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SYSTEMS

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THE WAY TO GO?**

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1992 has been a difficult year with plenty of change and disruption in Scientific areas and only time will let us see the wisdom of the changes now in place. I trust that chemists will now be able to get on with the task of performing science and be somewhat less preoccupied with matters political. It now remains for me to wish all members and their families a pleasant festive season and a relaxing holiday. I look forward to hearing of great exploits among chemists in 1993.

## EDITORIAL

### *Christmas & New Year Greetings from the Editor.*

Many chemists have had a busy 1992 with the completion of changes in public sector science to the Crown Research Institute system and the need to develop new relationships and allegiances. This issue has two articles relating to some of the changes that have affected chemists. At times the editor has had a shortage of suitable copy to produce an interesting journal. This has improved of late with each Branch in turn taking responsibility for providing copy. The real problem as it has been for several years is the shortage of revenue from advertising. This problem has to be addressed if Chemistry in New Zealand is to survive. Lack of urgency will very likely spell the end of Chemistry in New Zealand. Even a cheaper substitute if the present magazine format changes will still require regular adequate advertising support. We refer you to the publishers note below. We intend that 1993 will bring positive solutions.

## THE PUBLISHER

### *New advertising Manager -*

High praise is due to Mr Carl Roze for the many years service he has given Chemistry in New Zealand. Thanks to Carl's efforts as its Sales Manager the magazine has survived through very tough times to the present. The magazine now requires a new direction and new impetus in advertising and sales -consequently we are pleased to announce the appointment of a new Advertising Sales Manager - Mr Michael Edgar.



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**Chemistry in New Zealand:** Published on behalf of the New Zealand Institute of Chemistry (Inc) PO Box 12-347, Wellington Ph: (04) 473-9444. Fax (04) 473-2324

President: D.S. Winter, Hon. Gen. Secretary/ Executive Officer: Alan A. Turner, Hon. Treasurer: D.P. Karl.

Published six times a year in February, April, June, August, October and December.

**Editorial:** Technical and scientific article should be submitted to the editor no later than 1st of the month of publication, but much earlier for long articles. The editor will always welcome commercial and industrial news on product design, development and testing processing techniques, company and personal news etc.

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**Publisher:** Promotional Options, PO Box 101-189

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**Watch out for February's special feature:**

**SPECTROSCOPY  
UVVIS & AA**

# AUTOMATED ANALYSIS - THE WAY TO GO?

by Roger Whiting

---

## Introduction

In recent years the trend in analytical laboratories in New Zealand has been to increase output while decreasing staff. The pressure for increased output has come from the need to improve the quality of New Zealand goods and services by increasing the frequency and sophistication of analyses.

The pressure for decreasing staff has come from the need to compete with overseas competitors on price. The overall result has to reduce the number of people employed on routine bench testing but requiring those remaining to use more sophisticated equipment with higher sample throughputs. Automation of the laboratory is seen as one way in which this change can be achieved.

Laboratory Automation can be divided into a range of levels of increasing complexity.

## AUTOSAMPLERS

The elimination of sample handling is one of the key aims of laboratory automation. One of the most obvious ways this is done is by fitting an autosampler to a laboratory instrument. These have become a common feature of many chromatography systems over recent years. Chromatographic methods involving run times of ten minutes or more can represent a frustrating drain on skilled manpower. Although theoretically an analyst can perform other tasks while the chromatogram is running in fact this is seldom very successful. Thus the objective has been to develop systems which can be set up and be left to run either while the analyst performs other tasks or overnight.

The addition of the autosampler to a laboratory instrument has been a common approach. Initially introduced in the hospital laboratory for AutoAnalyzers, the earliest autosamplers merely fed in the samples via a tube connected to the peristaltic pump of the analyzer. The sample sequence was dictated by the position of the sample in the carousel. The incorporation of autosamplers to chromatography required the development of means of injecting samples into the instrument. Once this was achieved advantages became apparent as the reproducibility of injection improved.

Graphite furnace AA is also a technique which has benefited from more reproducible sample injection. The introduction of autosamplers has aided sample application and improved the reproducibility of results with such devices as the Hitachi SSC-300 auto sampler. In the SSC-300 it becomes possible to layer reagents and sample into the carbon furnace to enhance the performance - something very difficult to do without automated sample introduction.

More recently the incorporation of sample derivitisation into the autosampling procedure has also improved reproducibility of results. An example of this is peptide sequencing which has benefited greatly from the automation of derivitisation for chromatography. Both the SpectraPhysics Spectrasystem autosampler and the ICI Aminomate allow samples to be taken from the sample tray and then reacted with a derivitising reagent prior to being injected into the chromatograph. This field is undergoing a lot of development as the interest in

peptide sequencing and biotechnology develop.

## WORKSTATIONS

The addition of computers to the instruments has enabled automation to mean more than just allowing the instrument to run on its own. The use of chromatography workstations such as the Spectra STATION allows the analyst to run calibration sequences as desired or even to run standards to bracket the sample values. The worst nightmare of automated analysis is returning to find some malfunction has meant that the instrument has produced unusable results. Thus the drive has been to include some control procedures into the systems. An attempt to answer this problem has been made in the ICI DP900 Chromatography management system. In this PC based system the instrument runs calibration standards and then checks the results of these against criteria set by the analyst (these can be based on a variety of sources). In the event of non compliance of the standards a statistical analysis to remove outliers is carried out and a reevaluation done. If the system still is not conforming it shuts down. This institution of feedback is a necessary step towards full analytical automation.

## MULTIVENDOR CONNECTIVITY

Each manufacturer has developed a range of devices and software to automate their particular instruments and many are incompatible. A new trend in the market is to towards what has been termed "MULTIVENDOR CONNECTIVITY". This is the aim of a software package offered by PE NELSON which enables the analyst to connect together a variety of instruments, samplers and detectors and control them using a central computer. This also has the advantage of centralised data handling which should streamline report preparation and control.

## CONTINUOUS FLOW SYSTEMS

The autosampler plus a workstation automates the sample loading and data handling of the existing analytical equipment. Another approach to automation is to use systems that run continuously and the samples pass through. These systems are inherently automatic.

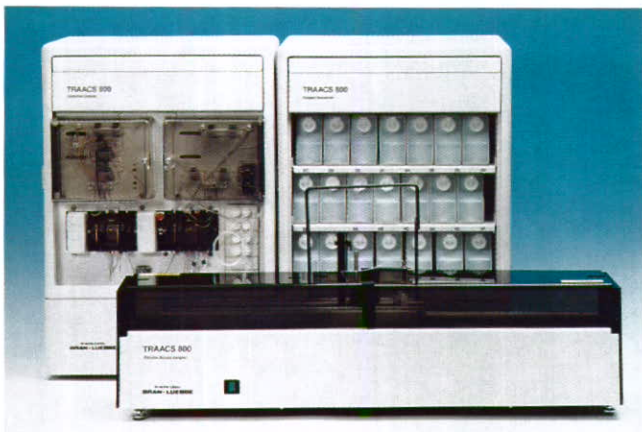
# TRAACS 800 Wet Chemical Analyzer

Bran + Luebbe's thirty plus years of experience in automated wet chemical analysis with their AutoAnalyzer systems has been embodied in a new generation continuous flow analyzer, the TRAACS 800. TRAACS incorporates all the benefits of continuous flow analysis – reproducibility, flexibility, sensitivity and reliability – in an innovative design to give a fully automated analyzer that offers high throughput, lower reagent consumption and less operator interaction.

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- Streamlined compact vertical design which occupies as little as 1.0 metre of linear bench space.
- Bubble-through-the-flowcell and small bore tubing allowing typical throughputs of 120 samples/hour.
- 120 place random access sampler including standards and QC sample rack and dual probe capability.
- Multispeed pumps for allowing fast system wash-out for quick changeover of chemistries and intermittent operation to conserve reagent usage during standby.



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- Comprehensive data analysis software including continuous real-time printout of results and peak traces with flagged anomalies, multitasking and re-analysis of stored data.

## Methods

There are over 800 separate Bran + Luebbe methods available on the AutoAnalyzer and most of these are now available for the TRAACS. The most common methods are listed overleaf. Many environmental methods have US EPA or NPDES approval. All methods are guaranteed to meet specified minimal performance criteria.

