performance rather than prescribing a means or method of compliance is not as easy as it first appears. The first problem is to ensure that **all** the required performances have been determined. As an example consider the underlying performance of a reinforced concrete wall as prescribed for a Type D Flammable Liquids Dangerous Goods Storage Depot.

- What is the purpose of the wall?
- Is it intended to prevent a fire outside the depot from reaching the stored dangerous goods inside?
- Is it intended to prevent a fire inside the depot from spreading?
- Is it intended to resist an explosion resulting from a fire in the dangerous goods?
- If the wall's primary function is to resist fire, can it's performance be specified as a Fire Resistance Rating (FRR)?
- Timber framed, gib-board clad walls can attain 3 hour ratings. Is this the same as the reinforced concrete wall?
- Is the performance of these walls the same as a reinforced concrete wall in a real fire?
- Is any other performance implied by the reinforced concrete wall?
- Does the wall need to be impact and abrasion resistant? A fire wall with a hole in it rapidly looses it's FRR.

The danger of poorly specified performance-based Regulations is that not all the performance has been elucidated. In the above example it would have been easy to have overlooked the need for abrasion resistance and durability, implicit in the reinforced concrete wall.

Good performance-based Regulations have the ability to allow a number of means of compliance. As they are not dependant on a particular means or method, they will readily accommodate new technologies and advancements in material science.

As scientists we must applaud the development of performance-based Regulations. As scientists we must assist MfE in elucidating all the required performances and we must assist in determining suitable parameters and acceptable values for use in the Regulations. If we do not, we will return to the wilderness of descriptive performance and the results are likely to be unpalatable. At worst incomplete specification of required performance may reduce rather than improve safety.

Between now and the next round of public consultation on the HSNO Regulations, it is imperative for us to put our energies and technical abilities into obtaining data on which to develop **good Regulations.** A good place to start would be to derive the implied performance embodied in prescriptive style legislation currently applying to your place of work. What measurable performance (lower explosive limit, ignition energy etc.) would provide the same or improved safety?

Industry sectors and larger companies should be starting to develop Codes which ERMA could approve. In many cases these may be created form an adaptation of current documents.

Some notes on my involvement with hazardous substances:

As a member of the New Zealand Institute of Chemistry (Auckland Branch committee), I chaired the Dangerous Goods sub-committee and made comment on the draft of NZS 5433:1983. I made substantial comment on the first revision of this document during 1988 and received a letter of appreciation from the Standards Association for my contribution.

Chemie-Tech is a member of the New Zealand Chemical Industry Council. I have served two years on the Executive (1991 - '93), during which time I was Co-Convener of the Health and Safety Committee. I am a member of the newly formed Technical Advisory Board.

During the period, December 1991 to May 1994, Chemie-Tech was retained as a Consultant by the MfE and I have provided technical advice on aspects relating to the drafting of the Hazardous Substances and New Organisms Bill.

In early 1994, Chemie-Tech was engaged by the Land Transport Safety Authority to make recommendations on the content of a technical document to replace NZS 5433. This work was completed in May 1994.

In 1994, I completed a review of the Approved Solution F3/AS1 "Hazardous Substances and Processes" for the Building Industry Authority as part of a review of Clause F3 of the Building Code.

Also in 1994, I was invited to become a member of the Air Transport Dangerous Goods Council, whose purpose is to improve the safe transport of dangerous goods by air.

During 1995, I was invited to join Standards Australia / Standards New Zealand Joint Technical Committee CH/9 Safe Handling of Chemicals. I am involved in the rewriting of "The storage and handling of toxic substances" and "Safe Warehousing of Dangerous Goods".

Chemie-Tech has carried out further project work for the Ministry for the Environment, contributing to the development of the Hazardous Substances and New Organisms Regulations.

I have recently completed a report on packaging standards for dangerous goods for the Civil Aviation Authority. This report made a number of recommendations for changes in the process of approval for packaging.

I was a member of the "Working Group" referred to in paragraph 2 (page vii) of the Red Draft of Rule 45001: Land Transport Safety (Dangerous Goods).

Chemie-Tech currently has a contract with the Ministry of Transport to update the publication "A Guide to the Transportation of Hazardous Substances".

In October 1995 I became the only New Zealand representative on the Co-ordinating Group for the Harmonisation of Chemical Classification Systems. This group is supported by five specialist UN Organisations and the OECD. The task is to globally harmonise the Hazard Classification and Hazard Communication. This effectively means melding the UN system with the occupational health and safety criteria of the EU, Eastern Block and North America. The aim is to elucidate a workable scheme by the end of 1997 and have it implemented by the year 2000. Dr S R Vaughan of MfE has also become a member of this committee.

In March 1996 I was elected Chairman of the New Zealand Air Transport Dangerous Goods Council.

NZIC CONNECTS TO THE WORLD WIDE WEB

Daily we hear about the Internet and the effect it will have on our future. The NZIC has joined the information age and has established a home page at:

http://webtwo.rsnz.govt.nz/www/nzic/nzic.html.

The front page is shown in Figure 1 below. Each header is the link to information about the NZIC.

About the NZIC is a document with basic information about the Institute. In it you will find information about the aims and ethics of the NZIC, a list of Council members and their Email addresses, membership information, the publications of the NZIC, and a calendar of NZIC activities.

Branches and Specialist Groups is a listing of the contact people for the branches and specialist groups. It also lists links to New Zealand University Chemistry and Biochemistry Departments and to other chemical societies worldwide.

Prizes and Awards contains information about the various prizes and awards sponsored by the NZIC.

Conferences and Meetings lists information and, in some cases, links to conferences in New Zealand.

News is regularly updated with Council News and articles by Nath Pritchard.

In this month's issue, writing in *"From the President"*, Nath Pritchard discusses the importance of improved communications to the role of the Institute and that timely communication needs to be based on our computers. The Web page is the first step in addressing those needs and I hope it will change to meet members needs (it has already changed to mention the President).

Already I have received suggestions for improvements. Some of these are: - listing overseas conferences, placing job advertisements, providing a searchable database of members and their skills, joining with the American Chemical Society for the International Chemistry Celebrations in April 1999.

Universities and many research institutes are connected to the Internet. Many of you will have a computer sitting on your desk. The page must evolve to meet your needs.

So get clicking and send me your comments!!

Grant Boston
Web Page Coordinator
Manawatu Branch
Email: nzic.manawatu@nzdri.org.nz

NEW ZEALAND INSTITUTE OF CHEMISTRY

Please note that these pages are developing. Some links may not be active. Please bear with us and direct any questions or comments to Grant Boston.

