

Analytical Laboratory Informatics 2004

Tony Davies

External Professor, University of Glamorgan, UK,
c/o Creon Lab Control AG, Europaallee 27–29 50226 Frechen, Germany

Introduction

This issue's column is dedicated to the Analytical Laboratory Informatics conference, which is being hosted at the end of June in the London Heathrow Sheraton conference centre. The core direction of the conference is also the direction that we have been taking in this column over the years so we hope you will agree it is a good use of the space to encourage your participation!

From 21 to 25 June this year the Analytical Laboratory Informatics Conference and Exposition will be run at the new Sheraton Heathrow Hotel conference centre in West Drayton, UK. The conference is timed to influence developments in a rapidly advancing field by bringing together the major users and providers in the broad field of Analytical Informatics.

This meeting will be following in the footsteps of the Linking and Interpreting Spectra through Molecular Structures (LISMS) conference held in September 1996 at Warwick, UK, and COMPANA/LISMS held during September 1998 in Duisburg, Germany.

The first international conference on Analytical Laboratory Informatics will be hosted by and organised for all people actively involved in day-to-day laboratory informatics. The conference is targeted at decision makers, policy strategists, problem solvers, advisors, researchers and consultants in the fields of chemical and laboratory informatics.

The conference chairman Mohan Cashyap summed up the business issues by stating: "In the current business environment 'First to Market' demands novel approaches to problem solving. Major strides have been made in technology and the ability to generate vast quantities of data continues unabated. ALI 2004 will be a watershed where Vendors and Users seek to reach consensus on how the

environment needs to be developed to meet the challenge: Data to Information to Knowledge."

Conference format

In a departure from its predecessor meetings it has been decided to hold the conference over the whole week. The core scientific programme will run from Tuesday 22 to Thursday 24 June with manufacturers and vendors running their own seminars on Monday 21 June and Friday 25 June.

Key topics

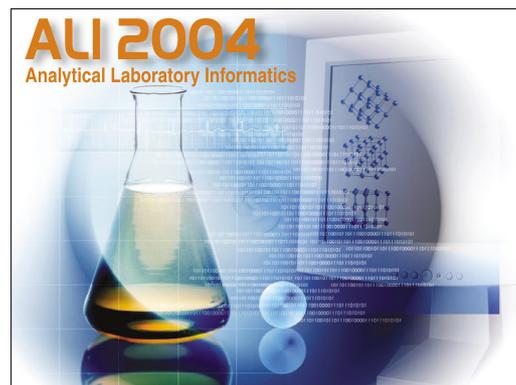
With the various aspects of reliable and secure long-term analytical data archiving being now driven as a regulatory matter and not just the interest area of long-sighted champions in individual organisations, these matters will receive particular attention. The conference will benefit from support financing in various areas especially through the EuroSpec project and the International Spectroscopic Data Bank (IS-DB). The key topics will be as follows.

21 CFR part 11

With the confusion that currently exists around the new interpretations that the FDA is placing on 21 CFR part 11 following the withdrawal of the initial guides the meeting will aim to clarify the key points with speakers from both regulatory bodies, vendors and pharmaceutical manufacturing.

CROMERRR

What the FDA can do so can the EPA for environmental electronic data. Some have stated that the EPA guidelines could have a wider impact on far more industrial sectors than 21 CFR part 11 has had in



the pharmaceutical world. This claim will be investigated!

Archiving strategies

There are differing opinions on the best strategies to adopt with a lively debate currently underway in several sectors between IT professionals and the laboratory users as how best to retain and present data generated within the labs. ALI 2004 will highlight some of the issues and the pros and cons of the different approaches.

Electronic laboratory notebooks

E-Lab Notebooks are (finally) coming of age. The wide range of functionality now available, the ease by which these replacements for the old fashioned paper can now be deployed as well as the ability to embed into the corporate IT environment has finally put all the pieces in place for the breakthrough to happen. But will they be accepted? Let's review and discuss.

High throughput informatics

With the advance of ever faster robotic synthesis and array-based analytical systems, the volume of data being produced is increasing exponentially. CPU speeds are also increasing, but how can we really begin to cope with the amount

of analytical data needing to be analysed. Automated software analysis packages are slowly becoming available which will handle much of the daily grind, allowing the analyst to concentrate on the critical cases where their specialist training can be best utilised. What measures do we need to have in place to ensure these critical cases are correctly identified and how do we validate these automated analyses?