## Options

- Reagent Sequencer for automated start-up and shutdown, and automated changeover on Multitest chemistries.
- On-line Micro-distillation Bath
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## TRAACS Methods: Summary

### Water

Acidity  
Alkalinity  
Aluminium  
Ammonia  
Boron  
Chloride  
Cyanide (with UV digestion and on-line distillation)  
Dissolved Organic Carbon  
Fluoride (with on-line distillation)  
Hardness  
Iron  
Magnesium  
Manganese  
Nitrate  
Nitrite  
Phenol (with on-line distillation)  
Phosphate  
Silicate  
Sulphate  
Sulphite

### Detergent

Phosphate  
Silicate

### Soil

Ammonia  
Calcium  
Magnesium  
Phosphate  
Potassium  
Sodium

### Chlor-alkali cell liquor

Chlorate  
Chloride  
Hypochlorite  
Hydroxide

### Tobacco

Ammonia  
Nicotine  
Nitrate  
Phosphate  
Sugars; reduced and total  
Urea

### Fertilizer

Calcium  
Nitrogen (total N)  
Phosphate

### Blood

Alcohol  
Glucose  
Urea

### Wine

Glucose  
Fructose  
Lactate  
Malic acid  
SO<sub>2</sub>, free and total  
Reduced Sugars  
Volatile acidity

### Food, Animal Feed

Amylase  
Ascorbic acid  
Calcium  
Diastatic power in malt  
Glucose  
Iron  
Lactate  
Phosphate  
Protein (Kjeldahl Nitrogen)

AFFIX  
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The earliest to gain wide acceptance was the AutoAnalyzer by Technicon in the medical field but since then a variety of companies and systems have entered the general market.

The first systems used Segmented Flow. This involves the incorporation of air bubbles in the flow which make the liquid at the tube walls move along at the same speed as the bulk fluid. This is essential to stop the samples tailing and intermixing. Thus when setting up and starting up an analytical procedure much time, effort and concern was spent on the pattern and behaviour of the bubbles flowing through the apparatus. The segmented flow system did however allow a long distance between sample input and the detector. Thus the technology is well suited to chemistries that require long reaction times or multiple steps. Once set up and running the system is capable of throughput in the range 60 -120 per hour with several analyses being carried out on each sample.

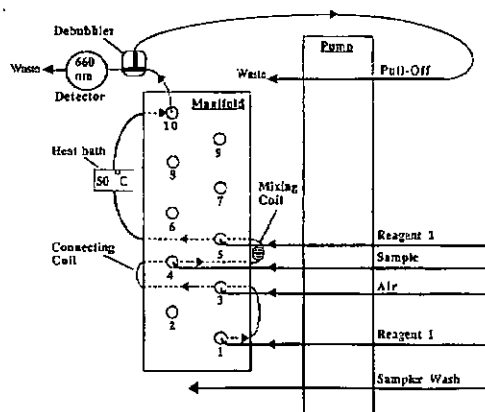


Figure one Generalised flow diagram showing reaction manifold

The alternative to segmented flow is Injection Flow Analysis. Here the tubing diameter is much smaller (0.5mm instead of approx 2mm i.d.). The sample is injected into the reagent flow to form a small plug of sample in the reagent stream. As this plug flows along it mixes by convection and diffusion with the reagent and is measured as it passes through the detector. This mixing process makes a short distance from the sample injection to the detector an important feature. Thus it is best suited to chemistries that are simple and single step. However the sample throughput can be 200 to 300 per hour.

The two technologies are now available in one package in the ALPKEM Flow Solution Analyser. This instrument incorporates a random access autosampler, a valve module to allow flow injection analysis and multispeed pump for segmented flow analysis. A variety of cartridges are available which incorporate the chemistries of the various methods. Detection is via UV-vis and data handling by a dedicated PC based system. The data handling is a key feature as it allows out of range samples to be resampled and diluted to yield usable results without the operator having to reset up the sample batch.

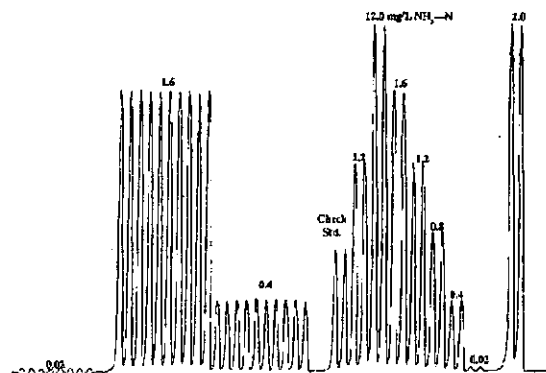


Figure two Typical data obtained on the Flow Solution (0.02 - 2.0 mg/L ammonia nitrogen, 103 samples/hr)

### LABORATORY ROBOTS

Another approach to automation is to take to older existing manual methods and automate them completely by use of laboratory robots. Here the action of the analyst is duplicated and the various sample handling steps are automated and performed by the robot. The major model in the field is the Zymate system. The range of analyses available is almost unlimited. Examples exist of systems for tensile testing, density determination, autotitrator operation, chromatographic derivitisation and injection and weighing and ashing procedures. One of the major advantages of the robotic approach is the ability to handle solids automatically. Most of the previous systems deal with liquids successfully while solids must first be weighed and digested manually. Unfortunately these devices have remained expensive and a large sample throughput is required to make them cost effective. More suited to the New Zealand scale of operations is the BenchMate which has some of the feature of the full robotic system. However undoubtedly time will see the costs fall and laboratory robots will become more common.

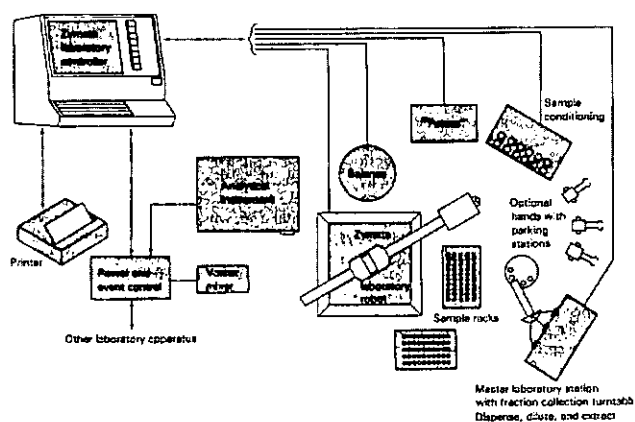


Figure three a robotic laboratory system

### CONCLUSION

The application of automated systems is becoming more common as New Zealand industry consolidates its analytical activities into more centralised facilities. More and more the training of analysts will cease to be in manual techniques but in the use and maintenance of systems.

# AUTOMATION AT THE NEW ZEALAND DAIRY RESEARCH INSTITUTE.

By Alan Matheson - DRI

---

The Applied Mathematics Section of the New Zealand Dairy Research Institute has successfully implemented automated analyses for the microbiological assay of several water soluble vitamins. Procedures have also been completed to measure total colour in milkfat.

Automation of folate assays, for example, is carried out in two steps. A Zymate robot is used to weigh milk powder samples, dissolve the powder in buffer, heat treat the solution at 100 C, incubate with added enzyme, titrate to precipitate casein and centrifuge to obtain an extract suitable for microbiological assay. A Gilson auto-dispenser is used to dispense media and sample extracts before manual sterilization/ and inoculation, and is later used to read the optical density of tile resultant solutions, The Gilson system is currently used for the analysis of five water soluble vitamins.

The assay for total colour also uses the Zymate robot. Milk samples are Saponified, the carotenoids are solvent extracted and the concentration determined by absorbance at 450nm.

We estimate that technician time required for folate assays has been cut from eight hours per day to less than four. The remaining time is spent on housekeeping chores, autoclaving and inoculation of samples and interpretation of results. A marked improvement in the quality of results has been noted since the automation program began.

The technician time required to analyse two hundred samples daily for total colour has been reduced from an estimated eight hours to one hour.

Our equipment layout has been designed so that we can change from one assay protocol to another by changing a program disk and supplying the appropriate reagents.

This flexibility is an important aspect of robotic systems and makes the assay of small hatches economically feasible.

Application of a carefully chosen automated system will improve output and increase the quality of results, but there are rules that should be followed when choosing and implementing equipment.

