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There is a paradox at the heart of this year’s Laboratory Informatics Guide. On the one hand, we have an article showing how technology developed for the consumer market can help drive down costs and improve efficiencies in the work of the analytical laboratory. But we also have an article lamenting how the sort of information sharing that consumers take for granted – think Flickr or Facebook – is currently impossible in laboratory informatics.

For very good reasons, change tends to be slow in this discipline. No one can play with electronic systems to see how to make them more efficient or cheaper – not if those systems have to conform to regulations issued by the US Food and Drug Administration and counterpart bodies in other countries. Change has to be carefully orchestrated.

However, the pressure for change never goes away. Analytical laboratories, whether in discovery or quality control, have to justify their cost and demonstrate to higher management that costs are being driven down.

As Robert Roe’s article on page 26 demonstrates, sometimes the change comes from technologies developed in entirely different spheres for entirely different purposes. Mobile phones and tablet computers, developed for the consumer market, are forcing informatics vendors to modify their systems to allow for the input, processing and analysis of data through these devices.

Peter Boogaard reports on the progress being made towards the integrated and paperless laboratory on page 4. However, the lack of common standards for interchanging laboratory data is an obstacle to the further development of informatics and progress has been frustratingly slow, as John Trigg discusses on page 10.

So this year, the glass is half-full. Let us hope that by the time next year’s Laboratory Informatics Guide is published, we can report that the cup is brimming over!
Joining up the laboratory

Peter Boogaard reviews efforts to make the laboratory an integrated operation

It is easier to get data into scientific databases than to get valuable information out of it. For years, we have been spending time and money to integrate systems and processes in the laboratory’s knowledge value chain. Many laboratory integration projects are under pressure to deliver on their expectations, as defined at the kick-off of. So why is it that laboratory integration is so difficult? What are the obstacles to creating value for the consumers of the laboratory data? Do we know what these users need and how they would like to consume this information?

Imagine that in the music world, each label has its own proprietary music file format. How would you be able to share music? By default, standards make it easier to create, share, and integrate data. Do we know the requirements of such a data standard? What about managing metadata-controlled vocabularies? Data standards are the rules by which data are described and recorded. In order to share, exchange, and understand data, we must standardise the format (data container) as well as the meaning (metadata/context). As of today, there is no unified scientific data standard in place to support heterogeneous and multi-discipline analytical technologies. There have been several attempts but they are limited in scope, not extensible or incomplete, resulting in recurring, cumbersome and expensive software customisations.

**PAY ATTENTION TO THE CONSUMER OF THE DATA**

Integrating laboratory instruments started when instrument vendors, such as Perkin-Elmer and Beckmann Instruments, created the first laboratory information management system (LIMS) software, in the early 1980s. The initial objective was to support the laboratory manager with tools to create simple reporting capabilities to enable the creation of simple certificate of analysis (CoA) reports. These systems were initially designed to support a single consumer, namely the scientists and lab managers. In today’s world, consumers of laboratory data can be found across the entire product lifecycle, and may include external organisations such as CROs and CMOs (Table 1). A different mind-set is required to adapt to this expanded view of the world. It is critical to first analyse who these new lab-data consumers are, and get an understanding of what their objectives are. Often forgotten, but as important, is to investigate what their perspective is on usability. The newcomers may be a non-technical audience! Stephen Covey phrased it very nicely: ‘Seek first to understand.... And then to be understood.’ It may sound obvious, but it still remains a valuable statement before starting any automation project.

**Stephen Covey phrased it very nicely: ‘Seek first to understand.... And then to be understood.’ It may sound obvious, but it still remains a valuable statement before starting any automation project.**

<table>
<thead>
<tr>
<th>Consumer</th>
<th>Objective</th>
<th>Impact / benefit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Patient</td>
<td>Assure secure instant access to medical data for doctors.</td>
<td>Better healthcare at lower cost</td>
</tr>
<tr>
<td>Fellow scientist</td>
<td>Re-use experimental data and leverage learning. Higher efficiency and quality. Consistent meta and context data</td>
<td>Higher efficiency and quality</td>
</tr>
<tr>
<td>Legal</td>
<td>Protect company IP</td>
<td>Consistent externalisation processes (CROs)</td>
</tr>
<tr>
<td>Finance</td>
<td>Understand overall life-cycle cost of operation</td>
<td>Holistic overall view</td>
</tr>
<tr>
<td>Customer care</td>
<td>Product complaints and product investigations</td>
<td>Secure branding image of company</td>
</tr>
<tr>
<td>Regulation</td>
<td>Faster responses to compliance inquiries</td>
<td>Simpler mechanism to audit heterogeneous scientific data</td>
</tr>
<tr>
<td>Management</td>
<td>Identify areas for continuous improvement in process. Reduce costs</td>
<td>Risk-based information across heterogeneous data systems</td>
</tr>
<tr>
<td>Stability labs</td>
<td>Simpler mechanism to create e-submissions. Ability to submit standardised e-stability data packages</td>
<td>Faster responses during studies, increased efficiency</td>
</tr>
<tr>
<td>CRO/CMO</td>
<td>Focus on lowering cost/analysis by decreasing IT complexity and overhead</td>
<td>Acceleration move from paper to ‘paper-on-glass’</td>
</tr>
<tr>
<td>IT</td>
<td>Reduce bespoke/custom systems. Consolidation of systems. Reduce costs</td>
<td>Unified systems. Simplify IT processes</td>
</tr>
</tbody>
</table>

**Table 1: Selected consumers of laboratory information data**
Secure and multidisciplinary enterprise knowledge management solutions

Web-based platform designed to enable real-time collaborative research internally and with CROs

Search, browse and share structured and unstructured data stored in multiple and diverse data sources

**BROWSER**
- A tool for integrating, querying and browsing multiple data sets at once
- Images as well as chemical, biological, analytical, and many other types of data can be unified and presented to users in a single view
- Schedule searches and automatic trigger email notifications

**REGISTER AND BIORegister**
- Adaptable chemicals and biologicals registration systems
- Designed to meet specific requirements of scientists, regulatory officials and administrators in education, government and industry

**VORTEX**
- Scientific data analysis and visualization solution
- Designed to dynamically import, combine, mine and analyse large datasets including chemical structures, biological assays, text and numeric data
- Includes a set of scientific property calculators and functionalities designed to assist scientists from diverse disciplines

**STUDIES NOTEBOOK (ELN)**
- Multi-discipline, highly customisable ELN
- Configured to fulfil the informatics requirements of different laboratories within an organisation
- Integrated with chemical registration and sample inventory tools
- Designed to capture and manage all types of biological studies
- Incorporates a powerful plate management

![Figure 2: Studies Notebook for Chemistry](image)

![Figure 3: Studies Notebook for Biology](image)

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For the scientific researcher, the ability to record data, make observations, describe procedures, include images, drawings and diagrams and collaborate with others to find new chemical compounds, biological structures, without any limitation, requires a flexible user interface.

For the QA/QC analyst or operator, the requirements for an integrated laboratory are quite different. A simple, natural-language based platform to ensure that proper procedures are followed will be liked.

To investigate a client’s complaint professionally, the customer care employee requires a quick and complete dashboard report to look at metrics for all cases, assignments, and progress in real-time, by task, severity, event cause, and root cause. The devil is in the detail, and that’s where the laboratory data may give significant insights.

Legal: Instead of saying ‘we saw that a couple of years ago, but we don’t remember much about it’, sensitive information can searched and retrieved, including archives.

During regulatory inspections ‘show me all the data during this time frame, which raw material batches were involved and show me all the details’.