Welcome to the NZIC homepage

About the NZIC **(Last changed 19 April 1996)**

Branches and Specialist Groups **(Last changed 19 April 1996)**

There are 6 Branches and 10 Specialist Groups. There are also some Links to other chemistry sites in NZ and overseas.

Prizes and Awards **(Last changed 31 March 1996)**

Conferences and Meetings **(Last changed 19 April 1996)**

News **(Last changed 5 May 1996)**

Throughout these pages two navigation icons appear, they are:

Go to the top of the current page

Return to this, the NZIC homepage

Page maintained by Grant Boston, Manuwatu Branch.
This page is generously hosted by the Royal Society of New Zealand.

Figure 1: *The NZIC home page*

MOLECULES FOR THE FUTURE

NATIONAL CONFERENCE
of the
NEW ZEALAND INSTITUTE OF CHEMISTRY
and the
NEW ZEALAND SOCIETY FOR BIOCHEMISTRY AND MOLECULAR BIOLOGY
DUNEDIN, 2-6 DECEMBER 1996

Planning for the NZSBMB annual conference, this year held conjointly with the New Zealand Institute of Chemistry (NZIC), is well underway; the Planning Group is Brian Robinson, Mel Carr, Jim Simpson, Kevin Farnden, Nigel Perry, Jim McQuillan, Ross Grimmett with Wayne Temple and Keith Hunter assisting with sections of the programme.

We are keen to involve all sections of the New Zealand Institute of Chemistry and the New Zealand Society of Biochemistry and Molecular Biology in the programme and to have a mix of pure and applied science. An exciting and stimulating programme has been organised around the following themes and sub-themes (in brackets):

Analytical/Environmental (marine and atmospheric chemistry, advances in analytical methods) Organiser: Keith Hunter

Biological and Organic Chemistry (flavanoids, proteins, drug design, proteins and enzymes, gene structure/function, cell signalling, plant pigments, cell walls) Organisers: Kevin Farnden/Nigel Perry/Dave Larsen

Colloids, Surfaces and Materials (colloids and surfaces, theoretical and spectroscopy, new materials, energy) Organiser: Jim McQuillan

Plenary Speakers:
Conference Speaker: Dr John Emsley (Imperial College)
Analytical: Professor Frank Millero (Miami)
Biological: Professor Nick Carpita (Purdue University); Professor Raymond Brouillard (Universite Louis Pasteur, Strasbourg), Dr Jenny Martin (University of Queensland)
Surfaces: Professor Roger Horn (Adelaide)

Keynote Speakers from both New Zealand and overseas will be associated with each sub-theme. A highlight will be a mini-symposium on Friday (6 December) on Chemical and Biological Hazards. This is being organised by Wayne Temple and it will feature a panel discussion and contributions from Government departments, industry etc. It will be targeted at people working in the education sector, public bodies, government departments, industry and researchers.

The 1996 Watson Victor Award Lecture will be delivered (nominations for this award are requested elswhere in this issue of *NZ BioScience),* as too will award lectures associated with the New Zealand Institute of Chemistry.

The Main Programme runs on Tuesday, Wednesday morning and Thursday with a mix of Plenary and invited speakers. Poster sessions are on Tuesday and Wednesday evenings. Wednesday afternoon is free and the Conference Dinner is on Thursday evening.

The Trades Exhibit will be held throughout the Conference but with specific lunch-time presentations.

We have had a good response to the first circular and are planning for 200-250 for the main conference. The conference fee will be relatively low — $160 (for NZSBMB/NZIC members), $200 (non-members), $30 (student NZSBMB/NZIC members) and $60 (student non-members).

There will be associated student oral and poster paper competitions and travel assistance for students. Details of these are supplied elsewhere in this issue of *NZ BioScience*. The second circular will be available in June 1996 and will be sent to those who responded to the first circular.

For further information contact:
Dr R M Carr,
Chemistry Department
University of Otago
P O Box 56
DUNEDIN
Phone (03) 4797932
Fax (03) 4797906
Email: Diana@alkali.otago.ac.nz

NZIC NEWS

MEMBERSHIP REPORT

The following have recently been elected to the various grades of membership as indicated:

Honorary Fellow

Manawatu	MALCOLM, Geoffrey Norman

Fellow

Auckland	NORRIS, Rodney John
Waikato	DAWSON, Peter Alistair
Wellington	SANDFORD, George Alexander William

Member

Waikato	GILKINSON, Richard William

Associate

Auckland	MITCHELL, Lorna
	TONEI, Deborah
Otago	BAXTER, Anthony
	GHOLAMI, Majtaba
	KERR, Joy

Student

Auckland	DANSTED, Paul
	CLARK, Russell
	CRAIG, Peter
Otago	SMIT, Ruben

Deceased

It is with sadness that we record the deaths of the following members:

Auckland	GALLAHER, P J
	ROGERS, J
Waikato	JOERIN, M M
Wellington	NAISH, G
Canterbury	HOUNSELL, E R

COUNCIL NOTES

Council met in Wellington on 7 March 1996 and Professor Brian Robinson (1996 Conference Chairman) and Mr Robert Lyon (Journal Editor) were also in attendance. The focus of the meeting was the strategic review but other highlights included the following:

Overseas Visitors

A grant from the Overseas Visitors Fund was made to assist Dr Malcolm Gerlock from Cambridge University visit all six Branches. He lectured on the roles of the *d* electrons in transition metal chemistry.

A letter of appreciation for financial assistance was tabled from Professor Deeming of University College, London, following his visit to Branches and University Chemistry Departments late last year.

Financial

A draft budget was presented by the Treasurer Mr Dennis Karl which assessed income at varying rates of subscription, as discussed in the Strategic Review. As the income level will dictate the level of expenditure for the ensuing year, a business plan is being drawn up which will prioritise the services and benefits to members. This will be reviewed/adopted at the next Standing Committee meeting in May.

Consideration is also being given to changing the current financial year (1 May to 30 April), to a calendar year with a similar change for elected members of Council.

Membership

It was with considerable pleasure that Council unanimously elected Professor Geoff Malcolm, recently retired from Massey University, an Honorary Fellow of the Institute. The membership report appears earlier.

Honours/Awards

It was noted that Dr Stan Simpson received an OBE for services to the wool industry and that five members were recently elected to Fellowship of the Royal Society of New Zealand - they were Kevin Tate, Patrick O'Sullivan, Peter Steel, John McKinnon and Lawrence Creamer. Letters of congratulation have been forwarded.