As a first step, consult the vendors of laboratory robots and automation systems. Look for those who offer complete packages and can provide effective after sales service. The vendors will carefully examine your methodology, advise on suitable equipment, and predict throughput. Such advice is free.

Systems should provide an audit trail and write analytical reports to floppy disk, preferably in spreadsheet format. The ability to interface to a laboratory information system network could be an advantage.

Staff training is essential. Most reputable vendors offer intensive training in the use of their products and advise a familiarisation course before delivery. Trained staff can quickly reconfigure a system for another method and solve the day to day problems that will occur.

Select personnel carefully. The technician who is to work with the system should be enthusiastic, able to make decisions, carry out simple mechanical repairs and be familiar with computers.

Unfortunately equipment prices have escalated recently. Expect to pay up to \$80,000 for sophisticated liquid dispensing systems with built in weighing, vortex mixing solid phase extraction and interfaces to laboratory instrumentation. Full robotic systems may cost from \$180,000 to \$300,000 depending on their sophistication. The cost of systems should be recoverable over a three year period, if the application is suitable.

## NATIONAL MILK ANALYSIS CENTRE INSTRUMENT AUTOMATION

By Michael Walker - Livestock Improvement

---

At the National Milk Analysis Centre we are equipped to process in the vicinity of 60,000 samples a day. We carry out three analyses on each sample. This involves the use of Milkoscan 605 to determine the percentage of Milkfat and Protein and Fossomatic 360 to count the number of Somatic Cells in the sample. These instruments are high throughput instruments designed and built by Foss Electric of Denmark. The Milkoscan is an Infrared absorption instrument capable of processing up to 600 samples per hour for one parameter, we generally analyse for two parameters which reduces the throughput to 450 per hour. The Fossomatic is in broad terms an automated microscope. Each of these instruments is controlled by a built in microprocessor capable of

monitoring all the critical functions, and alerting the operator to any failures. These failures may be of a mechanical, electronic, or physical nature. By physical we mean things like temperature or flow rates. The samples are feed along the instrument by conveyor, being subsampled and analysed as they move from one position to another. The data is logged electronically into an in house system developed for us by the Electronic Company of New Zealand. This system allows us to record, edit, report and transmit to a larger data base with a minimum of manual input. This system is modular, thereby allowing processing to continue should one section fail. At present we are operating 22 analysers, 24 hours per day, 5 days per week.

# NZ WINS MEDALS AT CHEMISTRY OLYMPIAD

The 24th Chemistry Olympiad was held this year in Pittsburgh, Pennsylvania and Washington, D.C. It is the first time that this international event has been held in America, all previous Olympiads having been held on the continent. Appropriately, 1992 is also the year which marks the quincentenary anniversary of Christopher Columbus' historic voyage from Europe.

On July 8, the first NZ Chemistry Olympiad team set off for the US from a different side of the world accompanied by Dr. Robert Maclagan from the University of Canterbury. The team, Nicholas Cutfield from Otago Boys High in Dunedin, Michael Pleming and Henry Liu, both from Auckland Grammar, and Andrew Lowe from Selwyn College, Auckland departed on flight CO2. As the NZ Herald commented, this was an appropriate flight for a team of chemists. It was indeed an auspicious beginning

as CO<sub>2</sub> was to feature substantially in the exams which the team sat in Pittsburgh. The team was met by their other leader, Dr. Sheila Woodgate, University of Auckland, in New York where a two day stay was scheduled to overcome jet lag. Not surprisingly the members of the team actually wanted more to do sight-seeing and shopping than spend time sleeping in the hotel. As a result the Kiwi contingent braved the 90°F heat to visit the Statue of Liberty, art museums, Wall Street, Central Park and the UN. The leaders and two of the boys who are talented musicians attended a performance at the Metropolitan Opera and greatly enjoyed the quality entertainment. The rest of the team enjoyed entertainment of another sort - breaking into the suitcase of one of the more cultured team members.

Our first sight of the other competitors and their leaders was at JFK airport where many of the teams gathered for a chartered flight to Pittsburgh. Much to our delight, many of the competitors and leaders were anxious to get acquainted, and most were competent English-speakers. Henry Liu, our resident Chinese interpreter, was very useful in helping to communicate with a Taiwanese girl who was trying very hard to practice her English.

Upon arrival in Pittsburgh we met the team guide, David Cliffel a previous silver medalist and current- graduate student at the University of Austin in Texas. It is Olympiad tradition that since the team and mentors are separated during the first days of the competition that each team have a bilingual guide who is responsible for the welfare of the students. Our guide wasn't bilingual when we met him, but at the end of 11 days he could at least understand if not speak Kiwi. We also on the night of our arrival first experienced the generosity of our American hosts from whom we received a deluge of gifts donated by various sponsors and \$US75 spending money from the Olympiad committee itself. The giving of spending money is in accord with the Olympiad regulations to allow countries with strict currency regulations to participate. This year a record 33 countries



*Left to right: Dr. Sheila Woodgate, Michael Pleming, Henry Liu, Dr Robert Maclagan*

participated, 23 from Europe, 4 from the Americas and 6 from the Pacific Rim.

The Olympiad is characteristically for both the students and their leaders a mixture of hard work and fun. The first day is characteristically touristic to allow competitors who have just arrived to recover from their trip. We were all taken on a bus tour around Pittsburgh, during which we were shown some chemistry in action - namely how potent acid rain can be in damaging historic buildings and how a polluted industrial city can be converted to a clean, pleasant metropolitan area. The opening ceremony was held during the first evening in the Convention Centre of the University of Pittsburgh. Although there was no extravagant ignition of the Olympic flame, each delegation marched into the hall carrying their national flag while their national anthem was being played. We were one of only two countries that proudly displayed a mascot, in our case a stuffed Kiwi.

The students had their first taste of things to come with an extensive safety tutorial the next morning. They continued their tourism in the afternoon with a visit to the Carnegie Science Center. In the meantime the mentors were required to check the lab stations which were stocked by the Fischer Scientific sponsor with digital pH meters, electronic balances accurate to four decimal places, and a huge selection of various glassware for each of the 132 students. They also received a draft version of the instructions for the experimental task proposed by our American hosts - Study of the Effect of Dissolved CO<sub>2</sub> on the Solubility of Calcium Carbonate. Whilst there was no change made to the experimental details, the text and marking scheme was the subject of about a five-hour discussion. After the official American version was decided upon, the various countries were faced with the task of translating into their own language. The other "English"-speaking countries finished their translation and final printing about 11 pm.

While the students endured a five-hour session in the

laboratory, the leaders were treated to a tour of the Carnegie Museum with its notable dinosaur and mineral and gem collection. The students had their chance to unwind from the practical exam the following day when they were taken to a local aquatic park which featured a big collection of water slides. While they were enjoying themselves, the leaders thrashed out with the leaders from 32 other countries the alterations to the theoretical exam proposed by the Americans, again a late night for the translators both into other languages and English. The test consisted of nine questions and lasted five hours.

The Olympiad has a very fair system for marking both the theoretical and practical exams. Each student's paper is marked both by his/her leaders and also by the Scientific Committee from the host country. The marks are compared at an adjudication session. If the marking by the host country is higher, this is accepted. If it is not, discussion is entered into by the leaders to try to justify a higher mark for their student. This is sometimes successful, other times not. In our case, the balance was in favour of gaining marks for our students. Our students had done relatively well in comparison to marks in other recent Olympiads, and any suggestion that New Zealand students could not cope with the level of the exams was put to rest. However, this is a ranking exercise and we had the feeling that the exam had not discriminated well as it was long, but somewhat easier than previously. This however was only a feeling as leaders keep their students results very much to themselves.

The leaders and students were brought together on the evening following the theoretical exam at a picnic which featured various outdoor sports, including square dancing and ended with a spectacular fireworks display. Although the work was over for the students, the leaders left early to complete their marking as the adjudication exercise for the theoretical paper was the following day.

After the adjudication exercise, the work was over for the leaders as well. Thus began the second very important aspect of the Olympiad, that is cultural interchange. During the first days when the emphasis is on the competition, mixing (for both the teams and leaders) is somewhat limited. The student interteam competition was a very effective getting to know you exercise for the students. Each team consisted of one member from an English-speaking country with three others from countries which all spoke different languages.