HETEROGENEOUS SCIENTIFIC CHALLENGES
The lack of data standards is a serious concern in the scientific community. It may seem a boring topic these days, but the need for standardisation in our industry, has never been higher. Without such standards, automating data capture from instruments or data systems can be challenging and is expensive. Initiatives such as the Allotrope Foundation are working hard to address these badly needed common standards.

The Allotrope Foundation is an international not-for-profit association of biotech and pharmaceutical companies building a common laboratory information framework for an interoperable means of generating, storing, retrieving, transmitting, analysing and archiving laboratory data, and higher-level business objects such as study reports and regulatory submission files. The deliverables from the foundation, sponsored by industry leaders such as Pfizer, Abbott, Amgen, Baxter, BI, BMS, Merck, GSK, Genentech, Roche and others, are an extensible framework that defines a common standard for data representation to facilitate data-processing, data-exchange, and verification. One of the ultimate goals is to eliminate widespread inefficiencies in laboratory data management, archival, transmittal, and retrieval, and to support a start-to-finish product quality lifecycle, which would enable cross-functional collaboration between research, development, quality assurance and manufacturing.

The framework will include metadata dictionaries, data standards, and class libraries for managing analytical data throughout its lifespan.

<table>
<thead>
<tr>
<th>Why traditional hierarchical was initially abandoned</th>
<th>The SQL a success story</th>
</tr>
</thead>
<tbody>
<tr>
<td>Complex architecture</td>
<td>Extensible open architecture</td>
</tr>
<tr>
<td>Slow responses</td>
<td>Split physical &amp; meta data</td>
</tr>
<tr>
<td>Vendor bound</td>
<td>Product independent</td>
</tr>
<tr>
<td>Inflexible and fixed data schemas</td>
<td>User definable flexible ad-hoc queries capabilities</td>
</tr>
<tr>
<td>Required mindset change</td>
<td>Availability of faster computers and networks</td>
</tr>
<tr>
<td>Invasive technology</td>
<td>Single database language</td>
</tr>
</tbody>
</table>

GLASS HALF FULL OR HALF EMPTY?
The deployment of computerised database systems started in the 1960s, when the use of corporate computers became mainstream. There were two popular database models in this decade: a network model called CODASYL; and a hierarchical model called IMS. In 1970, Ted Codd (IBM) published an important paper to propose the use of a relational database model. His ideas changed the way people thought about databases. In his model, the database’s schema, or logical organisation, is disconnected from physical information storage, and this became the standard principle for database systems. Several query language were developed, however the structured query language, or SQL, became the standard query language in the 1980s and was embraced by the...
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Available today.

Are you ready?

BSSN Software
The benefits of open data standards

- entire industry. Vendor specific proprietary extensions (e.g. PL/SQL) were allowed in the concept, allowing individual vendors to extend capabilities.

Now back to the laboratory. The current situation is that there is no framework for scientific data standards. Formats are vendor bound, product dependent, and in many cases based upon a closed architecture and are complex in nature. There are plausible reasons why, at this moment, our industry has no general accepted raw-data and metadata standards, but should we not learn from other industries and adopt best practices?

The Analytical Information Markup Language (AnIML) is the emerging ASTM XML standard for analytical chemistry data. The project is a collaborative effort between many groups and individuals and is sanctioned by the ASTM subcommittee E13.15. An AnIML is a standardised data format that allows for storing and sharing of experimental data. It is suitable for a wide range of analytical measurement techniques. AnIML documents can capture laboratory workflows and results, no matter which instruments or measurement techniques were used.

E-Workbook Suite (IDBS) allows spectra files to be dropped in from the experiment whereby they are automatically converted to AnIML and rendered. The rendering application then allows the scientist to annotate the spectra with searchable chemical structures, text, hyperlinks to other systems and records. The AnIML data is also indexed alongside everything else allowing specific searching of metadata and properties. These processes are non-invasive meaning that the originals raw data files are also kept.

An application programming interface (API) specifies how some software components should interact with each other, allowing customers and third parties to extend the types of spectra that are supported by writing new raw data to AnIML converters or plug-in in third party components.

Other examples of changes in the way laboratories may operate in the future relate to how balance and titration instrument vendors are increasing the value of their instruments by implementing approved and pre-validated methods in their instruments. This may sound a small step, but it may have a significant impact on validation efforts in the laboratory and manufacturing operations, such as fewer points of failure during operation, less customisation of software and better documentation.

The desire to convert manufacturing processes from traditional batch-oriented processes to a continuous operation has accelerated process analytical techniques (PAT) technologies as a way to create sustainable and flexible approaches for manufacturing operations. PAT is expected to grow significantly in the next decade. Over time, in-line, @line and on-line analysis will complement and potentially substitute off-line (batch oriented) laboratory manufacturing processes. International regulatory authorities such as ICH, FDA and ISPE are evaluating these new processes intensively and developing new workflows. These processes will have a high impact on how QA/QC laboratories will operate in next decade. International industry standards such as ANSI/ISA-88 (covering batch process control) and ANSI/ISA-95 (covering automated interfaces between enterprise and control systems), are commonly used in manufacturing. By

### Table 3: Applying standards requires a different mindset

<table>
<thead>
<tr>
<th>Glass half empty</th>
<th>Glass half full</th>
</tr>
</thead>
<tbody>
<tr>
<td>The market is too disperse</td>
<td>Technologies are emerging rapidly</td>
</tr>
<tr>
<td>Technology not available</td>
<td>XML and AnIML are accepted as standards</td>
</tr>
<tr>
<td>Vendor protection</td>
<td>Empowered customers</td>
</tr>
<tr>
<td>Poor performance</td>
<td>Consistent unified long time archive process</td>
</tr>
</tbody>
</table>

References

1. The 7 Habits of Highly Effective People – Stephen Covey 1990
3. PL/SQL (Procedural Language/Structured Query Language) is Oracle Corporation’s procedural language extension for SQL and the Oracle relational database
5. Technology Management In The Age Of The Customer - Forrester research 2013
incorporating these standards, scientists will be able to mine information from development and manufacturing for improved process and product design. In addition, information is more readily transferable between systems. For example, a recipe delivered in early development can be rapidly transferred to a lab execution system for API manufacture and then to a method execution system for mainstream manufacturing. ERP and MES applications are using these standards and it is very likely that integrated laboratory data management capabilities will be included within their software capabilities.

**CONCLUSION**

Empowered customers are disrupting every industry. Technology managers must broaden their agenda to consider not just infrastructure and traditional internal IT processes, but also activities to ensure they deliver value for their ‘client’. The power of an integrated laboratory environment is its ability to find detailed answers to support the overall business process. It is pure waste to perform labour-intensive hunting for information across multi-vendor, multi-technique databases, manual transcription checking and to manually create reports. Having a common industry standard framework will decrease process variability resulting in better quality and overall consistency. Non-invasive processes have proven to be successful in other industries. It is now up to the industry, regulatory bodies and vendors of scientific instrumentation and software platforms to make it happen. Integrating laboratory information really means integrating scientific data collected in the laboratory and beyond. Time will tell if this industry has been able to adopt such a strategy.