Conference

Professor Brian Robinson tabled the draft programme of the 1996 conference to be held in Dunedin in early December. The theme will be "MOLECULES FOR THE FUTURE" and will cover several fields of chemistry from analytical, through biological to new materials. One session is in the education area and will deal with chemical and biological hazards. The conference fees have been set at a relatively low level and should ensure a good turnout of members to the conference.

The American Chemical Society is drawing up plans to hold an INTERNATIONAL CHEMISTRY CELEBRATION in 1999 to herald the new millennium! It is our intention to participate.

The NZIC *In Action*

CHEMISTRY OLYMPIAD UPDATE

The Chemistry Olympiad Training camp was held in Auckland April 10-15 1996. Seventeen students attended (7 from Auckland, 1 from Tauranga, 1 from Wanganui, 4 from Christchurch, 1 from Nelson, 1 from Te Puke, 1 from Wellington and 1 from Waipukurau). Two students from Auckland and one from Christchurch were female. Dr Sheila Woodgate organised the camp with the help of Dr Jan Giffney who teaches at St Cuthbert's College in Auckland, Irine Oeng also provided valuable assistance. Irine is a bronze medallist from the 1995 Olympiad team.

The students attending the camp were among the thirty-two who were selected on the basis of a test they sat in October, 1995. A larger number of students was selected this year as it has become apparent that the student's knowledge of chemistry reflected by performance in a theory exam does not necessarily indicate the extent to which the same student will rise to the Olympiad challenge. Considerable commitment as well as the ability to study independently is required. It was the intention to exclude some of these students before the camp; however this was not necessary as during the January to April interval, those interested in continuing with training diminished to the seventeen described above.

During the period after selection and before the camp, the students were given both textbook and purpose-written background material relevant to the set of Preparatory Problems supplied by the Russian Olympiad Committee, the host for the 1996 Olympiad in Moscow. The purpose-written material proved popular, and more will be developed by Sheila Woodgate next year. A series of assignments and two tests during this period helped to begin to discriminate between students in the group.

The camp consisted of four workdays, each having two hours of lectures and two hours of problem-solving relevant to those lectures. The problem sessions were very lively, and each and every student, irrespective of their previous performance, tried very hard to come to grips with concepts on which they had just been lectured. On three of the four days there was a three hour laboratory session in the afternoon. Two of these focused on titrations, and the third on organic preparative chemistry. Preparation of cinnamic acid, one of the laboratory exercises suggested by the Russian Olympiad Committee and executed by these high school students is done by advanced organic chemistry students at the University of Auckland. All students took the tasks very seriously, and all three supervisors were kept extremely busy assisting the students with their experiments. Gratifyingly, it was obvious that the laboratory sessions were enjoyed immensely by all candidates.

Team selection was based on a three hour examination on the fifth day and on performance in the practical exercises carried out during the camp. The members of this year's team are Ben Clark (Wellington College; bronze medallist from the 1995 Chemistry Olympiad held in Beijing, China), Derek Caudwell (Tauranga Boys High School), Michael Townsend (Te Puke High School) and Geoffrey Lau (Westlake Boys High School, Auckland). The non-travelling reserve is Ashok Raj (Auckland Boys' Grammar School).

Great effort is being put into making it possible for students who have not been accelerated and who are from smaller centres to have Olympiad success. It was therefore very rewarding that two members of the team are from smaller centres and a different pair did not sit Bursary Chemistry last year. Only one team member had a mentor other than his teacher during the training period before camp. In an early letter to the training group they were told that "each and every one of you has a real chance to go to Russia." Obviously the boy at the bottom of our initial selection list took this seriously, and he made the team. Olympiad success isn't dependent on what students already know but on what they're prepared to learn!

The team will be accompanied in their journey to Moscow by Dr Jan Giffney and Dr Robert Maclagan who is currently on leave at Rice University in Houston, Texas. Thanks also to Time Oughton from Christchurch College of Education who has helped with fund-raising and who made the travel arrangements.

NZIC PRIZES AND AWARDS

SGS PRIZE

This prize of $1,000.00 and a plaque has been donated by SGS (New Zealand) Ltd.

1. The prize shall be awarded to a member of the Institute who, in the opinion of the Council, has made a significant contribution to some branch of chemical science, the contribution to be judged by research work published during the five years immediately proceeding 30th April in the year of the award.
2. Applications by members or nominations which may be submitted by Branch Committees or individual members must be received by the Executive Officer, P O Box 12347 Wellington by 30th June each year and must be accompanied by copies of papers presented in support of the entry. The Council itself may nominate candidates for the award.
3. A nomination or application, once made, shall stand for five years and material which fails to satisfy clause 1 shall automatically be deleted and additional material may be presented at any time.
4. If, in the opinion of Council, there is no candidate of

NZIC COUNCIL ELECTIONS

Rule 16.2 states:-

"The President, Vice-Presidents, Honorary General Secretary and Honorary Treasurer shall be elected annually from nominations made by Branches, or by any six corporate members, and forwarded to the Executive Officer by June 30".

Please forward nominations to reach the Executive Officer by 30 June 1996.

P O Box 12-347
WELLINGTON
Fax (04) 473 2324

A A Turner
Honorary General Secretary for Council

sufficient merit, the Council may refrain from making the award.

5. The prize shall be presented at the Annual Conference of the Institute or at a meeting of the Branch to which the prize-winner belongs.

6. A member to whom the prize has been awarded shall not be eligible for re-nomination.

SHELL PRIZE FOR INDUSTRIAL AND APPLIED CHEMISTRY

A prize of $1,000.00 and a certificate will be awarded annually by Shell New Zealand Holding Co. Ltd. to further the recipient's studies in industrial chemistry and to commemorate the achievement.

1. The prize will be awarded for meritorious achievement in the field of industrial or applied chemistry.

2. The prize will be restricted to financial members of the New Zealand Institute of Chemistry of any grade of membership. In the case of joint work the prize may be shared between two or more members.

3. Applications should include a written statement of the industrial or applied chemistry activities or achievements of the candidate(s) and their significance in terms of improved technology, new products or other benefits to industry or the community. Supporting documents and publications may be submitted with the application and **will be held to be confidential to the assessors.** If possible, the value of the work should be attested by an accompanying statement from the manager or directors or head of the organisation. There is no limit on the period of time over which the work was carried out.

4. Applications for the prize may be made by individual members or nominations may be made by Branch Committees or by corporate members of the Institute. A nomination or application, once made, shall stand for five years.