The competition was held the day after the exam and involving sporting exercises with chemical names (such as fullerene transfers - kicking a soccer ball through a slalom course; gas effusion - throwing a frisbee through a hoop). The day was topped off by a river cruise with dinner and dancing at which all competitors received prizes. The remainder of the Olympiad was devoted to tourism and mixing between competitors and leaders of various countries. We travelled by bus to Baltimore and visited the aquarium at the waterfront. A meal that evening was to introduce two of the more adventurous eaters of the team to alligator. Unfortunately the local delicacy, Maryland crab, didn't agree with one team member. After dinner we travelled to Washington where we were housed at Georgetown University. Leaders and students were separated again for our first day in Washington, with the students attending the King's Dominion Amusement Park in Virginia with the large collection of roller coasters, and the leaders visiting The Mall: the site of the Smithsonian Museums, the Capitol, the White House, the Supreme Court and the Lincoln, Washington and Vietnam memorials. The students were to have an opportunity to see this area later in the week. Maryland was added to the list of states visited as we had the treat of seeing a Chemical Demonstration Show at the University of Maryland done by Ron Showalter, the demonstrator on the Hoffman Chemistry videos. One of the most memorable events of the visit was a reception that afternoon at the State Department. Upon arrival, the guests had to display their passports and pass through the metal detector before entering the lift. As we came out of the lift, we were all overwhelmed by the playing of a string quintet and the luxurious setting in the most elegant Benjamin Franklin room. Waiters roving about brought us nibbles on silver platters. It was a beautiful setting and was as big a treat for the Americans as the foreigners. The Second Secretary of the New Zealand embassy was there to greet us and took us to the NZ embassy in Washington afterward.

The leaders were then involved in the serious business of deciding the medal cutoff points. Roughly 60% of students received bronze (30%), silver (20%) or gold (10%) medals. The code used to disguise the marks during the cutting lines decision exercise was not deciphered before the closing ceremony which was held in the National Academy of Science. The ceremonies began in a most delightful way with a ten minute video

of the events during the Olympiad in which each student featured. Short speeches by two Nobel Laureates, Gertrude Elion and William Lipscomb, preceded the medal presentation. The Americans had prepared medals for all participants with the lowest category being copper. These were read in alphabetical order. When the reading of the "M's" began, it was apparent that two of our team members, Michael Fleming and Henry Liu, had received medals. From their marks, we realized that Nicholas Cutfield and Andrew Lowe had just missed out on bronzes. The two bronze medal winners and the leaders were the subject of many congratulations as it was regarded that two medals in the first year of competing was a good performance. The Olympiad finished with a dinner that evening in which the leaders each received a copper



*Left to right: Michael Fleming, Nicholas Cutfield, Dave Cliffel, Henry Liu, Andrew Lowe.*

medal and themselves distributed a greeting card and NZ tourist board information as a memento to the other leaders. Tired and ready to go home, the team left Washington National airport after a remarkable two weeks. The preceding is a composite of the student and mentors reports of what happened at the Olympiad. The concluding paragraphs were from the student's report: Apart from being tourists, competitors and leaders, we also acted as cultural ambassadors. During the two-week long Olympiad, we had a lot of opportunity to get to know participants from various cultures all over the world. We have learned how to exchange opinions, tolerate views other than our own and realized how easy it is to build long-lasting friendships in such a short period of time. In fact some of the members of the team have already planned to apply for jobs at the New Zealand embassy in Mexico City and the New Zealand Embassy in Sofia, Bulgaria. Others are still wondering if New Zealand has any diplomatic relations with Latvia and Taiwan.

On our way home, we were suspected terrorists at the airport while we went through the metal detector with our medals in our pockets. Although our flight CO2 got reduced to CO 1 on the return trip, our interest in chemistry certainly has not been reduced in the slightest manner. On the contrary, the invaluable experiences and enjoyment gained from this trip has obviously facilitated our decision on our future career.

To conclude, the Olympiad brings together a group of talented students from diverse communities and cultures to work together in an environment dedicated to a wider understanding of the part played by science in the world in which we live.

The team and leaders would like to thank all those who helped us succeed in Pittsburgh, especially Dr. Robert Smith, Otago University, Drs. Peter Steel and Peter Harland from the University of Canterbury and the staff of the Chemistry Department of the University of Auckland who contributed to the May camp.

We wish to acknowledge the support of the New Zealand Institute of Chemistry and in particular two officers - Arthur Williamson who was always encouraging and Alan Turner who acted as Treasurer. We acknowledge financial support from the following organizations: Chemical Education Trust, Dynavac New Zealand, Fay Richwhite, John Ilott Charitable Trust, the committee of "Chemical Processes in New Zealand", Mobil Oil New Zealand limited, New Zealand Refining Company Ltd, Nuplex Industries Limited, Rohm and Haas N.Z. Ltd, New Zealand Section, Royal Society of Chemistry, New Zealand Biochemical Society, Tasman Pulp and Paper Company Limited, Thermoplastic Engineering Limited, and Union Carbide Chemicals (N.Z.). A number of NZIC members made contributions. Support in kind was received from Commercial Union Insurance Company Limited, Continental Airlines and McGraw-Hill Book Company, New Zealand Limited. You will note that no support was received from any Government department or the Lottery Board.

A number of individuals have also given significant support - Sheila Woodgate from Auckland organized the camp and undertook the training of the Auckland students. Drs. Peter Harland and Peter Steel from Canterbury set three exams and marked them. The Chemistry Departments at Auckland and Canterbury have also given considerable support in kind.

# INDUSTRIAL RESEARCH LIMITED

by Geoff Page

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**Industrial Research Limited came into being on 1st July this year, bringing together parts of DSIR Chemistry and DSIR Physical Sciences with all of DSIR Industrial Development. We now have almost 400 staff across four sites; Auckland, Palmerston North, Wellington and Christchurch.**

We are a Government-owned company dedicated to conducting viable world class research that leads to internationally competitive added-value opportunities. Building on the reputation for quality and reliability inherited from DSIR, the new commercial freedoms afforded Industrial Research will enable us to relate with commercial companies as a business partner rather than as a Government department.

As a company we will be working together with New Zealand manufacturers, processors, transport operators and others to assist in developing and maintaining their competitive edge.

We have a wide variety of skills in topics ranging from fruit storage to pharmaceuticals, from silicon chips to safety tests. The common element across all our work is a dedication to excellence - both in terms of the quality of our science and the quality of service given to our clients.

Basic research will not be neglected in our research and development mix. I see long-term basic or strategic research as crucial to the long-term viability of the company both in scientific and financial terms. This type of research will continue to be funded by the Government through the Public-good Science Pool administered by the Foundation for Research, Science and Technology.

Specifically with regard to chemistry our research is based primarily in Wellington.

Our expertise in organic chemistry synthesis, carbohydrates and plant pigments forms part of the Natural Products Processing group and is teamed with separation technologies and biochemical processing with the objective of maximising the synergies which exist between these areas.

Our inorganic and physical chemistry expertise is contained within the Materials Science and Performance group that now links together research into chemical aspects of materials with their physical properties and engineering applications.

We will also maintain continued collaboration with others for example, DSIR and MAF jointly funded the acquisition of the 500MHz nmr which is based on the Gracefield campus.

This facility is now jointly owned by AgResearch (the pastoral CRI and ourselves, and provides a significant increase in our scientific capability.

I look forward to the prospect of a growing synergy and partnership with the Crown Research Institute and others in the area of chemistry in general.

# DISPOSAL OF SURPLUS OR DANGEROUS CHEMICALS

by Jenny Butcher

A committee of the Auckland Branch has been considering the issue of unwanted chemicals in schools, and in August a questionnaire was sent out to a number of schools in Auckland and Northland in order to get an idea of the extent of the problem: that is, specifically what surplus chemicals schools were holding, and in what quantities.

From our own experience, we know that many school (and other) laboratories tend to have surplus chemicals lurking in dark cupboards. In schools this comes about in various ways: sometimes the syllabus changes, and less emphasis is put on a particular experiment; sometimes a new textbook is introduced and the routine changes slightly; sometimes a directive is issued from on high that a particular chemical is now considered carcinogenic or too dangerous. Busy school teachers and technicians often don't have time to look at each substance individually and decide how it should be disposed of, and local Council safety officers may not have the expertise to deal with the more obscure items.