Peter Boogaard is an independent laboratory informatics consultant.
Why can ordinary consumers share their data when the laboratory informatics community cannot? Sharing and collaboration are becoming second nature in the consumer world where the ability to communicate and transfer data over the web has become a routine part of everyday life, to the point where the terms ‘upload’ and ‘download’ are part of everyday vocabulary. A simple example is the ability to take a photograph on a camera phone, and immediately upload it to a photo-sharing site, or email it, or ‘message’ it or tweet it. The ability to do this is totally dependent on standards; the internet provides the infrastructure; wi-fi or telecoms provide the messaging; and the device (camera/phone) generates the data (photo) in a format that can be used by other applications. It’s a process everyone takes for granted, without having to worry about the data format of the photo and whether the recipient will be able to open it. It may be thought a simplistic example, particularly when compared to the complexity of laboratory systems that serve an extensive range of measurement and other services, but the underlying principle paints a vivid picture of how laboratory systems ought to work more efficiently and effectively if there are common standards for exchanging data. On the other side, the vendors argue that standards would constrain innovation in the development of tools for capturing and processing data. In the background is a more political viewpoint: proprietary data formats facilitate a commercial ‘lock-in’ for the vendors, and the adoption of open data standards would disrupt the marketplace, not only for the vendors, but also for the third-party systems’ integrators.

Few people could argue against the benefits of data standards. Laboratories would welcome the ability to acquire data and then process it, view it, store it, share it, re-analyse it, and preserve it without the constraints of proprietary data-capture software and integration tools. The advantages include not only ease of use, but also the reduction in costs associated with third party and custom solutions to interface laboratory devices and systems. A less obvious benefit is the ability to archive data in a human-readable format over the long term. One of the consequences of the transition from paper to digital technologies is that we are going into the unknown, and we will become totally dependent on technology in order to access electronic records. Basically we will no longer have any physical artefacts that represent our accumulated records of laboratory experimentation and their outcomes. It will all be digital, the IT industry has a poor track record when it comes to digital preservation.

However, the long-term preservation of electronic records does present one example of where a standard – PDF or PDF/A – has been adopted in the laboratory world. However, electronic document standards, such as PDF and PDF/A, have a very different purpose from that of data interchange standards. With regard to the write-up of an experiment, PDF or PDF/A can preserve a rendition of the data generated in the experiment, but does not preserve the data itself. In order to preserve the data and to maintain the capability to use and re-use it over the long term, then a data interchange standard is necessary.

One of the consequences of the transition from paper to digital technologies is that we are going into the unknown, and we will become totally dependent on technology.

The transition from paper to electronic lab notebooks created the need to be able to preserve, for several decades, the integrity, authenticity, and readability of experimental records to support business and scientific requirements. PDF and PDF/A both have ISO registration as open standards, and are typically used to provide the electronic rendition of the experimental ‘document’. The primary purpose is the preservation of a flat document, including the text, fonts, graphics, and other information...
needed to display it. PDF/A is a version of the portable document format (PDF) developed specifically for archiving electronic documents. It differs from PDF by omitting features that are unsuitable for long-term archiving, such as font linking (as opposed to font embedding). It identifies a ‘profile’ for electronic documents to ensure that they can be reproduced in exactly the same way over years to come. Key to this reproducibility is the requirement for PDF/A documents to be 100 per cent self-contained. All the information necessary for displaying the document in the same manner every time is embedded in the file.

The business case for data interchange standards is quite clear, as companies focus on: productivity (cost reduction); outsourcing or externalisation; and innovation:

- Improved productivity is increasingly dependent on automation and the elimination of inefficient steps and manipulations in data handling. Standards for data interchange would simplify instrument interfaces, cut interfacing costs, reduce errors, and simplify validation;
- Outsourcing, or externalisation, involves communicating and sharing data across wide geographic areas and disparate technologies. Standards for data interchange can facilitate these communications by removing the dependence of the data on the application that created them. In other words, the data can be stored, viewed, and manipulated in applications other than the one in which it was created; and
- Innovation arises from correlating, mining, visualising, and making sense of data from multiple sources. Again, these processes can be easier and faster, if data can be stored and accessed in standard formats.

A few standards for interchanging laboratory data do exist, but they have not been adopted on an industry-wide scale.

If the business case is so strong, why is it taking so long to make any progress? From a technology perspective, there has never been a better time to exploit the potential of standards: the development of a global infrastructure in the form of the internet has provided a platform that other consumer and business domains are taking full advantage of, as the example of photo sharing illustrates. However, digitising the laboratory has been a slow journey,

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stretched over four decades. As laboratories become progressively ‘paperless’, progress towards a fully integrated environment will depend on overcoming the limitations posed by the current lack of data standards.

Organisations such as the Pistoia Alliance, the Allotrope Foundation, and the Consortium for Standardisation in Lab Automation (SiLA) have recognised and taken action to address the issue from the standpoint of ‘industry associations’.

As Peter Boogaard explains in the previous article, the Allotrope Foundation (www.allotrope.org) is an international association of biotech and pharmaceutical companies that are collaborating to build a common laboratory information framework for an interoperable means of generating, storing, retrieving, transmitting, analysing, and archiving laboratory data, as well as higher-level business objects such as study reports and files of regulatory submissions. In a recent press release, Allotrope Foundation announced its partnership with Osthus to build the framework, which will have three interacting components:

1. Open document standards based on XML, JSON or other formats that support structured data;
2. Open metadata repositories containing dictionaries to provide accurate metadata input into laboratory systems;
3. Open-source class libraries that will produce and consume content from the first and second components;

The Pistoia Alliance (www.pistoiaalliance.org) is a global, non-profit, precompetitive alliance of life science companies, vendors, publishers, and academic groups that is aiming to lower barriers to innovation by improving the interoperability of R&D business processes. The Pistoia Alliance is trying to identify the root causes of inefficiencies in R&D and to develop best practices and pilot technology. Pistoia is not a standards group, but the membership recognises that their organisations are tackling common precompetitive problems – aggregating, accessing, and sharing data that is essential to innovation, but provides little competitive advantage. The ELN project (ELN Query Standard) initiated by the Pistoia Alliance has ground to a halt, but could be revisited if there were sufficient interest amongst members. However, there is good progress with the release of the HELM (Hierarchical Editing Language for Macromolecules), a standard open source
tools for biomolecular representation.

The consortium for Standardization in Lab Automation (SiLA, www.sila-standard.org) is developing and introducing new interface and data management standards to allow the rapid integration of lab automation systems. SiLA is a not-for-profit membership corporation with a global footprint and is open to institutions, corporations, and individuals active in the life science lab automation industry. Leading system manufacturers, software suppliers, system integrators and Pharma/Biotech corporations have joined the SiLA consortium and participate in and contribute to different technical work groups.

The long history of incremental adoption of laboratory technologies has left a legacy of proprietary approaches to interfacing laboratory and business systems

In addition to the strategic activity of these industry associations, the most prominent initiative in developing a data interchange standard is AnIML (anlml.sourceforge.net). AnIML is a standardised XML data format that can be used for storing and sharing experiment data. It is suitable for a wide range of scientific disciplines. Its origins are in the analytical chemistry, but the scope has been extended to include biological data.

AnIML documents can capture laboratory workflows and results, irrespective of the instrument or measurement technique used. To achieve this, AnIML provides a generic data-container that permits the storage of sample information, method information, measurement results, instruments and software used, as well as workflow information that ties experiments and samples together. AnIML is being developed by the ASTM E13.15 subcommittee on analytical data, which consists of volunteers from industrial, academic, government, and vendor communities.

It is far too soon to estimate what the industry associations will achieve, and there is a risk that the industry may end up with a multitude of standards. The diversity of laboratory types, the wide range of different data generators spanning different technologies and vendor communities, and the range of informatics’ tools all conspire to add enormous complexity to the challenge. Furthermore there is the need to agree not only the technical format of a data standard, but also the ontologies and vocabularies for relevant laboratory data elements. It is not unusual to find misunderstandings of data definitions within a single company, let alone across an industry!