5. Two or three assessors will be appointed by the Council of the Institute to consider the applications and make recommendations. The final decision on the award will be made by the Council. Council reserves the right to make no award in the absence of a suitable candidate.

6. Applications or nominations must be received by the Executive Officer, P O Box 12347, Wellington by 30th June each year.

AWARD FOR CHEMICAL EDUCATION

Council of the Institute has established an award for chemical education consisting of a certificate and a prize of $250.00. The award is to be made in compliance with the following rules:

1. The award will be made annually unless, in the opinion of Council, there is no candidate of sufficient merit.

2. The award shall be made to a person who, in the opinion of Council, has made an important contribution to Chemical Education in New Zealand. (Note: the award will normally be made to a secondary teacher actively involved in teaching chemistry.)

3. The award shall consist of a certificate and a prize of $250.00.

4. The award is not restricted to financial members of the Institute.

5. Application for the award may be made by individuals, or nominations may be made by any Branch Committee or by any individual financial member of the Institute.

6. Applications or nominations must be received by the Executive Officer, P O Box 12347, Wellington by 30th June in the year of the award. Each application or nomination must include a full curriculum vitae and two independent supporting statements from referees commenting on the educational activities of the candidate and their significance to chemical education.

EASTERFIELD AWARD

The Medal was donated by the Royal Institute of Chemistry (now the Royal Society of Chemistry) in honour of the late Sir Thomas Hill Easterfield KBE MZ(Cant), PhD(Wutzburg) FRSNZ, FRIC, HonFNZIC, who was well known for his contribution in the field of chemistry and will be remembered particularly for the inspiration and encouragement he gave his students during the many years he was Professor of Chemistry at Victoria University College and for his infectious enthusiasm for chemical research.

Sir Thomas was the first chairman of the New Zealand section of the Royal Institute of Chemistry and also one of the early presidents of the New Zealand Institute of Chemistry. It is therefore fitting and in accordance with the wishes of the Council of the Royal Society of Chemistry that they should act in association.

1. The medal shall be awarded to chemists in New Zealand in recognition of the quality and originality of their research work.

2. Candidates must be under 35 years of age at 30th April in the year of their application for consideration for the award.

3. The award will be open to all chemists whether or not they are members of the Royal Society of Chemistry or the New Zealand Institute of Chemistry.

4. The major portion of the candidate's research work submitted must have been carried out in New Zealand.

5. No person may be awarded the Easterfield Medal more than once.

6. The successful candidate will be requested to deliver a lecture on the subject of his/her research at the Annual Conference of the New Zealand Institute of Chemistry or on some other suitable occasion.

7. The medal shall be awarded biennially and presented to the successful candidate on the occasion of his/her lecture.

8. The Selection Committee reserves the right to make no award in any year if the standard of work submitted is not of sufficient merit.

9. Expenses necessarily incurred by the Medallist in connection with the delivery of his/her lecture will be defrayed.

10. Applications by or on behalf of candidates for this award must be received by the Executive Officer, NZIC, P O Box 12-347, Wellington, by the 30th June and must be fully supported by all relevant papers (either published or unpublished).

11. The award will be made by the President of the Royal Society of Chemistry on the recommendation of a selection committee comprising the New Zealand corresponding secretary of the Royal Society of Chemistry, the President of the New Zealand Institute of Chemistry or his/her personally nominated representative and a Professor of Chemistry from one of the New Zealand universities.

This committee will have the right to co-opt one suitable person in an advisory capacity.

NZIC BRANCH NEWS

MANAWATU

Branch members took part in a wine trail in the Hawke's Bay region on Saturday 9 March. Participants travelled to Waipukurau in their own car and joined a charter bus to visit five wineries in the Hastings/Havelock North area - Te Mata Estate Winery, Vidal's of Hawke's Bay, St George Estate Winery and Restaurant (where lunch was held), Cross Roads Winery, and Stonecroft. It was a superb sunny day in the region. Some excellent wines were tasted or, rather sampled, however some were not so memorable. There was often a substantial difference between standard and reserve batches of the same wine. White wines included chardonnays, gewurztraminers, sauvignon blancs, and mu[illegible]d wines were generally cabernet, and cabernet/merlot including the famous Coleraine of Te Mata Estate. At Cross Roads a very lucid description of the wine varietie[illegible] at th[illegible]inery was given by Malcolm Reeves, [illegible]y in the Department of Chemistry at Massey University. Afterwards some participants had dinner at the Stray Cat [illegible]urant in Waipukurau before returning home by car.

Manuwatu branch members exploring the Crossroads winery

Professor Geoff Malcolm, Department of Chemistry, Massey University, who recently retired as Dean of Science, gave a talk entitled "A personal history of involvement in polymer science research" in the HortResearch seminar room on 27 March. There were about 35 people present including a good proportion of students, many of whom were present at the pre-talk dinner with Geoff Malcolm. Geoff Malcolm started his talk with reference to Herman Staudinger, the starting figure in the history of macromolecular research in the 1920s, and to W H Carothers of Dupont who synthesised polymers such as nylon. Geoff started his own work in synthetic polymer research in the 1950s, later moving to biopolymers. He initially researched the physical chemistry of electrolytes in solutions at Canterbury University but switched to non-electrolyte solutions and statistical thermodynamics when working for his PhD at Manchester University under a UK scholarship. Geoff moved in 1957 to Otago University to work under Professor H Parton and on the strength of developing the Barker theory for polymer solutions obtained a Nuffield Travelling Fellowship to Imperial College, University of London to research the thermodynamics of branched polymers. In 1969 Geoff took up the position of Professor of Physical Chemistry at Massey University and became involved in protein-water interactions and more recently has worked on the analysis of conformation of polymers in collaboration with Australian scientists. Geoff ended his talk with a number of sage tips to students on following a research career.

At the occasion of Geoff Malcolm's talk the NZIC Manawatu Branch Prizes were presented to the best Massey University students in Level 300 Chemistry and Biochemistry for 1995. They were Andrew Gilbert and James Stephenson jointly in Chemistry and Katherine Moore in Biochemistry. The prizes were presented by Professor Andrew Brodie, Head of the Chemistry Department and Professor Pat Sullivan, new Head of the Biochemistry Department, respectively.

