



TOF News



Inside this issue:

Just what is in your fuel?	1
Environmental studies	2
Forensics: LECO and the SAPS	2
Pathology by TOFMS	3
Metabolomic dabbling	3
Wines and Spirits	4
Water Safety	4
Who is LECOAfrica?	5
Contact Information	5
List of abbreviations	5

The Future of TOFMS?

Recently LECO Africa reviewed its installed base and the applications our instruments supported.

From a small base in Petrochemical analysis (page 1), to extensive use in environmental analysis (page 2), forensics (page 2), pathology (page 3) the LECO range of products certainly has seen it all.

More recent applications cover life sciences and metabolomics (page 3), alcohol adulteration and wine profiling (page 4), and finally water safety (page 4).

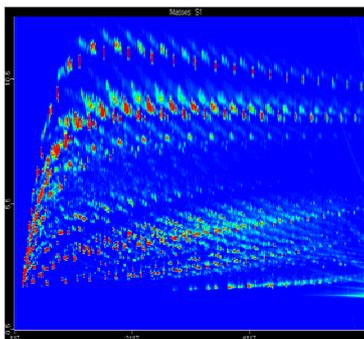
These applications are by no mean exhaustive, nor do they represent all the possibilities being explored world-wide by LECO users.

In these difficult times, LECO's market and potential keeps increasing, with sales already outstripping last year. In fact we have already nearly doubled last year's numbers.

LECO will be happy to expand on any of these areas in the next few months.



Just what is in your fuel?



Diesel, a simple mix of over 10,000 components.

Petrochemistry, an important industry in just about any country. South Africa is the largest producer of oil from coal, a complex process which is still being studied and refined.

From a humble beginning, a detector useful for heartcut 2D GC, a curiosity in the hands of an R&D lab, the LECO TOFMS has become a key tool in many projects at SASOL.

Over the last few years, the lab has expanded its arsenal, taking their initial GCxGC plunge by buying a GCxGC-TOFMS in 2005, upgrading their GC-TOFMS to full GCxGC capability shortly thereafter, acquiring a third Pegasus 4D in 2008 and finally financing an instrument at the University of Pretoria.

Applications in this field are immensely varied, from QC to catalyst monitoring, reactor profiling and product characterization.

Environmental studies, the LECO way.

A core expertise of LECO Africa has always been pesticides and Persistent Organic Pollutants (POPs). The rapid screening capabilities of the LECO Pegasus HT, harnessing the superior data collection capabilities of the TOFMS and the unsurpassed data mining abilities of LECO's ChromaTOF software, allow the analyst to not only pick up the targeted analytes, but also to pick up any unlisted components.

For really dirty samples, the GCxGC-TOFMS is recommended, allowing you to minimize your sample preparation and still resolve normally co-eluting analytes.

With 4 orders of magnitude available for quantitation, R values of at least 0.999 over this range, RSDs with internal standards on tighter calibrations as low as 0.1%, and sensitivity equivalent, if not superior to the MSD, the Pegasus would be a proud addition to any serious laboratory.

From Sheep wool to Cape Town air, the Pegasus has seen it all.

Forensics, LECO and the South African Police Service.

Recently, Senior Superintendent Roger Dixon presented at a ChromSA meeting some of the projects his group has been involved in.

This group has been involved in the analysis of some of the most interesting problems of all LECO users, often involving a potential environmental disaster.

From black sludge from incinerators buried under a concrete slab to a recycling plant leaking toxic waste into a river, to sampling crocodiles as they attempt to elucidate the recent spate of crocodile deaths in the Kruger Park, nothing phases this team.



A couple of years ago, fake olive oil hit the South African market. In order to make a quick buck, sunflower oil was artificially coloured and flavoured to resemble its more expensive cousin.

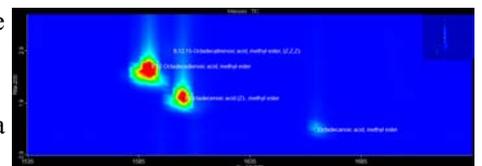
This event is simple to detect by harnessing the superior separation provided by a GCxGC-TOFMS.

Another area of concern for the SAPS is arson. Most of the time, your accelerant is destroyed during the combustion stage. Ultra-trace amounts may be found in the wreckage and is usually detected by MS/MS, if not MS/MS/MS.

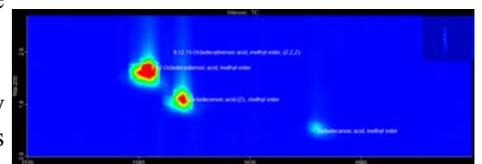
By employing a GCxGC system, the profile of the accelerant can easily be visually identified in any sample, making the whole process simpler as the answer just jumps at you.