Where will the laboratory informatics community stand if and when data interchange standards emerge? Firstly, laboratory integration would become easier, cheaper, and more effective. However, the long history of incremental adoption of laboratory technologies has left a legacy of proprietary approaches to interfacing laboratory and business systems. A data standard would be dependent on industry-wide agreement, approval by various regulatory bodies and other interested parties, and the willingness of the vendor community to cooperate. As strong as the business case may be, the task is therefore far from straightforward and has no guarantee of success.

However, there may be another approach, which will not be driven by the informatics community itself, but which may develop through the adoption of emerging technologies. The development of an ‘internet of things’ – where every ‘thing’ is uniquely identified and seamlessly connected into the information network – will depend on the adoption of data and communication standards to facilitate data capture, connectivity, and interoperability.

So, if every piece of laboratory equipment that generates data can have its own IP address and can be linked seamlessly into the networks, a truly integrated business ecosystem that incorporates laboratory data and information management becomes possible.

The relentless evolution of new technologies offers the hope that if all else fails, then the trends in integration, sharing and collaboration in the consumer world may provide the basis and incentive to address requirements in the laboratory.

John Trigg is director of phaseFour Informatics.
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INFORMATICS IN ACTION

From contact testing laboratories to multinational companies, informatics systems have an important role to play. Sophia Ktori spoke to some of the users

David Hawkins, CEO at Butterworth Laboratories

Butterworth Laboratories is a fully independent UK provider of contract analytical services. It offers method development, method validation, stability testing, and QC testing services to the pharmaceutical, medical device and chemical industries, including analysis of raw materials, active ingredients, and finished products. The laboratory is ISO 17025 (2005)-accredited, and GLP/GMP compliant, with specialisation in chromatography, wet and general chemistry, metals analysis, physicochemical testing, and elemental microanalyses.

Butterworth installed Autoscribe’s Matrix Gemini LIMS platform in 2007, following a review of its existing information management system, which was largely paper-based and inefficient, explains David Hawkins, chief operating officer and head of quality assurance and IT. ‘We realised back in 2006 that we needed a LIMS platform that would operate as a process management system. Required functions included overseeing the input, storage, retrieval, management and sharing of data, including client requests and quotes, along with sample receipt and tracking, the allocation of test specifications and requirements to our team of analysts, the management of laboratory and analytical data, results reporting to clients, and invoicing. Information from each stage needs to be visible to people in multiple departments, but we didn’t have the infrastructure to make that possible electronically, and in standard formats.’

Prior to implementing the Matrix Gemini LIMS, this information-flow largely involved passing sheets of paper with the relevant information from desk to desk between and within departments. ‘We even employed
an individual to ferry documentation from one department to another. Data entry was manual and labour-intensive, and, from a quality point of view, relatively high risk with the potential for errors, or information loss, which was far from ideal in a GMP- and GLP-compliant environment.

Butterworth had very specific requirements for its LIMS, in that the system would have to demonstrate significant flexibility due to complex technical specifications. ‘We tend to do the kinds of testing that our clients can’t, or don’t want to do in-house, which means each request is highly specific in terms of the type and breadth of analyses, as well as the sample type,’ Hawkins points out. ‘We don’t have a standard series of preconfigured analyses, such as those that would typically be run on finished pharmaceutical products, for example, or on wastewater or clean water samples for the utilities industry. We also send each client raw analytical data along with the certificate of analysis, so we needed the LIMS to interface with the electronic documentation system that we use to scan in and store each printout of raw results.’

The degree of flexibility and the ability to configure all aspects of the Autoscribe system has allowed Butterworth to use the LIMS as its default system for functions including data mining, generating management reports, and reagent inventory. ‘From a management perspective, we can even use the system to monitor and track the usage of each type of instrumentation and hardware, and calculate, for example, how much a particular technique has earned in a given time period,’ Hawkins adds. ‘Ultimately, the system has vastly improved efficiency, reduced the potential for errors, and provided business management and administrative benefits over and above its LIMS capabilities.’

Lloyd Colegrove, director of fundamental problem solving, statistics and modelling, Dow Chemical Company

Dow Chemical Company manufactures 5,000 products at 188 sites in 36 countries, and operates globally through six business segments; electronic and functional materials, coatings and infrastructure solutions, agricultural sciences, performance materials, performance plastics, and feedstocks and energy.

Within its manufacturing operations, the firm applies LIMS at a fairly basic level, to collect analytical data, carry out some basic data analytics inherent in the system, and communicate with the product-release process to confirm that the product meets specifications and allow product release, explains Lloyd Colegrove, director of fundamental problem solving, statistics and modelling. ‘The Thermo Scientific SampleManager LIMS receives and stores data from our chromatography data systems (CDS) and other instrumentation, and from there the data is used for laboratory management and quality systems functions. However, we really don’t use the platform to its full capability. It has many capabilities that we just haven’t tapped into. As one production manager once pointed out to me, we’ve got a 747 that we use as a crop duster.’

There are a variety of issues that have held back implementation of the LIMS platform to its full potential working. This will be especially relevant as Dow moves beyond running SAP R/3 to the next level, NEA, with which LIMS will also have to communicate.

Training LIMS users is another issue that holds back any incentive to use the LIMS to its full potential, he continues. ‘You have to ensure that expertise gained by one person who uses the system is passed on when new people are brought in.’ To this end, individuals within Dow’s larger sites are appointed and trained as experts in particular aspects of LIMS implementation, so they can support other users and pass on that knowledge. ‘We have also reached out to Thermo Fisher to provide a training curriculum that we can implement.’

Dow’s relationship with Thermo Fisher spans some 20 years, but the company probably hasn’t tapped into the expertise of its LIMS provider as far as it should or could have, which is not all that unusual. ‘I don’t necessarily want LIMS to do any more than it does already for us, even though I appreciate that we don’t exploit its capabilities fully. However, what I do want is for LIMS to be an easier solution to install and operate within the corporate system. We need to show Thermo Fisher exactly what we need and provide them with an understanding of how we use the platform, so they can build us a system that is suited to our particular workflows and processes, and show us how to make its implementation, customisation, and ongoing improvement less complex and more efficient.’
Latis Scientific is a UK contract testing laboratory and consultancy firm, accredited to ISO/IEC 17025:2005, that offers microbiology and chemical testing services to the water, food, recreational, and building-services industries. Three years ago the company installed an AIS LIMS to replace separate legacy systems in place at GR Micro and Oakland Calvert Consultants, the major parts of which were consolidated into the Latis Scientific organisation.

Latis offers a range of analytical suites that comply with legislative requirements, or can be designed to meet specific client requests. Operating two laboratories in the UK and 10 sample reception sites, the firm often has to transport multiple samples collected from reception sites to the different laboratories, so its informatics challenges start as soon as the sample is received at one of the laboratories. ‘We needed a system that could track and audit every sample from its arrival at the relevant testing laboratory, to logging of the sample on the analytical instrumentation, results generation, and data reporting,’ explains Michelle Idiens, the firm’s IT manager. ‘In many cases duplicate samples from the same origin will be transported to one of our facilities, but one sample will then be dispatched to our second facility for an alternate suite of tests. Using the AIS LIMS we can track every sample, while it is in transit, and know when it is live at a particular laboratory. AIS LIMS also provide a Labportal system that allows clients to go online and register their own samples at any time of day or location. This is then sent to the LIM system so that when the physical samples arrive they can be quickly processed. The tool also allows our clients 24/7 access to their results on screen, as a pdf or as an excel file.’

