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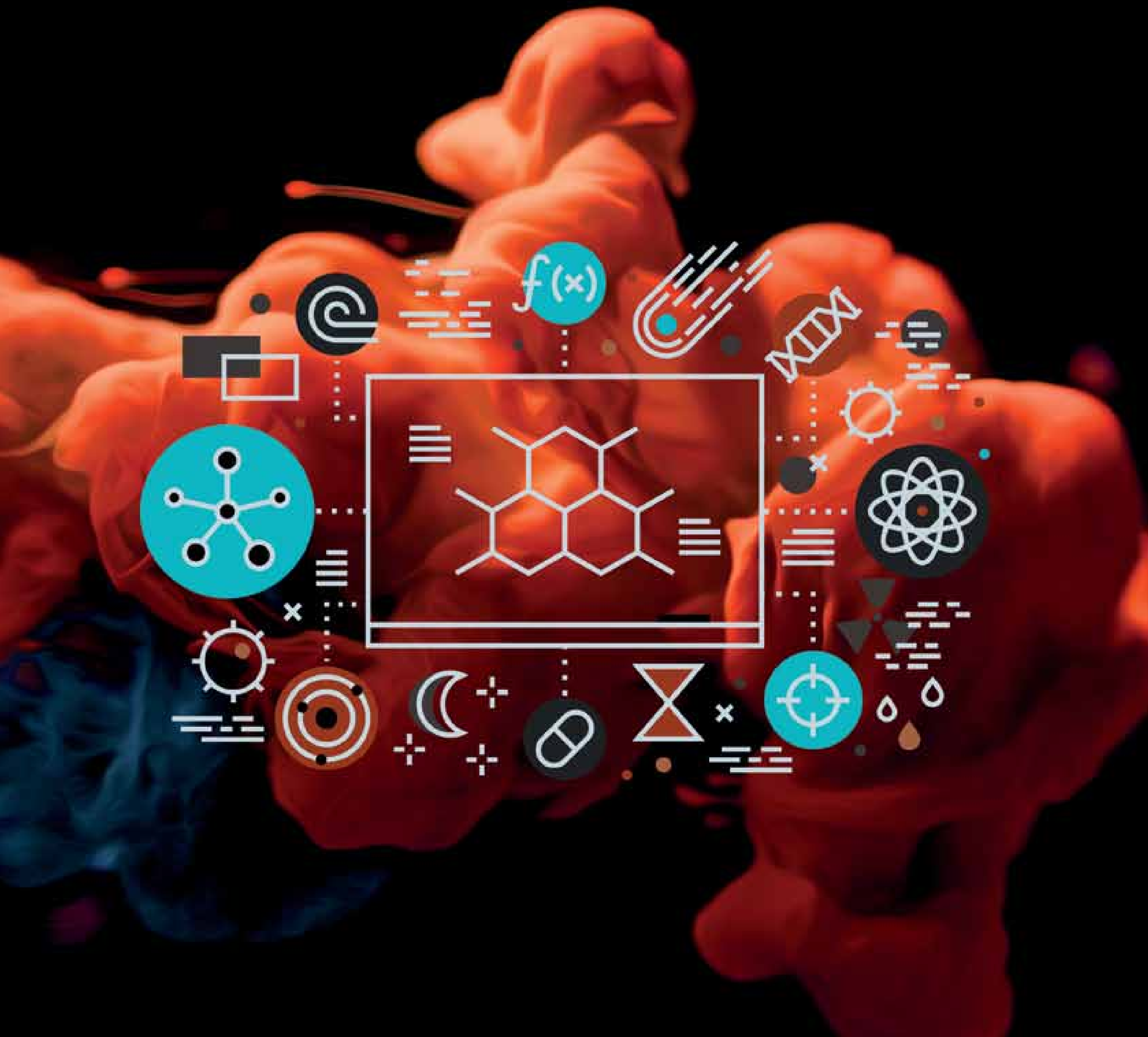


FROM THE PUBLISHERS OF

scientific computing world

ROADMAP TO DIGITAL CONVERGENCE

Peter Boogaard explains how laboratories can transform scientific information into actionable insight for their data consumers

The best way to predict the future is to create it.[1] Harmonisation, decreased financial budgets, increased privacy, regulatory and security requirements – plus the need to reduce overall system complexity – are all demands being made by modern-day senior laboratory managers. Despite all of this, many laboratory operations are predominantly paper-based – and, even considering the enormous potential to reduce data integrity for compliance and mandatory efficiency gains, implementing paperless processes are being questioned.