Pesticide	MSD S/N 4 Ion SIM	TOF S/N Full Scan
Heptachlor epoxide	4.4	56
DDT	18.4	92
Lindane	22.8	101
Methoxy-chlor	41.7	92

**A real sensitivity test, 4 pesticides in a matrix.
Who analyses OFN in any case?**



**Above: A suspected fake olive oil.
Below: The best match: sunflower oil.**



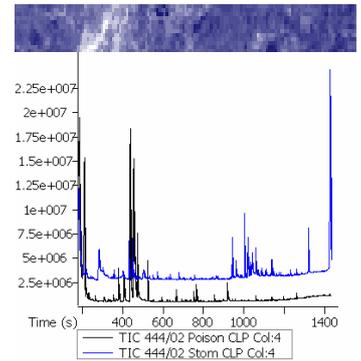
Pathology by TOFMS.

Cause of death is difficult in the best of cases. With blood samples made up of over 1,000 components, urine samples just as complex, not to mention kidney, liver and stomach content, an analyst has to be at the top of his game every day while manually trawling through a chromatogram.

In the last few years, LECO has made real inroads in this area, at the Department of Health's forensic chemistry laboratories in Cape Town and Johannesburg.

The added sensitivity of the LECO Pegasus, as compared to the MSD in full scan, has meant that several difficult cases could be closed. The high levels of data mining automation such as the COMPARE algorithm, coupled to the automatic peak detection and deconvolution, have provided these scientists with an additional layer of certainty.

No longer will a case rest solely on the ability of an analyst to pick out a needle in a haystack at these labs. Nor will cases be lost due to a trace analyte being missed.



Cause of death: industrial cleaners.

Metabolomics dabbling.

Metabolomics can largely be divided between profiling and fingerprinting. Before a biomarker can be categorised, it needs to be discovered and elucidated.

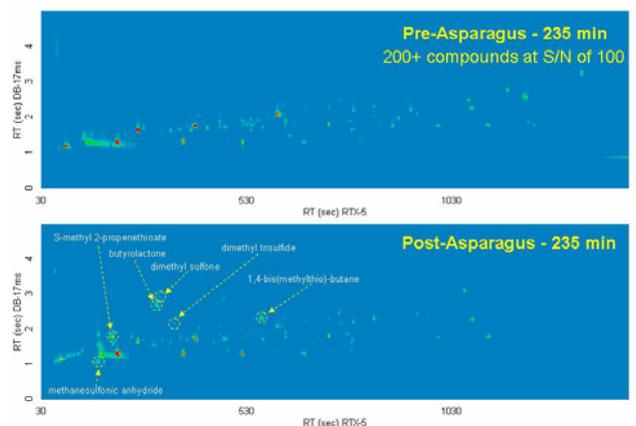
“Nuclear Magnetic Resonance (NMR) is the most important technique for structure elucidation[...]. NMR for metabolomic profiling has the advantage of being very reproducible[...]. On the other hand NMR used for mixture analysis has a poor resolving power for analyzing thousand of compounds in one single sample. The most severe problem are sensitivity issues compared to mass spectrometry. Depending on the sample technique mass spectrometry can be 1000-fold to million-fold more sensitive than NMR. Considering the different strengths and weaknesses of both techniques it must be concluded that they have to be used as complementary techniques for metabolomics”.¹



GCxGC simplifies the biomarker discovery process by stretching a sample from a 1D chromatogram into a 2D chromatogram. This makes minute differences much easier to spot. As an added benefit, our brains are geared to discern patterns, making data processing even easier as the exact retention time becomes less critical while the overall pattern becomes more relevant.

We look forward to presenting you with more information on such an application at the North-West University.

If the biomarkers are well known, then the high throughput of the GC-TOFMS becomes valuable, allowing you to reduce your runtime. Taking advantage of the full-mass range of the Pegasus and fast detection speed, the University of Johannesburg has run several hundreds of samples on the Johannesburg Forensic laboratory's instrument. This collaboration may yield insight on some tonic properties of plants.



GCxGC makes it easier to spot differences between samples.

References:

1) <http://fiehnlab.ucdavis.edu>

Wines and Spirits.

Our Peter Gorst-Allman's (our application specialist) love for wine is well known. As such it comes as no surprise that the Pegasus has been applied in this area of research.

The Pegasus' first foray in this field was through a collaboration with Quadru, Environmentek (a division of the CSIR), investigating whisky samples. Genuine Scotch Whisky is produced in accordance with strict manufacturing requirements to guarantee a drink of exceptional and consistent quality. As such it occupies an elite position in the liquor trade and consequently commands high prices. In South Africa unscrupulous manufacturers have developed alternative products which are marketed with names indicating a Scottish origin, and labeled as whisky. These products, while visually resembling genuine Scotch Whisky, are of inferior quality and lack the flavor components associated with the original.