**Working with the relatively small team at AIS LIMS enabled the platform to be tailored exactly to the requirements at Latis**

The legacy systems at GR Micro and Oakland Calvert were outdated, incompatible, and each had a number of drawbacks, Idiens points out. ‘As well as allowing for complete sample tracking, management and custody chain, the AIS LIMS platform is interfaced with the laboratory instrumentation, and has increased automation of both chemistry and microbiology testing through barcode scanning of microbiology microplates, and direct scanning of samples onto analytical instrumentation for chemical testing. This automation has reduced hands-on time, repetition of data input and potential sources of error associated with that data entry.’

Results reporting to the client was still very much a manual process using the old LIMS. Someone would have to generate a PDF after the laboratories had manually inputted all the results, and then e-mail the report to the client. Invoicing was another task that could take up to an hour in one system per client. ‘As well as providing a complete audit trail for each sample and set of results, the interface with our laboratory instrumentation means that the AIS LIMS generates and sends reports automatically to the client by email, in the correct format, and a flexible invoicing capability has dramatically reduced the time required for this operation.’

Working with the relatively small team at AIS LIMS enabled the platform to be tailored exactly to the requirements at Latis. ‘It’s a COTS (commercial-off-the-shelf) software that has been configured for the marketplace rather than by the industry, and the AIS LIMS team has listened to our requirements and built-in the features that we required. The system we now have in place has provided us with full sample tracking and auditing capabilities, as well as an interface with laboratory instrumentation, and this has allowed a major reduction in the need for manual data entry.’
Advanced Laboratory Testing Ltd (ALT) is a fully Irish-owned contract testing laboratory established in February 2013 to provide microbiology and chemistry testing services to the food industry in Ireland. The laboratory complies with ISO/IEC 17025:2005 for all analyses, offering customised solutions for testing raw and cooked foods, and water samples.

ALT carries out microbiology testing of cooked and raw food, and water samples in three separate laboratories at its site in Newbridge, Co. Kildare. Food chemistry testing is outsourced to the firm’s partners, so an installed LIMS also has to be able to track outsourced samples, and manage data coming back into the system from outside sources.

During 2013, ALT installed LabWare’s Enterprise Laboratory Platform LIMS, underpinned by the LabWare Contract Template Solution, which is ideally suited to the requirements of the Irish firm, explains Tom Tobin, who heads ALT’s LIMS administration. ‘We looked at the flow of samples through the lab, right from the point of sample receipt and entry into the system, through to reporting and invoicing, to see what our requirements were at every stage’. From our perspective, a LIMS had to be capable of allowing the processing of high volumes of samples, with the stringency to enable the highest levels of quality management,’ comments Graham O’Halloran, ALT’s technical manager.

One of the primary requirements of the contract food-testing sector is speed of turnaround and reporting to clients, Tobin continues. ‘LabWare’s Contract Template Solution has been designed around the needs of the contract-testing sector, and could be configured to our specific requirements, which are primarily centred on the need to manage sample volumes, enable sample throughput, and host a regulatory compliant, fully transparent audit trail. We were able to strip down the number of steps it took to book samples in to our laboratory, barcode them and assign each sample to the relevant laboratory, with a specific suite of tests, so that delays at each stage were minimised,’ adds Graham O’Halloran.

ALT also uses the LabWare LIMS to carry out results calculations, which are checked against specifications and highlighted and reported if a specification limit is exceeded. LIMS then produces the certificate of analysis, which is reviewed and approved before being sent out by the LIMS to the customer.

ALT is currently expanding to provide further on site testing for the environmental, food, and potentially pharmaceutical sectors.
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Abbott has announced version 11 of the its Starlims software-based laboratory information management system (LIMS).

It expands user functionality to include mobile device applications, advanced analytics, and HTML5 compatibility, enabling users to access LIMS information on any screen.

The software offers users advanced analytics capabilities with out-of-the-box dashboards that enable labs to optimise workflow and identify bottlenecks, viewing data with visualisations that are provided by advanced analytics.

Advanced analytics features include: forms that can be created by users to run system-wide on Chrome, Safari and other browsers for tablets and smartphones; two new control libraries, one for tablets and smartphones; two new control libraries, one for tablets and smartphones; two new control libraries, one for tablets and smartphones.

This version of ELN v2.2 includes new features with a collaborative and intuitive user interface enabling scientists to work with the ELN to support, complement or even replace the labs paper notebooks.

The upgrade includes improvements and new capabilities including improvement of the user interface with a more fluid usage, a new content editor and grid custom field’s improvements for PDF and printing exports; with a tree-view summary.

**AgileBio** is a provider of IT solutions specialising in web-based software for life sciences has announced the release of a new version of its electronic lab notebook (ELN), a complementary application to its LIMS, LabCollector. ELN is an efficient and simple notebook to store, organise, find and share all researchers’ laboratory experiments in a variety of life sciences and other industries as well as in academic research laboratories.

This version of ELN v2.2 includes new features with a collaborative and intuitive user interface enabling scientists to work with the ELN to support, complement or even replace the labs paper notebooks.

**Amphora** provides PatentSafe, a quick straightforward and cost-effective solution to the tricky problem of laboratory notebooks in today’s environment. Amphora believes that the best approach for users is to ‘get out of the way’. It eschews ill thought-out features and complex choices, instead allowing the users to be able to focus on science.

PatentSafe is particularly suited to modern approaches to research record keeping. Along with the increasing ‘externalisation’ of research activity, with collaboration across organisational boundaries, the America Invents Act brings new concerns. The focus is no longer solely on experimental write-ups, now scientists need to ensure they can account for the knowledge that is transferred to other parties and when. This takes the burdens of ‘lab notebook’ style record keeping into the project meeting and day-to-day collaboration.

**BioXM Knowledge Management Environment** is a fully customisable knowledge management environment that manages complex data and transforms it into useful information.

The system is designed to be configured easily; this makes it useful in several different areas. It is designed with a solution-building approach: rolling out a new application to end-users takes only weeks. The system is continuously adapted while staying in production, which is aimed at reducing costs.

BioXM technology enables expanding knowledge and integrating data from any source, refining decision making, connecting the dots explaining systems, and creating new hypotheses to visualise relationships between data networks.

**Bruker Dash Reporting** is a new system which brings customised reporting to all users of the EVOQ liquid chromatography mass spectrometer (LC-MS) and the SCION gas chromatography mass spectrometer (GC-MS). This new capability centres on Dash Designer, a purpose-built application that enables customers to position and closely format report elements and preview reports with relevant data.

Bruker’s Pacer software is
designed to match the hardware advances in the EVOQ liquid chromatography mass spectrometry (LC-MS) range. Pacer provides exception based data review to significantly reduce the error rate for quantitative analysis, by enabling chromatograms to be reviewed by exception.

www.bruker.com

BSSN Software has released Seahorse Scientific Workbench, a vendor-independent software suite for capturing, analysing and sharing analytical data. It consolidates raw and result data from multiple experimental techniques in a single tool, based on the emerging ASTM AniML data standard.

Seahorse Scientific Workbench captures each step of a workflow and presents it in its entirety. An intuitive navigation model allows scientists to explore experiments and samples, independent of the original vendor software. Visualisation, annotation and reporting features provide the necessary support.

www.bssn-software.com

Certara’s D360 is used for the query, analysis, and visualisation of drug discovery and development data. It can be used to analyse, and visualise existing data and entire workflows can be saved as a ‘widget’ to be shared or reused.