On 16 April, Nath Pritchard, NZIC President, gave his Presidential Address "Chemistry in Peculiar Places" at the HortResearch seminar room. Prior to this Nath had dinner with committee members and members at Periwinkles Restaurant in the Massey University business complex. At the dinner some lively discussion ensued on the future of the NZIC and its proposed reshaping. In his address Nath provided an overview of the myriad of opportunities for chemistry in thermal power station operations. Potential chemical problems were discussed relating to the use of oil, fuels and water; corrosion in boiler systems etc.; atmospheric discharges (e.g., stack and cooling tower emissions); and aqueous discharges (e.g., process water, stormwater, leachates, cooling water). Nath mentioned the important links that had been formed in recent years with scientific and testing staff in relevant organisations such as ECNZ (Electricity Corp.), CRANZ (Coal Research), IRL (Industrial Research), ESR (Environmental Science and Research), NIWA (National Institute of Water and Atmospheric Research), and a number of private analytical laboratories, to assist with monitoring and testing of power station processes. Nath concluded his talk by briefly discussing future energy generation options involving superconductors, coal gasefication, and fuel cells.

The Department of Chemistry at Massey University, Palmerston North campus, has welcomed a new chemistry lecturer, Dr Simon Hall. Simon comes from the Manchester Metropolitan University, England where he has been since 1991 on the lecturing staff, teaching analytical and physical chemistry. He also has had experience as a Tutor for the Open University. His postdoctoral experience was at the University of Wales, Cardiff where he collaborated with D R Williams, J R Duffield and M

I Barnett developing, among other things stability assessment methods for intravenous nutrition fluids and new predictive models for the behaviour of lipid emulsions. Simon completed his PhD with G A Wright at the University of Auckland in 1988 in the general area of electroanalytical chemistry. His MSc, also from Auckland, was with G R Clark in x-ray crystallography. He plans to continue with his interests in the environmental measurement of electroactive species, both metal ions and organic compounds, and is keen to develop collaborations with other scientists in the region.

Harry Percival

WELLINGTON

It has been quite a while since the last update on the comings and goings at the Wellington Branch. With nothing but good intentions this is the first of what will hopefully be a new, continuing series of updates, gossip and news.

The 1995 Branch AGM was held in October 1995 with 21 members in attendance. Dr David Bibby and Dr Linda Parker were standing down from the jobs of Secretary and Treasurer respectively. Our Chairman thanked both of them for their invaluble contributions during their tenure. A new Secretary and Treasurer could unfortunately not be found during the AGM. This left the Branch without them for a number of months. The situation was recently resolved and I am proud to present the new Wellington Branch Committee for 1996:

Chairperson:	Rod Tilbury (Victoria University of Wellington)
Secretary:	Cees Lensink (Industrial Research Ltd)
Treasurer (Acting):	Alan Turner
Branch Editor:	Graham Murray (St Patricks College)
Post-Graduate Representative:	Antony Fake (Victoria University of Wellington)
Members:	David Bibby (Industrial Research Ltd)
	Jim Ellis
	Sue Freitag (Works Central Laboratories)
	Jim Waters (Department of Health)
	John Reeve (AgResearch Ltd)
	Vince Gray

The average attendance at the monthy meetings during 1995 has been higher than the previous year and we hope to keep this trend going for 1996.

The meetings in 1996 started with a presentation in February entitled "glasses and thermodynamics, never the twain shall meet" by Richard Bowles, graduate student at Victoria University. This was followed in March with a presentation by Vince Gray on the greenhouse effect. The meeting was characterized by the attendance of a large delegation of the Sceptics Society. We have not been able to determine whether this was in support or not of Vince's "cool response to global warming".

The April meeting saw NZIC president Nat Pritchard visit the Branch. His lecture title "Chemistry in peculiar places" was most appropriate for an after dinner lecture at the Industrial Research Limited Gracefield campus.

The May meeting will be a combined meeting with Science Wellington (formerly Wellington Branch of the Royal Society).

The Wellington Branch can now be contacted by e-mail. The address is as follows: nzic.wgtn@irl.cri.nz.

Cees Lensink

OTAGO

On the evening of 20th March 1996 about 30 members and friends heard Nath Pritchard give a fascinating and entertaining account of diverse aspects of chemical and environmental problems associated with the Huntly Power Station where he is Chief Environmental Officer. We then dined at the Mellor restaurant and enjoyed the usual high standard of food preparation and presentation. The evening concluded with a report from our national President about the process of review and reform in the NZIC. Any significant changes to the NZIC will be considered at the AGM to be held during the December 1996 NZIC Conference in Dunedin.

Branch members visited Central Otago on the 12th and 13th April 1996. Friday evening began with a visit to the Benger Gold Juicing Company, hosted by their cider maker, Mark Simmonds. Benger Gold have increased their turnover sevenfold in the last three years, using the local apple crop. The first visit on the Saturday was to Crop and Food Research's Redbank Station, near Clyde. Malcolm Douglas talked about research on essential oils and medicinal herbs, and showed off the distillation facilities announced by Crop and Food Research. Finally, the group visited a relatively new vineyard, that of William Hill, near Alexandra.

The Chemistry Department, University of Otago, is currently enjoying a number of overseas academic visitors. Don Macalady is visiting for a year from the Colorado School of Mines and has research interests in aquatic chemistry and geochemistry. John Morris is from Strathclyde University. He is interested in polyborane cluster compounds and is visiting until May. Mike Benn is visiting once again from the University of Calgary. He is associated with the Plant Extracts Research Unit pursuing bioactive natural products as is Seung-Hwa Baek from Wonkwang, Korea. Steve Davies visited in April, from Oxford University. He also runs the commercial company Oxford Asymmetry, specialising in enantiospecific syntheses of high-value organic compounds. Chris Easton visited from the Australian National University recently, and lectured on his interests in amino acid radicals and cyclodextrin complexes

Nigel Perry

LIMS says Bob McDowall (*LC.GC International* **9** (1) 21-26) can mean: Labyrinth of Incompatible Machine and Software; Lost in the Machine Somewhere; Life is Made Slower, or Life is Made Simpler.

From the President ...

I am pleased to report that it has been both a reasonably busy, and pleasurable two months since I last spoke to you. I have visited a number of our Branches and have been pleased with the unbridled enthusiasm I have found in those attending the meetings. A large number of whom are in favour of change.

PRESIDENTIAL TOUR

On my "Presidential Tour" I have so far visited Otago, Auckland, Manawatu and Wellington Branches. I have enjoyed meeting some fine people. Three things spring to mind:

- The genuine enthusiasm and concern of those attending the meetings for the Institute;
- The age group of those attending;
- The need to bring in young members.

I was pleased to see a number of our Past Presidents at those meetings, still active, still retaining a real interest in the NZIC's activities. At Otago; Fred Fastier, Arthur Campbell and Stan Winters. At Auckland; Alan Mackney, Ashley Wilson and Bill Denny. At Manawatu; Harry Percival, looking really well after his operation. Finally Wellington; Brian Halton.