Shortly thereafter, a scandal rocked Peter's world as certain wines were found to be tampered with. Not content to let nature take its course, some producers added flavour components to enhance the value of their product. A study of the adulteration of white wines with methoxy-pyrazines was undertaken by the National Metrology Institute.

More recently, researchers at the University of Stellenbosch's chemistry department have used the LECO Pegasus to profile pinotage wine (amongst others) while the Wine-Biotechnology Institute uses our technology to expand on general profiling of wines and further adulteration studies.

Peter and Professor Rohwer at the University of Pretoria have also launched a series of wine appreciation evenings to link theory to practice.

Water Safety.

Last year, South Africa suffered from a lack of energy. Simply put, not enough new investment was put into power stations to keep up with the rapidly rising demand of a fast-growing economy. Recently alarm bells have been ringing, warning us of an impending crisis in our water-supply chain.

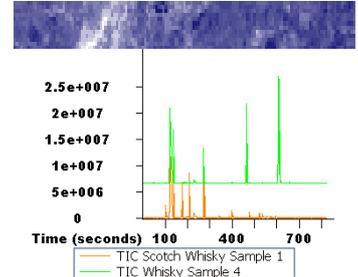
South Africa boasts some of the cleanest drinking water in the world, yet legislation ignores a whole class of contaminants: organic pesticides. Some testing labs heed their moral obligations and use the WHO recommendations to ensure that our drinking water is indeed world-class.

With the growth in potential contaminants, it is no longer viable for these labs to do target analyses for a select few analytes. A new approach, namely rapid screening by TOFMS, is required to ensure that all potential threats are identified prior to individual confirmation.

While this helps humans, our wildlife is also affected and has no voice to request proper analyses. In the last year, hundreds of crocodiles have been dying in the Kruger Park. An in-depth study has been launched by several labs to discover the reasons behind this event.

Scientists from the North-West University, the SAPS, NMISA and LECO Africa, among others have started tackling the problem, looking at all aspects of the problem, including sediment, water, plant, tissue samples.

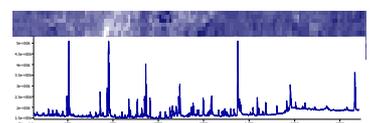
As part of the study, thermal desorption and the TWISTER are used on the GC-TOFMS, showing once again that any inlet solution available to the Agilent GC is simple to use on the Pegasus!



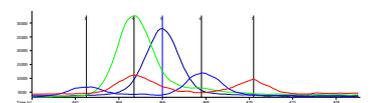
One of these whiskies lacks several flavour components.



Water. Clear? Clean?



**Above: A water samples
Below: Dichlorvos is automatically detected by the software.**



LECO AFRICA

LECOAfrica
 P.O. Box 1439
 Kempton Park
 1620

Phone: 082 771 7097
 Fax: 011 974 1848
 E-mail: alexander@lecoafrika.co.za

*Excellence through Customer
 Satisfaction*

www.lecoafrika.co.za

LECO Africa... Who are we?

LECO Africa is a wholly-owned subsidiary of the privately owned company LECO Corporation, USA, servicing the South African Analytical and Metallographic industries since 1976.

We provide LECO Analytical, Metallographic, Spectrographic and Separation Science equipment, consumables and related spare parts manufactured and assembled in the USA.

LECO Corporation Instrumentation Manufacturing Division is certified with the ISO-9002 accreditation, certification acquired April 29, 1993, registration number FM24045, issued by BSI Quality Assurance, United Kingdom. Today, ISO-9002 is accepted and preferred by many satisfied LECO customers as evidence of an effective quality system and approach.

LECO Africa serves the entire sub-Saharan region, with offices in South Africa's Gauteng, Western Cape, Mpumalanga and Kwazulu-Natal provinces, as well as distributors in the Eastern Cape, Namibia, Ghana and Tanzania.

Contact us! Our motto of "Excellence through Customer Satisfaction" is embraced by all LECO Africa employees.

We assure you of our commitment to service, quality instruments and operating supplies that deliver the right results.

Still not convinced? Then put us to the test. LECO Africa maintains an Applications Specialist, Dr Peter Gorst-Allman, who is more than happy to show you what we can do with your sample.

List of Abbreviations	
SIM	Selected Ion Monitoring
MS	Mass Spectrometer
HT	High-Throughput
Quad	Quadrupole Mass Spectrometer
Ion Trap	Ion Trap Mass Spectrometer
FID	Flame Ionisation Detector
TOF/TOFMS	Time-Of-Flight Mass Spectrometer
GC	Gas Chromatograph
EU	European Union
S/N	Signal to Noise Ratio
LOD	Limit of Detection