Phoenix WinNonlin is a pharmacokinetic/pharmacodynamic (PK/PD) modelling and non-compartmental analysis (NCA) software. The tools allow researchers to visualise and analyse their data which is stored in a single file. Key features include a library of PK/PD models, reusable workflow templates and bioequivalence determination.

Phoenix NLME is a data processing, modelling, and reporting product for population PK/PD analysis. Tools are provided for creating preliminary plots, determining a base model, covariate analysis, developing a final model and its evaluation.

www.certara.com

ChemAxon has launched JChem for Office, which provides chemistry functionality for MS Office users. Building out from the JChem for Excel product, the product provides productivity features including, embedding live chemical structures from existing files, supporting all major common chemistry file types and copy and paste functionality. The software can also be used to sketch and edit structures on the fly, directly in the original document and import structures and their associated data directly from remote corporate databases, or from other ChemAxon products like Instant JChem.

http://bit.ly/1BNak3S

Core Informatics provides LIMS, ELN and SDMS to customers across R&D industries including life science, food and beverage, clean technology, molecular diagnostics (MDx), genomics, energy, chemical, petrochemical and environmental. Core informatics products are configurable to match customers exact laboratory workflows and automation needs without programming.

Core LIMS includes inventory management, automated data capture and reduction, dashboards and reporting, workflow management and more. Core ELN helps labs capture, analyse, manage and share data to simplify the transition to a ‘paperless’ system. Core SDMS accelerates scientific decision-making by simplifying the capture and archive of vital instrument results files.

www.CoreInformatics.com

CSols Laboratory Informatics Software and Services solutions include links for LIMS, instrument interfacing and integration software. AqCTools for QC statistical analysis and charting of AQC and IQC samples for improved monitoring, exceptions management and reporting of AQC results, ensuring that analytical methods and instruments are performing optimally and within regulatory requirements.

They also offer the Remote Sampler mobile application to assist sampling and data capture in remote locations, designed to help to eliminate transcription and data entry errors and guide samplers in all routine activities. Optionally included are sat-nav software for route guidance and GPS coordinate recording for full chain of custody trails.

www.csols.com/home.asp

Dataworks Development has announced the release of a major new upgrade, version 6.0, to its Freezerworks Unlimited freezer inventory and sample management software program.

Freezerworks software is designed for user configuration; this has been implemented with expanded configurability in version 6.0. Most notable are improvements and greater capabilities in screen design and layout, as well as in adapting the shipping processes to the workflow of the biobank.

www.freezerworks.com

IDBS provides E-WorkBook Suite, a single platform proven to increase operational efficiency through flexible management of research and IP. It enables scientists and researchers to more effectively create and work in communities supported by trusted data.

E-WorkBook platform includes data management and workflow management. It improves data quality and compliance by enforcing business rules and reducing transcription errors. This enables the user to move beyond unstructured data capture and IP protection towards real-time data-centric collaboration.

E-WorkBook is available both via the web and as a desktop client to enable researchers to access, manage and share their data from the lab, at their desk or on the go. The platform provides a secure, searchable repository of corporate knowledge.

www.idbs.com

KineMatik has launched version 10 of its Electronic Lab Notebook, which now includes full mobile and tablet device support. Intellectual property is protected with full audit trails and 21 CFR 11 compliance.

Dotmatics has a new Dotmatics Platform, which includes Studies Notebook and Browser.

Studies Notebook is a web-based electronic laboratory notebook that covers all scientific disciplines in a single set of tools, including chemistry and biology. In this latest release, Studies Notebook incorporates configurations for formulations and analytical/ad-hoc biological studies.

Studies Notebook is designed to enhance information sharing and improve productivity in pharma, biotech and chemical companies, as well as academic institutions and research centres. Browser, the powerful and scalable query and reporting tool, allows users to search all fields within the Notebook. Through Browser, users can federate and search data from multiple sources, independent of the original database.

This release offers enhanced security features for using the system on your intranet, or on our cloud infrastructure.

www.dotmatics.com
The KineMatik ELN offers one-click publishing to automate the entire process of publishing, approving, and witnessing the experiment, as well as archiving the experiment for use in future research.

LabAnswer has produced multi-site systems that perform tasks such as assessments, vendor/product selection, architecture/design, configuration, system/instrument integration, validation, training, data load/migration, organisational change management, deployment, and support outsourcing. They deploy integrated systems comprising of ERP, ELN/LES, LIMS, SDMS, and CDS functionality. Aiming to provide strategic and technical information from which informed investment decisions can be made. LabAnswer’s experience with enterprise informatics solutions ensures the development of a scientific data management system that optimises application portfolios while maximising value, increasing compliance, and achieving business objectives.

LabLite LLC is a LIMS software company offering multiple products including LabLite SQL LIMS, LabLite Process Control, LabLite CS, LabLite Stability and LabLite CMT. LabLite CS is used to track customer calls and complaints from receipt to resolution. LabLite Stability which is aimed at labs conducting rapid age testing and stability studies, features include inventory to track consumables, expiration dates and usage history, handhelds and tablets to collect field readings then auto-upload to LIMS. LabLite CMT to track your calibration, maintenance and training schedules. All of these products can be used alone or fully integrated depending upon customer’s needs.

LabWare’s ELN provides a familiar spreadsheet style environment, providing the capability to mix spreadsheet and document style templates. The system can operate in experiment driven, research environments and also provides a method execution mode suitable for QA/QC. The software provides instrument integration, flexible management of images and raw data files and comprehensive operation auditing.

LabWare ELN can be integrated with LabWare LIMS, delivering a cost effective, advanced level of laboratory automation capability with access to an extensive range of application modules and integrated instrument data acquisition technology.

Modul-Bio provides MBioLIMS BioBanking, a flexible LIMS dedicated to biobanks and cohorts studies, which has been deployed successfully at more than 100 sites. This 100 per cent web-based software provides perfect traceability of biospecimens, from reception to shipment. Its main functionalities include patient management, sample collection, processing, analysis, storage and distribution. MBioLIMS is compatible with MBioLABEL, a biological sample identification solution for long-term storage, which includes labels, barcode printers and scanners; and with eMBioBANK, a centralised bio-specimen inventory web portal for sharing bio-repositories’ sample collections with researchers.

NoteBookMaker is a legal notebook system for laboratory professionals but can also be used by anyone recording proprietary data, (easy to use data management). The solution was produced with FileMaker Developer database software; it is also 21 CFR part 11-compliant, a key feature for legal defence.

BioRails enables research scientists to capture experimental data and methodologies together in a single system, enabling them to quickly analyse assay results and refine study designs.

A key component of BioRails DM is Morphit, a spreadsheet technology for data analysis and reporting. It includes support for curve fitting, non-compartmental modelling for PK and statistical tests for in-vivo pharmacology.

Qlucore’s first product, Qlucore Gene Expression Explorer 1.0, is a software engine that visualises data in 3D and aids the user in identifying hidden structures and patterns. Major efforts have been made to develop a core software engine that is extremely fast, allowing the user to interactively and in real time instantly explore and analyse high-dimensional data sets with the use of a normal PC. The latest version, Qlucore Omics Explorer 2.0, represents a major step forward with the added support for hierarchical clustering, scatter plots and powerful log function.

One of the early key methods used to visualise data is dynamic resolution. LabLite Stability which is a LIMS software provides perfect traceability of biospecimens, from reception to shipment. Its main functionalities include patient management, sample collection, processing, analysis, storage and distribution. MBioLIMS is compatible with MBioLABEL, a biological sample identification solution for long-term storage, which includes labels, barcode printers and scanners; and with eMBioBANK, a centralised bio-specimen inventory web portal for sharing bio-repositories’ sample collections with researchers.