In previous issues of the *Laboratory Informatics Guide*, I focused on operational challenges in the laboratory. This year, I would like to focus on how laboratories can create value by transforming scientific information into actionable insights, and address the frequent misconception by management that the laboratory is a cost centre.

We are masters in finding ways to be perceived different, and we use all our scientific creativity to prove that we are right. While other sectors such as financial/banking, travel and healthcare adopted new ways of working, many of our processes are still the same as they were in the previous century. Even our tax authorities are moving away from traditional paper-based processes and introducing paperless new alternatives – achieving 20 to 40 per cent cost reductions, significantly improved turn-around times, and lower barriers to accessing relevant information.

For years, we believed that our pharmaceutical and biotech industries were unique in respect to regulation requirements and the ability to adopt new management processes. However, many other industries also have to comply with very strict safety and security regulations, and they have been able to adopt the transformation. So let's take a step back and answer some of the basics first.

DATA GOVERNANCE

Data governance is a set of processes to ensure that important data assets are formally managed throughout the enterprise.

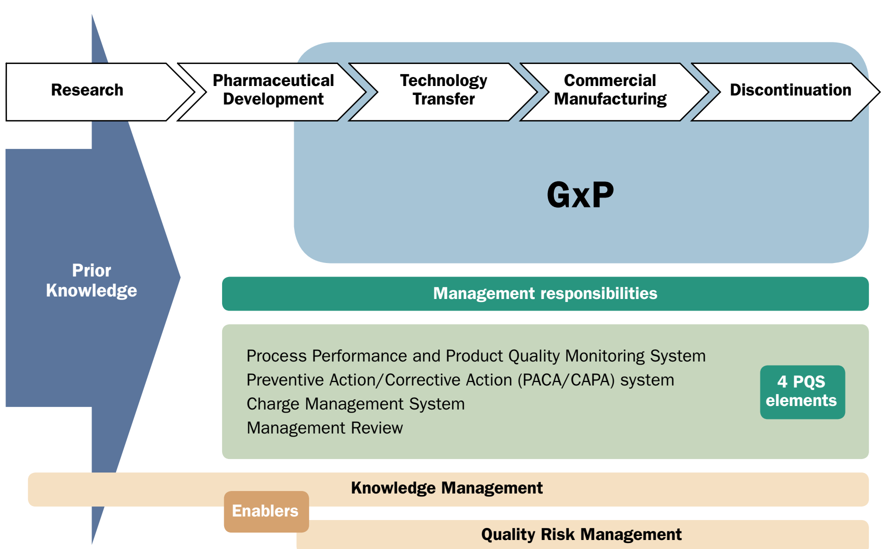
It ensures that data can be trusted, and that people can be made accountable for any adverse event that happens in the case of low data quality. It is about putting people in charge of fixing and preventing issues with data so that the enterprise can become more efficient. Data governance also describes an evolutionary process for a company, altering the company's way of thinking and setting up the processes to handle information so that it may be utilised by the entire organisation[2].

A good example is how, in the ICHQ10[3] lifecycle, the management layer plays a leadership role in assuring cross departmental data government engagements. ICH Q10 describes a comprehensive model for an effective pharmaceutical quality system that is based on International Organisation for Standardisation (ISO) quality concepts.