Once we had an idea of the nature and extent of the

problem, we hoped to be able to provide some help towards disposal/safety. We wondered if these chemicals could be passed on to someone who needed them; perhaps even sold on by means of some scheme which could make a profit, or at least be self-supporting. Some of the issues which arose were as follows:

- all schools need much the same things
- industries may not want pre-opened (and possibly contaminated) jars
- a permanent, central dropping-off point would involve expensive storage; quantities could be large
- legal problems arise regarding the sale of schedule poisons
- noxious items which are completely unwanted may need to be chemically 'neutralised' and this could be expensive.

Schools were asked to provide the following information:

Chemical name	Formula name	Common name	Quantity (g)	s,l,g	Opened or sealed
<i>eg</i>					
<i>potassium cyanide</i>	<i>KCN</i>		<i>500</i>	<i>solid</i>	<i>opened</i>

We received 30 replies, and in October we made up a list of chemicals based on these returns. It was clear that there was quite a demand for help relating to permitted chemicals, storage of certain substances, books and publications on safety, as well as information on disposal. Therefore the NZIC is now acting in a liaison capacity, and working with the Education Advisory Service on this project. Whatever information the NZIC, and our helpers, can provide, is being made available to the Education Advisory Service, so that a comprehensive body of material is being collected. Schools will have received a copy of the list of unwanted chemicals via the Education Advisory Service. A list is also being made up of chemicals which may need extra security in terms of being sought-after for illegal purposes. Any inquiries should be directed to: Kath Hills Education Advisory Service Private Bag 9260 1 Symonds St Auckland. Phone (09)3770881.

As well, we are trying to organize a day (this term, we hope) to hold a sort of swap-meet or "bring and buy" (in Auckland) for unwanted chemicals. As this will most likely be in association with commercial disposal firms, it is possible there will be a charge to schools for disposal of the things they cannot give away, but this should be less than if each school negotiated on an individual basis. Some things may even have a resale value. If any industries or commercial labs are interested in a copy of the list, or require further details, please contact the Education Advisory Service (as above). You may wish to get in early and contact any school on the list which has something that you require. We hope these efforts will help to address a very real problem faced by many schools.

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# THE SHELL PRIZE FOR 1992

The Shell Prize for 1992 has been won by the fertiliser chemistry section of the Department of Scientific and Industrial Chemistry based at Mount Albert, Auckland. The team of Andy Braithwaite, Tony Eaton and Phil Groom performed work both on and off site for the Bay of Plenty Fertiliser Company to develop a new commercial product. Team leader Andy Braithwaite was born in England in 1949 and moved to New Zealand in 1957. He was awarded a PhD in Chemistry in 1974 and then spent three years on Postgraduate Scholarships (in England) and on a Humbolt Scholarship (in West Germany). He returned to New Zealand in 1978 and briefly lectured at Auckland University before taking up the position of Physical Chemistry Section leader at the Fertiliser Manufacturers Research Association in South Auckland.

When this association was wound up 1986, D.S.I.R. developed a small fertiliser group as part of the Applied Chemistry group and Andy built up a team to provide both a research group and commercial unit. During their four years with D.S.I.R. the group twice won the Chemistry Division prize for commercial excellence.

After the demise of D.S.I.R. in June 1992 Andy joined the New Zealand Pastoral Agriculture Research Institute Ltd (Ag Research) in Hamilton as a processing scientist attached to the Soils and Fertiliser group and has been involved in promoting and marketing Ag Research in South East Asia. He has recently been involved in a study in Vietnam and has just returned from a promotional tour in Thailand.

Tony Eaton joined D.S.I.R. in 1978 as technical trainee, studying for NZCS whilst working in the Food and Water Sections doing routine analyses. He transferred to the Applied Chemistry Section after 2 years and worked in the industrial chemistry field, where the role became more of an investigative/problem-solving nature. During the 7 years spent in this area, Tony gained his NZCS in 1980 and shortly after was appointed the "Official Gas Examiner" for the Auckland and Hamilton areas. His role in this capacity was to monitor the quality of gas supplied to these areas for regulatory purposes.

In 1984 he was awarded the A.C. Kennett Award for the best paper on non-metallic degradation, presented at the annual A.C.A. conference.

Since 1987 Tony has been working in the fertiliser chemistry area, when a small group was formed. In this time he has contributed to research in the assessment of fertiliser materials, resulting in 6 papers to date being published internationally and numerous research contracts for commercial clients, one of which involved the production of a new fertiliser product which resulted in it being successfully marketed.

It is for this work that the Shell Prize is being awarded with the formation of Crown Research Institutes in July

1992, he now works for New Zealand Pastoral Agriculture Research Institute Ltd. Phil Groom was born in Napier and received a D.S.I.R. bursary for his BSc degree at Victoria.

He built a solid career in D.S.I.R. Chemistry in a variety of divisions including forensic work on the Rainbow Warrior and was made a fellow of the Institute in 1988. In 1988 he joined Andy Braithwaite in Fertiliser Chemistry and contributed to the research programme until he retired at age 60. The development work that was the basis of the award arose from changes in fertiliser strategy over the last decade.

The fertiliser industry in New Zealand had for many years been seeking a viable alternative to its traditional product, single superphosphate. During the 1980's a hybrid mixture of single superphosphate and "reactive" phosphate rock, called LONGLIFE, had been offered as an alternative.

However this product had become unacceptable to the farming community because of its inconsistent chemical analysis, its poor physical condition, and inhomogeneity. Accordingly one fertiliser company, Bay of Plenty Fertiliser Limited, (BOP), approached D.S.I.R. in 1987 to perform laboratory trials to assess the potential of an alternative product, a partially acidulated phosphate rock.

After the successful completion of laboratory trials D.S.I.R. and BOP applied jointly to the Emerging Technologies Board for a grant to study the potential of the product at works level. The application was successful and Dr Braithwaite and Mr Eaton performed trial work on site at Mt Maunganui for eight months over the period from April 1990 to February 1991.

A successful launching of a new product, called LONGLIFE SUPREME, followed in March 1991. The company now manufactures LONGLIFE SUPREME as an alternative to single superphosphate, production of LONGLIFE having ceased in March 1991. Such products as LONGLIFE SUPREME have been manufactured in other countries, but never using the low cost granulation systems used in New Zealand with Broadfield mixers and dens. The small capital outlay required to produce this product has resulted in a 10 to 15% saving in cost due to its higher P status, its more efficient P to S ratio, and lower transportation and application cost.



The product has been endorsed by MAF as a highly efficient fertiliser product. Key research work in defining its chemical assessment has been performed in the D.S.I.R. laboratory in Auckland by Mr Groom Dr Braithwaite, Mr Eaton (above) and, over a three year period, resulting in six international publications.

# CHEMISTRY IN THE NEW CROWN RESEARCH INSTITUTES

The DSIR exists no longer, with the new government owned CRI's now the major government science providers. Chemistry expertise contained within the old DSIR Chemistry has been diluted to a number of the new CRIs. However the majority of scientific staff have transferred to two new institutions, Industrial Research Limited (IRL) and the Institute of Environmental, Health and Forensic Sciences Limited (IEHFSL).

As well as chemists, Industrial Research Limited has a large proportion of the physicists who were previously with DSIR Physical Sciences and engineers of DSIR Industrial Development. Thus as in most of the other CRI's the principal resource is the scientific staff. The large number of physics, chemistry and engineering scientists places IRL exceptionally well to undertake research in the industrial area. The CEO of IRL is Dr. Geoff Page and board chairman Mr David Bone. IRL has six science management units which covers specific research areas and should allow for better and more specific client interaction. Two units (Packaging and Transport, and Production, Automation and Control) are situated at Parnell in Auckland and the rest are at Gracefield in Lower Hutt.

Materials Science and Performance is managed by Dr Don Smith and has research teams in the following

areas; superconductivity, high technology ceramics, corrosion, polymers, surface coatings, materials performance testing, metallurgy and materials analysis. Measurement, Applied Maths and Analysis Research is managed by Dr Kevin Duckworth and includes primary standards, calibration services, data analysis, mathematical modelling, and product testing and evaluation as major research components.

Natural Product Processing is managed by Dr Doug Crump and has research teams in the areas of biochemistry, biochemical engineering, organic chemistry, and environmental engineering.

Communication, Electronics, Sensing and Information Technology is managed by Dr David Bibby and includes research areas and services in silicon sensors, computer networks, information technology, information services, signal processing and microwave communication.