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The software can be used on a PC, notebook or any Mac IOS product to create, search, and print data, which can be imaged to pdf, or to paper for patent submission. The attachment field can embed virtually any file, including sophisticated scans, tables, sound, and movies. A page will also contain a body text field for scientific data; in addition to this NoteBookMaker can be setup in single-user or multi-user (peer to peer, or client/server).

The Edge software consultancy provides BioRails, an application suite designed for biologists and project teams. BioRails PTO is an assay request and tracking system used to enable project teams to track and optimise progress of small molecules and biotherapeutics drugs.

BioRails PTO enables scientists to plan, and schedule their work, improve turnaround times and remove bottlenecks.

BioRails Data Management (DM) is a solution for capturing, processing, analysing and reporting in vitro and in vivo biological data and workflows.

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Siemens Electronic Lab Notebook (ELN) allows researchers to capture experiment data of any type in electronic format, it is also fully integrated with the lab, being built on top of the Siemens LIMS. The software now offers a mobile platform that deploys all the assets of modern tablets in a simple user interface and a central data repository, allowing the search and re-use of knowledge from previous experiments. Full audit trail and access control for this data is available, facilitating intellectual property management www.siemens.be

QESTLab is Spectra QEST’s LIMS, specifically designed for the construction materials testing (CMT) industry. It is designed to improve efficiency and introduce best practice in all areas of the laboratory. The system can support centralised implementations and is a functionally broad system after more than a decade of continuous improvement and adaptation in a variety of markets.

QESTLab’s reach can be extended to the field with the adoption of the QESTField system which is designed to run on portable, hand-held devices. Further, the QESTLab system integrates well with Construction Hive, which is a web system for the management of CMT results. www.spectraqest.com

Studylog Systems provides Studylog Animal Study Workflow Suite, which aims to automate animal study work-flow, from collaborative study design, data acquisition, task scheduling & oversight, data analysis, graphing, reporting and data sharing. All results and methods are digitised, stored securely and accessible wherever and when you need them. www.studylog.com

Titian Software’s Mosaic is a sample management software suite, providing management of compounds, biological collections, reagents and standards. Designed to streamline sample inventory, tracking and ordering, in high-throughput biotech and pharma laboratories, Mosaic provides a solution to sample management traceability and sample supply chain. As a modular software platform, Mosaic is scalable and provides flexibility to support the sample supply workflows for all sizes of life science organisations in industry and academia. The latest version of the software, Mosaic 5.0, also permits extensive integration capability with a range of automated stores and dispensing systems for maximum productivity and complete workflow management. www.titian.co.uk

The Trilogy Group provides TAPS (sample planning and scheduling), which enables companies and consultants with environmental or sample collection field teams, to plan collections, create optimised sampler rounds, print bottle labels, estimate workload and cost, conduct monitoring and on-site

Thermo Scientific has launched SampleManager 11, a configurable version of its laboratory information management system (LIMS). It features tools and workflow capabilities that simplify implementation, allowing lab managers to model their processes in the LIMS. The LIMS workflow can automate the logical decisions, improving throughput by saving time and simplifying user interactions. SampleManager 11 puts power in the hands of users who can make logical choices about workflow, instrument integration and data reporting for management metrics or regulatory requirements. www.thermoscientific.com

The TIBCO Spotfire Analytics platform allows users to uncover insights hidden in data through intuitive visualisations, analytic dashboards, and applications. It is used to reduce reliance on IT and eliminate time related to data preparation, report building, and spreadsheet version control.

ENotebook 2014 is the latest version of TIBCO’s electronic laboratory notebook. It is used for capturing, recording and analysing scientific data, the notebook is also integrated with Datalytix query tool used for seamless data visualisations. Improved features include: inventory and registration integration, BioAssay including a library of standard protocols and the upgrade toolkit.

Ensemble is a solution for the management of data and the integration of workflows; it features a number of tools including inventory, registration, ChemBioDraw a chemical drawing tool and iLAB, an LES designed specifically for QA/QC. www.tibco.co.uk

UNIConnect supply laboratory process management software solutions for bi-molecular labs (MDx, CDx, OncoMDx, Crop Science, Aquaculture and Livestock). UNIConnect delivers software and professional services for the dynamic requirements of those driving the science and business of precision medicine and agriculture. Aiming to provide configuration flexibility, precise tracking and process detail that is comprehensive from first sample to final report. www.uniconnect.com
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HIPAA Accountability Act of 1996
HIPAA Patient Safety and Quality Improvement Act of 2005 (Patient Safety Act)

Compatibility:
☑ PC/MAC
☐ Tablet
☐ Smartphone
☐ Web-based
One of the biggest trends in informatics is the move to integrate mobile technology into the laboratory. The topic will feature repeatedly in presentations and round-table discussions at the Smartlab Exchange meeting in Munich in February 2014.

Similarly, many laboratories are switching to use software as a service (SaaS). The first reason is to restrict spending on data-centres and IT infrastructure especially for smaller companies that cannot afford to have large installations for data analysis. SaaS provides the opportunity to pay for these services when they become necessary, and removes the need to house data centres with large maintenance and power costs.

The second reason for the adoption of an SaaS model is so it can be used as a safe but temporary collaboration infrastructure – several companies can share a zone external to their firewall where collaboration can take place but without risking their intellectual property. This service can then be switched off once the collaboration is over, meaning that the companies do not incur extra costs or have to share parts of their own internal data-centres with competitors.

MOBILE TECHNOLOGY STRATEGY
Mobile technology presents its own technical challenges. Either discrete applications have to be created to take advantage of mobile devices, or the existing system has to be modified, for example, to enable the use of touch-screen devices. Informatics companies have adopted different strategies for tackling the integration of mobile devices. Stuart Ward, product manager for IDBS’s ELN product E-WorkBook, said: ‘We see mobile devices as having specific apps for very discrete types of transactions, rather than some sort of universal application like you could deliver on a desktop or a laptop.’

In contrast, Seamus Mac Conaonaigh, director of technology at Thermo Fisher, said: ‘Our approach is really to extend our applications to allow mobile use, rather than to develop single-use mobile applications.’ He went on to explain how the company’s software can enable the use of mobile-devices within the existing LIMS infrastructure. ‘We have a piece of middleware called Integration Manager which allows integration of basically any end-point with our LIMS system’. This enables users to develop functionality, on top of the existing LIMS platform, tailored to their specific needs.

CAMERA TECHNOLOGY
Mobile technologies can capture data better than conventional techniques in certain areas. The most effective and easiest to implement are: QR codes; bar-code scanning; and the use of cameras to photograph specific instances in the lab. Ward explains that very much like traditional ‘apps’, data-capture in the laboratory is most effective for very specific things: ‘Using the camera as a bar-code scanner or a taking a picture of an event. They lend themselves to specific types of data’. Mobile technology is not going to replace all the traditional methods of data capture. ‘You’re not going to have someone on a mobile device typing in 10,000 data-points, it’s just not going to work,’ he continued.

One problem is simply the lack of...
convenient keyboards when using tablet or phone-like devices. Similarly, browsing large amounts of data or conventional spreadsheets are unlikely with the current technology in mobile devices. Scott Weiss, IDBS director of product strategy, explains: 'Just trying to shrink them [big data sets] down to a mobile device and trying to cram all that functionality into a touch-screen – it’s not just a technical challenge, there’s an ergonomics challenge with the way you interact with that.’