Joined-up informatics

There are several vendors in the market place providing increasingly broad ranges of informatics solutions for the laboratory environment. Do we go with a single vendor to take the benefits of clear product integration across the board but at the possible expense of being the "best" solution in every case or is it preferable to allow each project to pick their own IT solutions regardless of platform and functional intercompatibility with the rest of the corporate IT environment?

Process analytics

Finally the FDA has published an initiative aimed at promoting innovation! Do we really think that process analytics have come far enough for us to grasp the carrot that the FDA is holding out of on-line real-time batch release? Have you tried? Are you planning to look at this opportunity for new plant or even re-engineering older plant because of the enormous advantages in time and productivity that such systems should bring?

Public reference data

The NIST Chemistry WebBook is maturing; the EuroSpec project has delivered the International Spectroscopic Data Bank; who cares? Are these public reference services of use to you in your work or not? Do they present the stored information in a way appropriate to your work? Have you been telling your colleagues "what we really need is..."? Come along at let us know. This happened at LISMS in Warwick and the result has been the €1.2 million EuroSpec project delivering the IS-DB, so your voice CAN make a difference!

XML and chemical data

XML, the Extensible Markup Language, is an excellent tool for moving database

content around. But when it comes to experimental data there are numerous drawbacks and a lack of standardisation. What are IUPAC and the ASTM, owners of the currently most widespread analytical informatics standards, doing about this?

Internet and publishing

Electronic delivery of scientific information is today the norm. It is, however, still a largely unregulated publishing field where laws equivalent to those covering the conventional publishing methods such as the requirement for deposition with national archives are missing. As the publishers have been at pains to point out they are not archivists! So if you have an electronic-only subscription to a scientific resource, who is to ensure that you will still be able to access it in the morning? Recent painful experiences with the withdrawal of electronic services in the USA and more recently the controversy surrounding the web portal strategy of a major European publisher have brought these issues to a head. How are you coping in your company? Let's share strategies and maybe lobby for legal change!

Outsourcing

Where are your systems written? Increasingly IT providers are employing software and support service groups in low-wage paying areas. Often the services and products developed by such subsidiaries are of excellent quality but how are you ensuring this is the case? What strategies are in use to oversee such developments? If you carry out company audits, what generic issues have arisen apart from the need to travel to interesting locations?

Where we receive sufficient numbers of (well argued!) timely requests to cover other areas, these will also be included in the conference programme.

Conference organisation

For the organisation of the day-to-day affairs of the conference we have been able to win two very experienced industrial practitioners in John Senior and Tom Heyes. Emma Lee, a forensic scientist from the University of Glamorgan, will assist them during the conference.

Mohan Cashyap from Glaxo Smith Kline chairs the International Organisation Committee, your author is responsible for the scientific programme, Jeff Seymour the exhibitors. Perry Hailey from Pfizer and Christine Kelly from Novartis are also on the team and will ensure that we stay on the right track.

Conference location

ALI 2004 will take place at the newly-renovated London Heathrow Sheraton, which has an excellently equipped conference centre within the hotel complex.

Conference exhibition

Such an event as ALI 2004 would be rather pointless without the active participation of our community's instrument manufacturers and software vendors. The participating exhibitors have the opportunity to run half-day or whole-day seminars on the Monday or Friday of the conference week inviting their own clients to the conference centre. On the Wednesday afternoon and evening there will be a conference exhibition. Those companies exhibiting will have space in the central exhibition area for tabletop demonstrations as well as the use of breakout rooms for meetings with up to 20 people.

As we want to promote active participation in the conference, especially in the discussions on strategic directions, all exhibitors will be required to register two full conference delegates. There might be some point in groups of end-users discussing where the vendors ought to be going as an industry but the relevance of such discussions will be greatly enhanced by input from our supplier industries.

Conference delegates—you!

Well hopefully you! you can register as a conference delegate through the web site at <http://www.ali2004.org>. Exhibitors can also register their interest here by following the link from the main conference site or going direct to <http://exhibitors.ali2004.org>. I am looking forward to a lively meeting with lots of topics and excellent speakers; so see you all in London in June!