Packaging and Transport is managed by Dr John Meikle and is involved with supplying research and services in controlled atmosphere storage, packaging properties, shock vibration testing, heavy vehicle stability and fuel performance. Production Automation and Control is managed by Mr Peter Conner and is involved with research and services in automated production systems, automated inspection systems, microwave applications and optical processing. The majority of the staff members are situated in Wellington on the Gracefield campus although head office is in Auckland and there are regional centres at Auckland and Christchurch.

The Institute of Environmental, Health and Forensic Sciences provides research, analysis and consultancy services in the fields of environmental health and forensic science. This includes such diverse fields as examining food, water and air quality, monitoring wastes, testing for illicit drug use, and carry out surveillance of communicable diseases. The CEO of the Institute of Environmental, Health and Forensic Sciences is Mr Mark Templeton and the board chairman is Mr Chris Mace. IEHFSL is organised on a regional basis to provide better service to the mainly regionally based clients. Four regional laboratories or science centres have been established as separate management units.

The Auckland Science Centre at Mt. Albert and NECAL at Mt. Eden is managed by Dr Merv Jones. The Wellington Science Centre at Gracefield is managed by Dr Terry Manning.

The New Zealand Communicable Disease Centre at Porirua is managed by Dr Martin Tobias and the Christchurch Regional Laboratory is managed by Dr Bill Swallow. With the exception of the Porirua laboratory the majority of the scientific skill in IEHFSL is chemistry based and include such diverse chemistry disciplines as pharmaceutical, food, environment trace organics and inorganics, water, and forensic chemistry. The Wellington Science Centre contains the majority of staff and head office is in Wellington.

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# PHD CHEMISTRY RESEARCH AT THE UNIVERSITY OF AUCKLAND

Here is a cross-section of abstracts of PhD research currently being carried out in the Department of Chemistry at the University of Auckland.

## OBSERVATIONS OF ATMOSPHERIC REDUCED SULFUR GASES/AEROSOLS AT SITES IN ANTARCTICA AND NEW ZEALAND

DAVID WYLIE

It has been proposed (by Chadson *et al.*) that reduced sulfur gases (RSGs) of marine biogenic origin may influence climate through an aerosol (CCN) cloud-albedo feedback mechanism. We have made measurements of RSGs, particularly dimethylsulfide (DMS), at two sites in New Zealand and one site in Antarctica. In addition, measurements of aerosol methanesulfonate (MSA) and aerosol non-sea salt sulfate (NSSS) have been carried out on a continuous basis at the University of Auckland's Marine Laboratory at Leigh, on occasions at Baring Head (Wellington), and at a coastal site on Ross Island in McMurdo Sound. At a remote site in Antarctica concentrations of MSA and NSSS in aerosols and surface snow have been determined and compared with their depositional history in ice cores. Research has been carried out in collaboration with the National Institute of Weather and Atmospheric Research (NZWIR Ltd). Changes in RSGs and aerosol concentrations are being compared with meteorological events.

## BIODEGRADABLE FOOD GRADE SUDACTANTS

RICHARD BARTON

AGMARDT PhD scholarship to investigate of the production of food grade surfactants from readily available materials. Aspects of interest include the investigation of interaction of Lamb Lingual Lipase and Tallow and tallow methyl esters without solvents or detergents, and including characterisation of reactivity with both raw and processed lipase. Also later investigation of the possible use of lamb lipase in the production of sugar fatty acid esters toward the same ends, with optimisation of the kinetic condition

## KINETIC INVESTIGATIONS OF AMINO/AMIDE RING CLOSURE

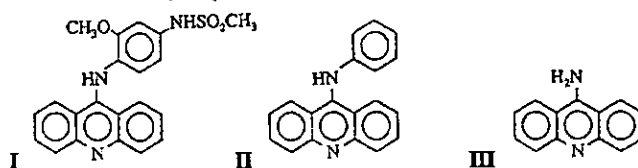
BRIDGET SYKES

The utility of internal cyclisation reactions as a means of hypoxia selective release of a mustard is being investigated. Amine nucleophilicity, stereochemistry and the nature of the leaving group have been identified as rate influencing. Some esters have also been investigated showing greater reactivity than their amide counterparts. Buffer studies are underway in order to elucidate some mechanistic aspects of the reactions.

## RAMAN SPECTROSCOPIC STUDIES OF COMPLEXES OF mAMSACRINE WITH CALF-THYMUS DNA

C.A. BUTLER

Resonance Raman (RR) spectra of the anti-tumour agent meta-amsacrine I in aqueous solution of varying pH (6.00-10.45) have been recorded and bands sensitive to changes in protonation of the molecule have been identified. The intensity changes of these pH sensitive bands appear to correlate with intensity changes observed in the surface enhanced Raman spectra (SERS) of I from silver electrodes at different potentials with the more reducing potential corresponding to a neutral species in solution. Excitation profiles (EP's) for RR bands of I have been obtained with excitation at wavelengths between 457.9 and 514.5 nm. The EP's were normalized against the intensity of an internal standard, MeCN, which was selected because its presence generated no detectable changes in the appearance of the spectrum of I.

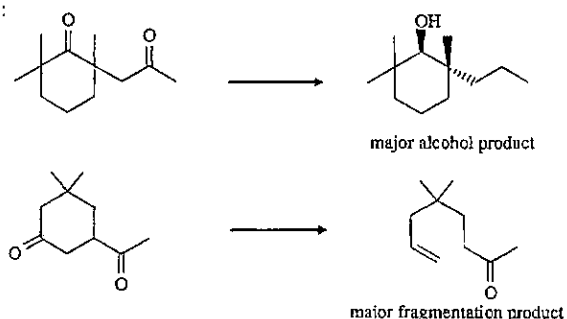


The UV-visible spectra of I, II and III were analyzed in conjunction with available X-ray crystallography data and the results suggest that the RR spectra of I exhibit the vibrational modes of the acridine chromophoric unit only. The RR spectra of calf thymus DNA-I complexes have also been recorded at a neutral pH for drug : base pair ratios of 1:2 to 1:20. To assist in interpretation of these spectra the acridine unit will be the subject of a normal coordinate analysis and molecular orbital calculations.

## REGIOSELECTIVITY IN THE CLEMMENSEN REDUCTION OF 1,4-DIKETONES

K.E. BAILEY

The Zinc-acid reduction of a range of 1,4-diketones has shown that a variety of pathways may be followed, depending on the structure of the dione. In some cases, the reaction shows a surprising degree of regioselectivity, e.g.:



## TASTANT INTERACTIONS WITH MODEL MEMBRANES

PATRICIA SHAW

The interaction between various tastants and their receptors on the tongue can be investigated using NMR methods. Since isolated human taste buds are unavailable, model systems are used. The biological organelles are considered to be essentially lipid membranes with embedded proteins and are mimicked using unilamellar phospholipid vesicles.

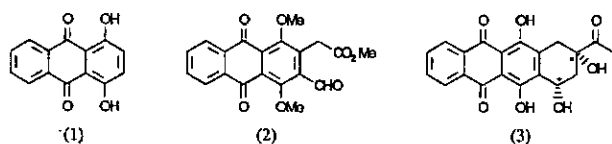
A wide range of compounds elicit the same sweet taste. Some of these are simple organic molecules such as glucose and saccharin. Others are much more complex such as the diterpenoids, glycyrrhizic acid and stevioside. Sweet proteins such as monellin and the thaumatins are also known. A major part of this work is unequivocal assignment of the  $^1\text{H}$  and  $^{13}\text{C}$  spectra of these naturally derived sweeteners.

No obvious structural similarities in all the sapid molecules are apparent. The taste response may be triggered by a specific molecular conformation when interacting with the receptor. We are determining the solution conformation of the tastants and monitoring the changes when in the lipid membrane environment. Changes in chemical shifts and  $T_1$  relaxation times characterising molecular constraints are observed.

## THE SYNTHESIS OF ENANTIOMERICALLY PURE 4-DEMETHOXYDAUNOMYCINONE (3)

JARED MILBANK

The synthesis of enantiomerically pure 4-demethoxydaunomycinone (3) and *ent*-4-demethoxydaunomycinone from quinin (1) is being attempted. The proposed synthesis can intellectually be divided into two sections; synthesis of methyl (3-formyl-1,4-dimethoxy-9,10-dioxo-9,10-dihydroanthracen-2-yl)acetate (2) as an achiral intermediate, followed by annelation. The first section, functionalization of quinizarin, makes use of the reductive Claisen rearrangement. The second requires the stereoselective introduction of two asymmetric centres (starred).