COMMUNICATION

I had the privilege during the month of lunching in Hamilton with the Minister of Science and Technology, The Honorable Simon Upton. That pleasure was shared with Peter Robinson, Waikato Branch Chairman and Don Llewellyn, Past President. The discussion revolved around the Institute and Chemistry. It proved to be a stimulating and thought provoking experience.

The Minister thought communication to be critical, and the timeliness and method of transference crucial. The new generation required information on the computer. He drew a personal analogy where he could, in the evening, in his office read that morning's English newspapers on the Internet. Not a week later in hard copy when the news was history. He questioned the value of the Institute journal!

Simon Upton

The Minister was supportive of the Royal Society and questioned our potential roles within it. What did the Royal Society offer the Institute? Much in the same vein as, what did the Institute have to offer its members?

If I was to take away four issues from talking to the Minister they would be;

- improved communication,
- identifiable image, role clarity, and
- it is a shame he was not a chemist!

On behalf of the Institute I would thank the Minister for affording the time to discuss the issues with us.

DILEMMA

Since my last notes to you chemistry has featured in the media in a big way. Two major issues hit the headlines; "mad cow disease" and 96 octane lead-free petrol. To digress for a moment, to my mind these two interesting issues well illustrate the difficulty and problems our Institute faces. Who would associate two such seemingly diverse topics with the one main stream discipline - chemistry? How does an Institute cater for such diversity?

Some of our fellow members have asked Alan Turner why there has been no NZIC response to these two issues. The 96 octane lead free petrol is a difficult one to respond to. I have a five page draft article on my desk. It landed there very early in the discussions on the issue. The difficulty we face as a professional body is how to be supportive of the chemistry involved, thus being constructive in the public's eyes. It would have been very easy to table an argument that was either controversial or negative and achieve little good for our profession and chemistry. *Your comments on this philosophy would be appreciated.*

CHANGE

The tasks set of the VPs are well in hand. Rob Whitney on the Secretariat/Business Plan and Alistair MacGibbon on Membership Structure are both beavering away. I am certain that both will have draft papers ready for the Standing Committee's consideration at the end of May. The procedure will then be to discuss the finalised papers at the August Council Meeting.

Again digressing, The Membership of the Institute is unaware of one significant change that has taken place over the last few years. I wonder how many of Council have recognized it? Council Meetings used to be a two day affair, with an overnight stop in the Capital. The opportunity to meet the "Local Branch" over libation and sustenance would be taken. A Council Meeting today barely lasts the full day:

- Agenda papers are circulated to delegates prior to the meeting. The Executive Officer deals with routine issues outside of the meeting.

A Council meeting is professionally run, efficient, and leaves little time for philosophical discussion.

I have asked Alan Turner to warn the Executive and Delegates that I should like the August Council Meeting to be a two day affair. The second day allowing the issues of the day and the VP's papers to be discussed. I have also asked Alan Turner to set the date in ample time to allow attendees to make their arrangements. It will be important for each Branch to send its Delegate or nominee to this meeting.

INTERNET

I spent some time at the DRI in Palmerston North in conjunction with my Manawatu Branch visit. An esoteric place. A far cry from my normal haunts. I learnt something about the dairy industry from an enthusiast, Alistair MacGibbon. I also had time to congratulate Grant Boston for his efforts in putting the NZIC on the Internet. Even if his first effort had omitted to mention the President! This is real progress. In light of the Minister's comments, merely the beginning.

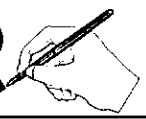
West Australia?; the recent inclusion of the NZIC's periodic table wall chart in *Chemistry in New Zealand* drew some interest from Western Australia. A correspondent asked for additional copies! Who said we can't replace RACI?

Thanks to Wayne Williamson and Lawrence Scot, who travelled from New Plymouth to Palmerston North for my Manawatu Branch Meeting.

Elections: by the time you read this article Institute election time will be fast approaching. Challenge the *status quo*! Nominate candidates for the contestable positions.

Nath Pritchard
President, NZIC

LETTERS TO THE EDITOR



Dear Sir,

In the last issue of *Chemistry in New Zealand* Ian Graves, Greg Olsen and Lisa Walker raised the point about the difficulties in maintaining student members as they move into the work force. To their credit rather than just complain about the current service the NZIC provides they offered some possible solutions. Unfortunately in the hard light of day the direction that they suggest the NZIC move may not be the most beneficial. The pros and cons of the NZIC becoming a "professional body" have been debated recently by the Manawatu branch. We would like to take this opportunity to inform the readers and NZIC members of our conclusions.

Firstly, the difficulty of maintaining student members or any members for that matter: The major factor is always cost. Today we live in a world where cost effectiveness is the reality. More and more the question "what am I getting for my fees?" is being asked. Today the answer for most people is NOT ENOUGH! Think about the situation from the point of view of a student. They pay a minimal fee $25 per year and get this magazine and get to go to a couple of meetings. The day they graduate they are then asked to pay $80 per year and, four years later, $140 per year for exactly the same services. Somehow the "prestige" of being able to put MNZIC after their name is not sufficient to balance a 178% increase in fees. Also there is a large number of qualified chemists in the work force whose jobs have very little to do with chemistry (one of the beauties of the qualification is its flexibility). Often they would like to keep some ties with the field were they gained their qualification. The present membership structure prohibits them from being anything but full members ($140 per year). This is often considered too much money for something that would be purely for interest. This is a loss to them and to the NZIC.

In simple terms there are two possible solutions:

1) become a real professional body.
2) drop the pretence and become a "friendly society".

Pros and Cons

1) The pros were clearly stated by the previous letter. However the cons represent a compelling argument. The requirements of a professional society are very demanding. Most professional organisations have stringent entry requirements and a correspondingly high membership fee. In return the member receives a licence to practice and its attached prestige, group representation in negotiations with their employer, and must contribute to an indemnity fund to pay for their, and their fellows, mistakes. All of these things cost money and not just $140 per year. In most cases professional bodies have significant charges. As there is not currently any requirement for a practising chemist to be a member of any organisation it is unlikely that the thought of fees of $600-$1000 per year will be attractive. One just has to look to other professional organisations, lawyers for example, to see some of the pitfalls that exist.

Will the NZIC be able to develop a professional organisation and will the employers accept it? We think not.

2) The pros of being a friendly society are the certainty of reduced fees. Here in the Manawatu there are a significant number of science professionals that would be happy to be members of the NZIC. However, the current fee structure turns many away. When you try and persuade someone to joint the NZIC there is often genuine interest right up to the point that you mention how much it costs.