Seamus Mac Conaonaigh, from Thermo Fisher, highlighted how bar-code scanners on mobile devices have already been implemented in a loading-dock scenario. ‘Historically, this was done with something like a bar-code reader attached to a workstation, which is not very mobile,’ he continued. With mobile devices, in contrast: ‘You can have the person who’s receiving the goods just basically walking around and scanning all the items no matter where they are, rather than bringing the items to a single location.’ This information is then automatically transferred to the LIMS or similar system. The inherent mobility of hand-held devices means that these types of activities, which used to create a bottleneck in the workflow, can now be carried out more efficiently.

Barcode scanning, combined with the GPS included in many smartphones, can make environmental sampling in the field more efficient. Mac Conaonaigh explained: ‘Previously you would need several pieces of equipment to do this type of thing. Your water-testing person just goes to a location – be it a river or lake – and scans the barcode that’s already attached to the test-tube, fills the test tube, bottles it up, enters the record and then its immediately transferred to the LIMS, so they have the complete chain of custody of where this sample was captured.’ This kind of sampling eliminates transcription errors and makes the validation process easier, as the system automatically records the GPS data.

**REVIEWING DATA**

Another key area for the integration of mobile technologies is to review the data that has been analysed. John Wise, executive director of the Pistoia Alliance, gave an example of data review out of the laboratory environment where two scientists may discuss how a chemical compound could be modified to aid targeting to a specific area for medicinal purposes. Traditionally this would have been done on paper, but applications can now be used to accomplish this on a mobile device.

Stephen Gallagher, CEO of Dotmatics, said: ‘We have implemented a feature in our chemical drawing app, Elemental, that enables the scientist to draw or annotate a compound or reaction on their phone or mobile device, and automatically push it to their Studies Notebook, Dotmatics’ electronic laboratory notebook.’ Wise went on to say how this type of procedure could be enhanced, ‘by connecting to the corporate chemical database and finding out that maybe you have got that molecule.’ There are other examples of the use of mobile devices to review data captured in the laboratory. Wise said: ‘If you wanted to check the status of an ongoing experiment then perhaps the mobile device would allow you to check.’ He was talking hypothetically – but this technology has already been implemented, according to Thermo Fisher’s Mac Conaonaigh. The company’s Data Manager module can be connected to chemical analysis instruments, for example chromatography. The software collects the data, which can then be viewed using traditional workstation-based computers or a hand-held device. Taking the raw data from the instrument, rather than a jpeg or pdf, means that a higher fidelity is obtained.

Mr Conaonaigh highlights the advantages: ‘On an iPad, you can connect to one of our applications and you can get at the original raw data. So if it’s a chromatograph you can...’
view the overall output and you can zoom in to view all the original peaks.’ He pointed out: ‘Frequently, you can have a situation where there is a very visible artefact at the gross level, which is actually just noise from the instrument, and then when you zoom in you actually see what you wanted to see – which may be in a totally different place. The pdf won’t show that type of thing.’

When implemented for mobile devices as well as traditional workstations, the software does not require the scientist to be in the laboratory. Now this review can be done anywhere as long as the device being used is connected to the internet and thus a web-based client. The device can also be notified when the instrument is finished with the experiment.

THE RISKS OF MOBILE DEVICES
The integration of mobile devices has risks, mainly those associated with the loss of a company’s data, but this has not stopped the adoption of the technology. This is because many of these risks have been associated with similar devices used by company personnel for a number of years. Mac Conaonaigh points out: ‘There is still a risk with mobile devices, but there has been for a long time with laptops anyway.’ He went on to say: ‘You can sandbox anything that’s to do with the enterprise, and if the device is lost or stolen then the IT organisation within the enterprise can remotely wipe that.’

With the ability to remotely wipe sensitive data from mobile devices, the perceived risks can actually work as an advantage. Ward stressed this aspect: ‘If you can have this all operating on a simple device that is relatively cheap, and you put your money into the server that’s actually doing the analysis, you have essentially got the analysis occurring in an environment that you as a business, paying for it, have much more control over.’

BUDGETARY CONTROLS (SAAS)
Some data can be dealt with over mobile devices, but large data sets are becoming more frequent and their analysis presents particular problems, especially for smaller companies. This issue has led to the development of a second technology trend in the informatics field. SaaS is an exciting prospect for many smaller companies as it can provide a high level of computing power for the analysis of large data sets, on a ‘pay as you go’ basis. This removes the financial burden of installing large data-centres. Ward explains: ‘I think the attraction on paper for many organisations to move to a SaaS model is budgetary control, in so much as “I don’t have to think now about setting up the infrastructure, buying servers, maintaining the servers, dealing with upgrades” so there are clearly potential cost-savings from just management of those kind of complex systems.’

Although the main advantage for companies using SaaS may be the management of the IT infrastructure, there are other advantages to using the model, such as being able to access large amounts of computing power at times when the workload for analysis increases. Mac Conaonaigh gives an example: ‘So if you’re in a situation where you have a huge amount of analysis to do, and it is going to take a month or more using your single server that you have sitting in your lab, you can certainly leverage SaaS infrastructure.’ He continued: ‘Just set up 30 instances, instead of your single instance: you get your results much faster and it doesn’t cost you anymore because you’re only running it for a fraction of the time and you only pay for what you use.’

COLLABORATION INFRASTRUCTURE (SAAS)
The case for SaaS is not restricted to just budgetary control, however. Its other advantage is as a collaboration infrastructure. It provides a tool for companies to share information in a safe environment without IP concerns or the classical association with moving sensitive information outside the firewall, or allowing people from outside the organisation to access information inside the firewall for a particular collaboration project.

Weiss outlined the concerns he has experienced from customers with existing collaboration methods: ‘We can create a space in your system and give your collaborators access to it. You open up the firewall and the ports – and that kind of makes them (customers) nervous.’ He explained why the SaaS model was such an attractive proposition especially for sensitive industries like pharmaceuticals: ‘The ability to spin up these open public spaces that are managed by your vendor, that allow people to safely collaborate and share content, but also allow you to extract that content back into your own infrastructure when you see fit.’

Dotmatics’ Gallagher has experienced similar requests for SaaS to promote innovative collaboration. He said: ‘We have seen a trend whereby many large pharma and chemical organisations with important internal IT infrastructure, choose to extend it with SaaS systems that enable them to work seamlessly with collaborators across the world.’

He added: ‘Not only does the SaaS model provide a safe framework to exchange data between organisations, but it enables true collaborative research with real-time knowledge sharing between researchers.’
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To enable today’s laboratories to be more flexible, efficient and compliant than ever, software must empower users and demonstrably improve productivity across a connected enterprise.

The hardest working LIMS in the industry now has advanced new tools and user-interface enhancements that improve laboratory process mapping management and automation.

SampleManager 11 puts decision-making power where it belongs, in the hands of users who can make logical choices about workflow, instrument integration and data reporting for management metrics or regulatory requirements.

Workflow capabilities simplify implementation, allowing lab managers to easily model their processes in SampleManager. As laboratory needs evolve, workflows can be modified to change with them.

SampleManager 11 At a Glance:

- Configurable workflow and extended lifecycle features
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- Flexibility in splitting and merging aliquots and samples
- User-Friendly Search Syntax, new Internet Explorer® features and improved support for Windows® 7 and 8
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For more information about SampleManager 11, please visit us at www.thermoscientific.com/SM11 or email us at marketing.informatics@thermofisher.com
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