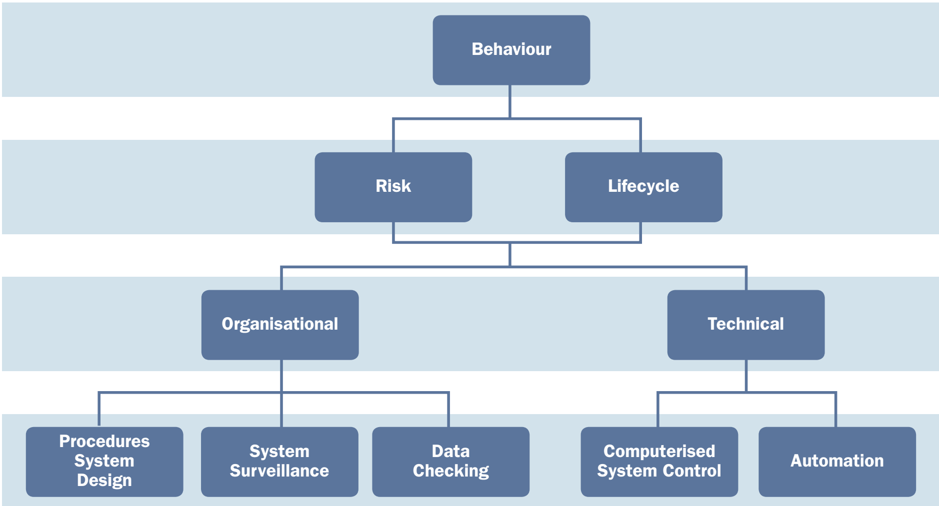
The model is based on a holistic data lifecycle approach, and gives organisation practical guidelines on how to implement risk management based processes. According to the FDA, to avoid data integrity issues, source data needs to be 'Attributable, Legible, Contemporaneous, Original, and Accurate' (ALCOA) to meet the regulatory requirements[4].

EXPAND AUDIT TRAIL USAGE

It is known that audit trails are a secure resource to maintain a record of activity in both system and application processes. They store a secure record of all individual user activity.



Product and data lifecycle requires holistic corporate participation



Source: GMP's Data Integrity Guidance Documents

Digital convergence requires a data lifecycle-based holistic view

Traditionally, audit trails assist in detecting security violations, performance problems, and flaws in applications for regulatory purposes. But there is more that we can do with this highly secured dataset. Wouldn't it be nice if we could use this trusted resource to improve operational excellence? Pro-active use of data analytics tools may identify and visualise existing process flaws, and present opportunities to improve operational excellence.

Deep dive analysis can predict and identify trends that may indicate more deep-rooted problems, such as faulty equipment, a lack of competence, or fraud – and they can be used to optimise existing scientific workflows. An additional advantage is that this information is available at no extra cost, has an outstanding quality and is readily available in many of our software application systems. We may combine CDS, MES, LIMS, LES, ELN, SDMS and ERP audit trail data in a joint process.

INTRODUCING NEW TECHNOLOGIES

Digital transformation is at the heart of all business strategies and begins with an executive mandate. It is essentially a commitment by organisations to innovate on the experience they offer for their customers[5]. At a boardroom level, the threat of digitally enabled competitors remains high on the list of concerns.

An essential element of generating innovative experiences and transforming operating models is the so-called Internet of Things (IoT). This technology underpins acquiring, analysing and activating data from a variety of devices in real-time. According to Gartner in 2018, 90 per cent of scientific R&D organisations will struggle to enter the 'digital era', thanks to hurdles with legacy laboratory systems and unfamiliar IoLT (L stands for laboratory) environments.[6]

IDC concludes that 58 per cent of companies believe IoT is strategic, and 33 per cent of all industry leaders will be disrupted by digitally enabled competitors by 2018[7]. Industry 4.0 is the current trend of automation and data exchange in manufacturing technologies. It refers to what has been called a "smart factory". The term was first used in 2011 at the Hannover Fair, and it consists of four design principles[8].

M2M LEARNING

Machine-2-Machine (M2M) learning is a generic term that explains how networked devices can exchange information and perform actions independently, without the manual assistance of humans.

M2M communication is often used for remote monitoring; examples include a vending machine that can sent a message to the distributor when a particular item, such as ice-cream, is running low. M2M communication is an important aspect of warehouse management, remote control, robotics, traffic control, logistic services, supply chain management, fleet management and telemedicine.

Key components of an M2M system include sensors, RFID, a Wi-Fi or cellular communications link and autonomic computing software, programmed to help a networked device interpret data and make decisions. Forrester recommends that IoT data and software should be integrated into existing business systems and operations, to leverage convergence of existing data[9].