The cons are the drop in the income that will be associated with reduced fees. The simple answer to that is: "What are we getting for our money now?!!". The fact that this question can be asked and is being asked more frequently every week begs the question "how serious would a drop in income be to the members?"

Last month our branch had the opportunity to discuss what the NZIC offers to its membership with the president of the NZIC. Upon being asked "What does the NZIC do for me?" The most common reply was it provides me with networking opportunities. This was supported by most of the senior members. Many of the less senior members noted that, in today's information age, the ability to network is no longer restricted to being a member of a specific organisation. If the NZIC is to survive into the 21st century (4 years away) it is going to have to look to the future not the past. The organisation has been wonderful for many of the current members, but it is clearly not fulfilling the expectations of the latest generations of chemists. Without new members the NZIC is doomed.

With the situation near crisis, immediate action is required. The choices are not going to be easy ones but they are vital and they cannot be postponed. We feel that the only real choice if the NZIC is to survive is to pull back from the current structure and enable a lower fee for simple membership. (Those who wish to have the initials MNZIC and FNZIC after their name can continue to pay for the privilege at the existing rate.) If services need to be cut due to reduced income, so be it. Let's get the membership back up to a level that will enable us to be a vigorous organisation again. Then if there is a demand for a service that the NZIC cannot afford we will have to review fees at that time.

If the NZIC does not change it is going to find itself supplanted by another similar organisation. The seeds of this evolution are already present in the form of the speciality groups. It is up to us to assure the NZIC has a future. Now is the time to act, while we still can.

Yours sincerely,

members of the Manawatu Branch Committee.

Dear Sir,

So, the Institute has finally been dragged into the computer age with the development of our own World Wide Web home page (http://webtwo.rsnz.govt.nz/www/nzic/nzic.html).

My hearty congratulations to Grant Boston for the excellent effort which he has made in putting this together. "Our" site matches anything else that I have seen on the Net, and provides a wealth of information about the Institute and associated activities.

The only minor point that I noticed is that our Secretariat does not appear to have a connection via Email, hence anyone using the home page cannot make easy contact with the Institute, though they can with many of the Specialist Groups and University contacts listed.

Maybe it is time to consider the usefulness of computers to the Institute and how they might benefit our members as a whole. I would guess that our membership list is held in a database on a computer system somewhere. Notwithstanding the provisions of the Privacy Act, it is necessary that this list should not be made freely available to those outside the Institute. There must be many members, however, who would be willing to act as spokespersons or give advice on a wide variety of topics and maybe this could be stored in a linked database which would be easily accessable, either through the General Secretary, or maybe even via the WWW Home Page. Only those members who specifically agreed would be included (information from the Annual Subscription Form?) and this would allow Alan Turner to rapidly find an appropriate contact person in response to queries from the Government, the media, business or private individuals. Email addresses could even be included!

Perhaps as part of our present considerations about our Institute we should look at the

computer facilities available to our General Secretary, and how these may be best organised to serve all of our members.

I would be interested in any comments from other members on this matter.

Yours sincerely,

Peter Robinson
Environmental Division
R J Hill Laboratories Ltd
P O Box 4048 Tel: (+64-7)-8552266
Hamilton Fax: (+64-7)-8549886
peter@rjhill.co.nz

"**ACTIVATION ENERGY:** The quantity of useful energy available in one cup of coffee"

Dear Sir,

The proposition that cot death is due to gaseous poisoning by one or more of the gases phosphine, arsine and stibine has led to an interest in the analysis of cot mattress materials for the elements phosphorus, arsenic and antimony.

Errors in such analyses have occurred as a result of incorrect sample preparation. The fact must not be overlooked that some compounds of these elements volatilise and are lost before they are decomposed into inorganic forms suitable for analysis. Failure to appreciate this point has resulted in some erroneous figures being reported - much less than the true values. This could result in unsafe mattresses being considered safe. In view of the importance of these analyses, therefore, the following comments are offered:

Samples must not be dry-ashed, as many compounds of the three elements are volatile. Wet methods must be employed using strong oxidising agents, the preferred reagent being nitric acid followed by perchloric acid. Even so, some compounds of phosphorus and arsenic will evaporate before they are oxidised. Care must be taken to cover beakers, and in some instances Kjeldahl flasks should be used.

Tests have shown that decomposition with sulphuric acid sometimes results in charring of the matrix and this reduces arsenic and antimony to volatile substances. This is especially so in the analysis of PVC for arsenic and antimony.

The use of a sealed "bomb" has been found necessary with some chemically resistant materials, and this technique should be used where decomposition of samples is difficult in open containers.

Compounds likely to be encountered include: (a) phosphate esters used as plasticisers, present as accelerators and antioxidants in some plastics and rubber formulations, and present in many natural fibres;

(b) arsenic organo-metallic compounds, such as oxybis-phenoxarsine (OBPA), a commonly used biocide; and arsenic/keratin compounds in sheep fleece and wool;

(c) antimony trioxide added as a fire retardant in PVC, and also present as an organic additive in certain types of plastic foam.

The method of analysis must be proved by using "spiked" samples.

The lower limits of detection should not exceed 10 mg/kg = 10 parts per million, expressed as the element.

Yours sincerely,

T J Sprott
Consultant

10 Combes Road
Remuera
Auckland

IS THERE A PROBLEM WITH DIETARY ALUMINIUM?

R. H. Molony, Molab Ltd
14 Goldie Street, St Heliers, Auckland

Over recent years there has been a considerable amount of concern about potential problems with dietary aluminium. Much of this concern is centred on statistical associations and aluminium residues found in bodies after autopsy. There seems to be very little consideration of the chemical properties of aluminium and the mechanisms by which aluminium can enter the body, be transported and have an effect. Aluminium compounds have a variety of special properties which make these compounds useful industrially. These particular properties are normally emphasised in chemistry text books and hence are not widely appreciated. A consideration of these properties may well shed some light on whether or not there is a problem associated with dietary aluminium.