## SYNTHESIS AND REACTIVITY OF BORON PORPHYRIN COMPLEXES

WARWICK BELCHER

Complexes have been prepared containing boron coordinated to tetra-*p*-tolylporphyrin (TTP) using  $\text{BCl}_3 \cdot \text{MeCN}$ ,  $\text{BF}_3 \cdot \text{OEt}_2$  or  $\text{PhBCl}_2$  as the source of boron. The resulting complexes contain one or two boron atoms with fluoro,

hydroxy or phenyl substituents. Interaction of the boron atoms with the porphyrin is markedly asymmetric, such that the four-fold axis through the ligand is lost.

## ASYMMETRIC HETERO-DIELS-ALDER RXNS

M. BERCIH

The synthesis of the C-glycosidic moiety of vineomycinone B2 methyl ester via an asymmetric hetero diels alder RXN is being studied. The use of homochiral boron vanadium and europium complexes as well as anthraquinone substrates bearing homochiral auxiliaries are being studied.

## SPECTROSCOPIC STUDIES OF ADSORBATE-PILLARED INTERLAYER CLAY CATALYST INTERACTIONS

S.A. BAGSHAW

FT-IR and Raman vibrational spectroscopic studies of organic 'probe' molecules have been undertaken in an effort to gain understanding of the properties, structure and behaviour of the surface of various pillared-interlayer clay catalysts (PILs). FT-IR spectra of adsorbed pyridine have been employed to study the behaviour of surface acid sites and Lewis/Bronsted acid ratios. FT-IR and Raman studies of adsorbed 2,2'-Bipyridine have been employed to study the interaction of a bidentate adsorbate and in an attempt to characterise interpillar spacing of various PILs. Further work is continuing.

## PHD CHEMISTRY RESEARCH AT THE UNIVERSITY OF OTAGO

*Continued from October issue*

## FIDELITY, INFIDELITY, DEVIANCE AND RELEASE

The messenger RNA (mRNA)-programmed synthesis of polypeptide sequences by the ribosome is arguably the most complex and information-intensive reaction in nature. mRNA-transfer RNA (tRNA) basepairing is the basis of the translation from nucleotide to amino acid sequence during initiation and elongation cycles. When the end of elongation is signalled by a stop codon it's a whole new ballgame: The stop RNA sequence is not recognised by any tRNA, but by a family of proteins; the Release Factors (RF).

Our interests in this fundamental process are manifold. Release of the finished protein from the ribosome is potentially a rate-limiting step in protein synthesis and hence in cellular growth. Bacterial cells spend a large proportion of their existence making proteins, so

optimisation of the protein synthetic machinery is crucial. Fran is studying the way the bacteria *Escherichia coli* fine-tunes and co-ordinates the amount of its two release factors. She has shown dramatic changes at different growth rates.

The freedom of the stop signal from the constraint of triplet anticodon base-pairing allows the cell a unique opportunity to escape the tyranny of the 20 amino acid, non-overlapping triplet genetic code and do deviant things such as incorporate a funny amino acid (e.g. selenocysteine), shift reading frame or readthrough a stop. Viruses, with incredibly compact genomes, are regular users of such 'tricks'. With the frameshifts of retroviruses (HIV in particular) and plant viruses in mind, Julie is using in vivo and in vitro translation techniques to study ways of up- or down-regulating the HIV frameshift event. Chris is using a similar approach to ask the rather profound question; what is a stop signal?, testing his theory that 4 bases, not a triplet, make an effective stop signal, and that the 4th base influences the efficiency or infidelity of termination. The 4-base stop model applies to eukaryotes as well as bacteria, and since it is the eukaryotic release factor (eRF) involved in deviant events in plant and animal virus protein synthe-

sis, Jason is working on isolating and sequencing the eRF from rabbit.

Deviations from the 'universal' genetic code are seen in mitochondria. During their evolution from symbiotic bacteria they have come to use some stop signals to code for amino acids. Kirsten is isolating the mitochondrial RF (mRF) from rat, comparing its functions to bacterial factors, and sequencing the gene. Rob and Nicola are studying the factor from yeast mitochondria, and Rob is further looking at the evolution of RFs by sequencing genes from bacteria across the kingdom. The divergence of parts of the RF sequences during evolution is an important guide to the functional roles of parts of the proteins. John has been identifying functional parts of *E. coli* factors using antibodies to fragments of the protein and by making changes to the genes to identify essential sites. Together these approaches will increase the understanding of how these factors both recognise, and sometimes fail to recognise, stop signals, whatever they may be.

Fran Adamski, Chris Brown, Nicola Collie, Jason Gray, Julie Horsfield, John Moffat, Rob Powell, Kirsten Timms.  
Supervisor: Warren P. Tate

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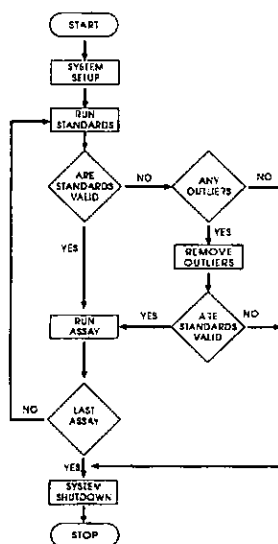
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5 Lake Drive, Redwood Gardens Estate, Dingley Victoria 3172 Australia  
Fax: +613 551 7440**

### SSC-300 Autosampler

Totally Automated Analysis for as Many as Eight Elements Increases Laboratory Productivity.

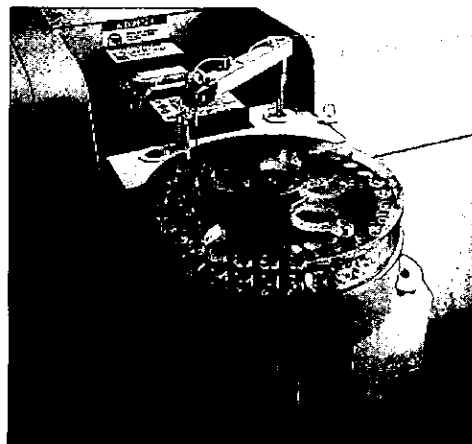
As many as eight elements and the sequence of their analysis can be user selected for automated measurement. Heated injection from 50 to 200°C is possible and can be combined with five different syringe speeds to accommodate the widest range of sample viscosities. The Heated Injection procedure also allows multiple sequential injections and drying of very dilute analytes for the measurement of extremely low levels of metals.

As many as ten standards can be assigned to each element, combined with the concentration values and cup positions. Working standards can also be automatically prepared from three different stock solutions. Dilution factors and volumes are calculated and displayed automatically.

Up to four different matrix modifiers are included and can be dispensed into the cuvette before and after the sample. This 'sandwich' deposition method ensures maximum mixing of the sample and matrix modifiers for efficient delay of the sample atomization.

To eliminate potential carry-over or contamination, from one to five complete rinses of the sample nozzle can be user selected.

Injection volumes can be varied from 1-100 µl in 1 µl increments. Optimum sample dilution, modifier and spike volumes are easily selected.



**For further information contact:  
Alphatech Systems Ltd.  
P.O. Box 37583 Parnell Auckland  
Ph: 09-377 0392 Fax: 309 8514**

## SEGMENTED & FLOW INJECTION ANALYSIS

The Flow Solution is flexible enough to meet all the wet chemistry needs of today's analytical laboratory. It combines the advantages of segmented flow and flow injection analysis into one integrated package. The result is an analyser that delivers the best of both technologies. For example, each of The Flow Solution models have automated valves that solve a number of sample handling problems. They provide direct sample injection, sample dilution or preconcentration, and sample filtration for clean-up.



### SUPER CARTRIDGE

To provide a greater degree of flexibility The Flow Solution includes a family of specially designed SuperCartridges. They provide the ability to run multiple or single tests on the same manifold. Using non breakable coils and unique polymeric connections, test changeover is faster and easier than ever before. Cross contamination is eliminated. The Environmental One SuperCartridge, for instance, is configured for nitrite, nitrate, total phosphorus and ortho-phosphate analysis using US FPA approved tests. A number of SuperCartridges are available to meet your testing requirements.