The medical evidence which suggests there may be a problem is varied and in some cases a little controversial. The original suggestion that aluminium is neurotoxic seems to date back to a US army research project by Kopeloff, Barrera and Kopeloff in 1942. Since then there has been a variety of evidence published including the following examples;

- The aluminium induced neuropathy of kidney dialysis patients is well known.
- There were deaths of babies in the USA which were associated with both aluminium contaminated milk formula and poor kidney function.
- Desferrioxamine was found to retard the progression of Alzheimer's disease in a 1991 study. The suggestion was that desferrioxamine, a chelating agent, was removing or inactivating aluminium present in brain tissue.
- Aluminium compounds have been used to induce brain lesions during neural pathway investigations in cats.
- A group of miners suffered brain damage as a result of the deliberate administration of aluminium compounds. These were administered as a preventative to silicosis.
- Two statistical studies, one in Norway and one in the UK, have shown a statistical concordance between aluminium in drinking water and Alzheimer's disease. The Norwegian study has been questioned.
- A recent study also found an association between dietary aluminium and frequency of hip fracture in elderly people.

In the environment, aluminium exists in a variety of forms, these are likely to vary significantly in bioavailability. The most common form in which the majority of the world's aluminium occurs is the alumino-silicate minerals. The bond between silica and aluminium is strong. During the chemical analysis of silicates, agents such as boiling hydrochloric acid, fused alkali, or hydrofluoric acid are required to break the silica-aluminium bond. It seems that alumino-silicates are unlikely to be affected significantly by the chemical conditions prevailing in the human intestine. The aluminium in these compounds is unlikely to be bioavailable. Aluminium produces complex ions with a variety of materials. One of these is fluoride. The fluoride-aluminium bond is very strong and it seems likely that in the presence of excess fluoride aluminium would be unavailable. The only bioavailable forms of aluminium would be simple aluminium compounds or aluminium complexes with metabolisable organic compounds.

Assuming that bioavailable aluminium is present, the next step is to consider its fate. Aluminium forms complex compounds with citrate. These can be either uncharged or present as a negative ion depending on the citrate:aluminium ratio in the complex. Aluminium absorbed into the blood stream (either as positively charged aluminium ions or as an organic complex) would react with citrate present in blood producing an aluminium-citrate complex. The aluminium-citrate complex molecule is of similar size to a sugar molecule and would presumably circulate throughout the body, possibly being able to pass through the blood/brain barrier. In areas of high metabolic activity local regions of citrate depletion are likely to occur due to the metabolisation of the citrate ion. When this occurs the highly reactive positively-charged aluminium ion would be released.

One of the industrial uses of aluminium is based on the ability of the positively-charged aluminium ion to crosslink and precipitate negatively-charged polymers. Glycoproteins are normally precipitated by aluminium. The association of the precipitated glycoprotein amyloid with neurological damage suggests the possibility of a link with aluminium. The positively-charged aluminium ion is potentially able to bind to negative charges on the surface of protein molecules. The binding of an aluminium ion to the surface of a protein would change the surface charge at that point from a negative charge to a positive charge. This would alter the antigenic properties of the protein molecule opening the way for an auto-immune attack. Theoretically a level of 250 micrograms of aluminium is capable of changing the antigenic properties one gram of a typical protein. There have been recent suggestions that Alzheimer's and some other diseases have an auto-immune origin.

Silica and silicate react in aqueous solution with aluminium ion producing insoluble aluminosilicates. This was the theoretical basis for the disastrous use of alumina dust as a preventative for silicosis. There is a suggestion in some of the scientific literature that many of the supposed benefits of dietary silica are not due to silicon being an essential element, but rather due to the detoxification of aluminium by silica. For example, the suggestion that silica can favourably influence bone strength could be due to removal of aluminium, which is known to affect the crystal structure of hydroxyapatite in bone.

Aluminium in the diet can come from a variety of sources. Aluminium compounds are used to flocculate and precipitate impurities present in natural waters. Correctly used aluminium compounds do not introduce a large amount of aluminium into the treated water. Unfortunately this is not always the case as the operating parameters for obtaining low residual aluminium levels in water plant discharges, are rather stringent. In foods, aluminium compounds are sometimes added as baking powder components. In New Zealand large amounts of baking powder containing alum as the acidulant are being imported and sold in large commercial packs. This is occurring despite the fact that under New Zealand law alum is not permitted in foods. Very small amounts of aluminium may be added in the form of insoluble aluminium lakes used to colour some foods. Aluminium cans would not be a significant contributor to

dietary aluminium unless the can lacquer was faulty. Aluminium cooking utensils are likely to be a significant contributor to dietary aluminium particularly when acid foods are being cooked. In pharmaceuticals, aluminium compounds may be used in antacids and in tablets as a processing aid.

In water treatment the use of aluminium can be completely avoided by using the more expensive iron compounds. Iron produces a more stable floc over a wider pH range than aluminium. The iron floc is heavier and settles more rapidly than the aluminium floc in many cases, enabling a smaller plant to be used for the same throughput. There are no good reasons for the use of any bioavailable aluminium compounds in food. Alum just happens to be the cheapest acidulant. Very few foods are coloured with aluminium lakes and the colouring is not an essential component. Aluminium cooking utensils are easily replaced by stainless steel. There is therefore no good reason for food or beverages to contain any significant amount of added available aluminium.

There are currently no legal restrictions on the level of bioavailable aluminium in foods. While the connection of dietary aluminium with Alzheimer-like diseases may not have been proven conclusively as one of cause and effect, the evidence suggests a connection. Is this suggested connection enough for the introduction of legislation restricting bioavailable aluminium in foods or do we have to wait for conclusive evidence with potential long-term health effects for very many people?

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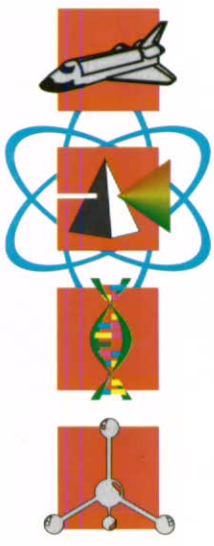

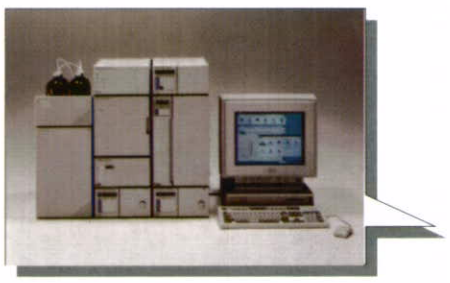

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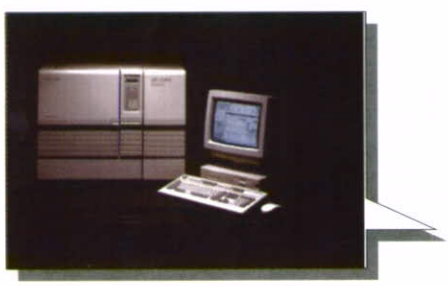

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