### THE CHECK REAGENTS

To guarantee reliable, consistent results every time, a family of prepackaged kits called "The Check Reagents" have been developed. They eliminate weighing and preparation errors; are available for a variety of applications; and all reagents are formulated according to the standard reference methods of organisations such as US FPA and AOAC. Used together, the SuperCartridges and Check Reagent kits provide total assurance of

regulatory compliance and consistent analytical performance.

### FULL AUTOMATION WITH ADVANCED SOFTPAC™ PLUS

To provide today's analytical lab with true hands-free automation, ALPKEM developed SoftPac Plus. Under the control of this versatile 12 channel data package, The Flow Solution provides automatic recalibration at user-defined intervals. It can automatically control the random access sampler, dilute and rerun off-scale samples, automate pump start-up/shutdown and detector autozero. Softpac Plus easily handles segmented and FIA

data collection. It offers US EPA Contract Lab Testing protocol, real-time display of peaks and has an integral spreadsheet for reformatting reports.

**For more information contact:  
Sci-Tech, P O Box 633 Dunedin,  
Ph 03-477 7860 Fax 477 7870**

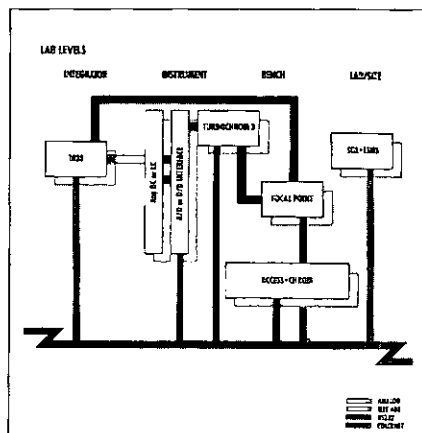
### TRUE INTEGRATION FROM PE NELSON PERKIN ELMER NELSON SYSTEMS

(PE Nelson) is dedicated to the development and support of computing solutions for the analytical laboratory. PE Nelson provides integrated multivendor solutions

which optimize the latest computer technologies, adhere to accepted industry standards, and protect the user's investment in analytical instrumentation, computer hardware, and software applications. Solutions that make sense today and tomorrow. Laboratory managers and directors are challenged to choose the best product for the particular job - and to knit together integrated computing solutions that serve the goals of the entire laboratory. While these two agendas appear to conflict - the use of the best solution for a particular problem produces a multivendor environment which makes integration difficult - a solution achieving both goals is available.

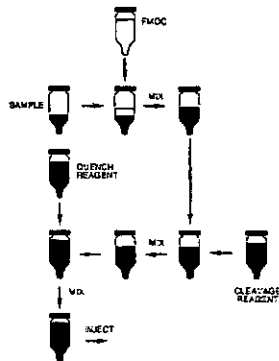
For PE Nelson, responding to customer requirements means delivering products that can function in a multivendor environment. It means working with customers on whatever technological approach is best for them. It means helping customers develop computing solutions that work both today and tomorrow. The typical laboratory has a number of different vendors' integrators, chromatographic data handling systems, computers, workstations, and network protocols. Each product has a different form, fit, and function which causes inefficiencies because each produces data in its own format, making data comparison and interchange difficult. Through strategic partnerships, PE Nelson can integrate your chromatography instrumentation, bench level data system and workstation, and laboratory information management system (LIMS) to function as a single system - eliminating data interchange difficulties and effectively linking your laboratory and your whole organisation together. The successful laboratory must integrate data from a variety of instruments, convert the data into useful information, and make this information available quickly and easily to the entire organisation. Each level in the laboratory computing hierarchy must communicate with the next level regardless of the instruments, data systems, computers, and networks involved.

**For more information contact  
Perkin Elmer PO Box 22159  
Otahuhu Auckland Ph (09) 276  
2230 Fax (09) 276 5602**



## ANIOMATE

Aminomate provides a complete validated procedure based on proven 9-fluorenylmethylchloroformate (FMOC) pre-column derivatisation chemistry for both primary and secondary amino acids. The derivatives are stable and highly fluorescent, providing reproducible and accurate results at femtomole sensitivity. Aminomate guarantees outstanding separation and resolution of 17 amino acids within less than 25 minutes and without interference from FMOC by-products (figure 1). Automation Aminomate's PC based Chromatography Management System provides comprehensive data analysis, report generation and validation. Total interactive communication and control of the autosampler and the multisolvent pump are key features of the system. Aminomate is pre-programmed for immediate turn-key operation (figure 3). The flexibility of the data system allows you to tailor the method to suit your specific analytical requirements. The full robotic capability of the autosampler enable highly accurate vial to vial liquid transfer and thorough liquid mixing (figure 4). To prevent cross contamination, all liquids are isolated during transfer and the needle is washed after each transfer of a reagent or sample.

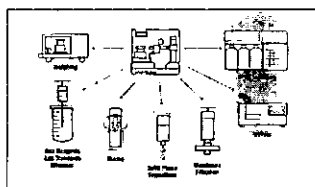


The chromatogram is displayed in real-time and can be autoscaled at any stage during the sample run. At the completion of analysis, Aminomate automatically activates a shutdown sequence to protect system by flushing all solvent lines and then maintaining the pump in a stand-by mode. Validations & Diagnostics Aminomate utilises a comprehensive set of validation parameters that enable single and group validation during the analysis. The validation routines are executed after every sample analysis. The unique automation capabilities of

Aminomate allow you to enter a command sequence that will be performed depending on the validation results. Validation of the results includes the ability to check the variance of peak area/height, retention time, plate count, peak shape, resolution, and many more. Confidence limits can also be set for statistical outliers so that they may be removed from the calculations. **For more information contact ICI Instruments PO Box 68330 Newton Auckland Ph(09) 373 5765 Fax(09) 3600683**

## BENCHMATE WORKSTATIONS

The BenchMate sample prep workstation is a versatile, smart "extra pair of hands" for all of those SPE manual tasks that eat into your lab's productivity. The BenchMate lets you easily automate the SPE sample prep techniques you're using now, takes the kind of care with every sample that you would, and keeps a detailed and accurate record



of every action. In addition to SPE, the BenchMate performs extremely precise dilutions, reagent and internal standard additions, vortex mixing, and membrane filtration. The BenchMate also performs HPLC and UV/Vis autosampling. An internal balance monitors every liquid transfer or addition with four-place precision, time after time. You'll not only get more done, you'll improve the reproducibility of your results. Build methods quickly and easily on any PC. Intuitive pull-down menus let you create a procedure in minutes, even with no previous hands-on experience. Save procedures on a diskette; use the diskette to run the BenchMate. No dedicated computer (or computer genius) necessary. It's simple, the BenchMate lets you work more productively by working smarter.

**For more information contact Alphatech Systems Ltd PO Box 37583 Parnell Auckland Ph (09) 377 0392 Fax (09) 309 8514**

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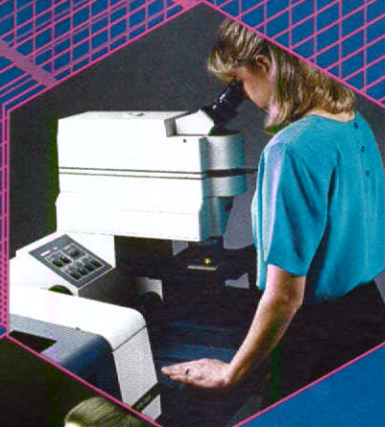
Molecular identities emerge quickly and easily with state-of-the-art FT-IR spectrometers and accessories.



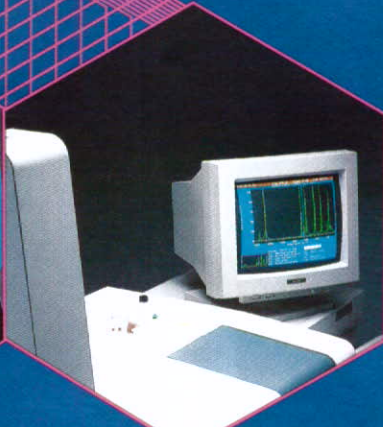
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*The new Bio-Rad FT-Raman spectrometer is the first to offer precision step-scan capability.*

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