On almost every occasion, the laboratory may be a trusted provider of scientific data to support the overall data and product lifecycle. As part of creating this publication, I have surveyed the laboratory software and equipment suppliers and contacted a number of pharma and consumer goods companies.

My initial conclusions are that, while in our personal life IoT is introduced and becoming accepted – with smart devices for energy consumption, electric and hybrid cars, and smartphones – in our professional life we are not familiar with these new capabilities and hesitate to apply them. Based upon my experience and exposure in the global market, I foresee a significant potential in the scientific community. BioVia, iVention, and Agilab for example, have capacity with their software, to include IoT capabilities.

'Many of our processes are still the same as they were in the previous century'

IoT is on the march and will reshape not only the world of consumers, but also the role of the products and services our industry supplies. L'Oréal has for example launched the UV Patch (www.appcessories.co.uk/

Industry 4.0 Design principles	
Interoperability	Ability of machines, devices, sensors, and people to connect and communicate with each other via the Internet of (Lab) Things (IoT/IoLT) or the Internet of People (IoP)
Information transparency	Ability to create a virtual copy of the physical world by enriching digital plant models with sensor data
Technical assistance	Ability to support humans by aggregating and visualising information Ability physically to support humans by conducting a range of tasks that are unpleasant, too exhausting, or unsafe
Decentralised decisions	Ability of cyber physical systems to make decisions on their own, and to perform their tasks as autonomously as possible

Tatsianama/Shutterstock

Selection of Internet of Lab Things (IoLT) devices	
Spectrometers	Ovens
Balances	Refrigerators
Pipettes	GPS sensors
Thermometers	Biometric ID bracelet
Tablets	(Mobile) phones
Heads up display safety glasses	Wearables

loreal-my-uv-sun-patch), which is an exciting new digital way for people to monitor their UV exposure.

The usage is pretty simple. All you need to do is stick the stretchable L'Oréal My UV Patch on the area that you want to monitor. Consumers can compare this to the everyday use of wearable devices these days – be it fitness trackers or smartwatches.

But the grass is not always as green as we might hope; there are downsides and worries.

As with all public internet applications, data collection, transfer, curation and cross-selecting data between personal and company lives, privacy and security need to be addressed securely. IoT data raises unique issues of data ownership, privacy and security.

These unique characteristics have created new theories of liability for the creators and users of this data; the industry and authorities will need to re-group in the way we currently do consumer research, adopting learnings from new and existing social media and consumer services. A good example is the Information Governance initiative (IGI) – a cross-disciplinary consortium and think tank dedicated to advancing the adoption of information governance practices and technologies through research, publishing, advocacy and peer-to-peer networking. The IGI publishes freely-available research, benchmarking surveys, and guidance for practitioners[10].

WIRELESS INTEGRATION IS MAINSTREAM

During the Paperless Lab Academy congress in 2015, I challenged the audience with the provocative question: 'Can Bluetooth simplify laboratory instrument integration?'[11]

In our laboratories, a significant amount of data is created and stored in LIMS, ELN, LES & SDMS systems. With the exception of automated chromatography systems (CDS), not so much has changed in how we capture experimental data from instruments in our daily laboratory work. While more than 75 per cent of laboratory experiment or analysis starts with some kind of manual process, such as weighing – or measuring a temperature or a pH – the majority of these measurements are still written down manually on a piece of paper or re-typed in in a computer or tablet.

Many modern ELN, LIMS and LES systems can connect electronically to a network, but you still need to be an IT professor to enable an easy transfer to your laboratory automation software. While the perception is that we reduce transcription errors, the reality is still often the opposite.

So why is it, that many capabilities offered by new technologies are not implemented in the laboratory? I like to challenge the industry to have a fresh, realistic view of how we may learn from other industries and adopt best practices and optimise them for our purpose. We should embrace initiatives such as SiLA consortium[12] (Standardization in Lab Automation), AnIML[13] (Analytical Information Mark-up Language), Allotrope Foundation[14] (ADF Framework) and Pistoia Alliance[15] (HELM – single notation standard that can encode the structure of all biomolecules) to develop these common standards for the community.

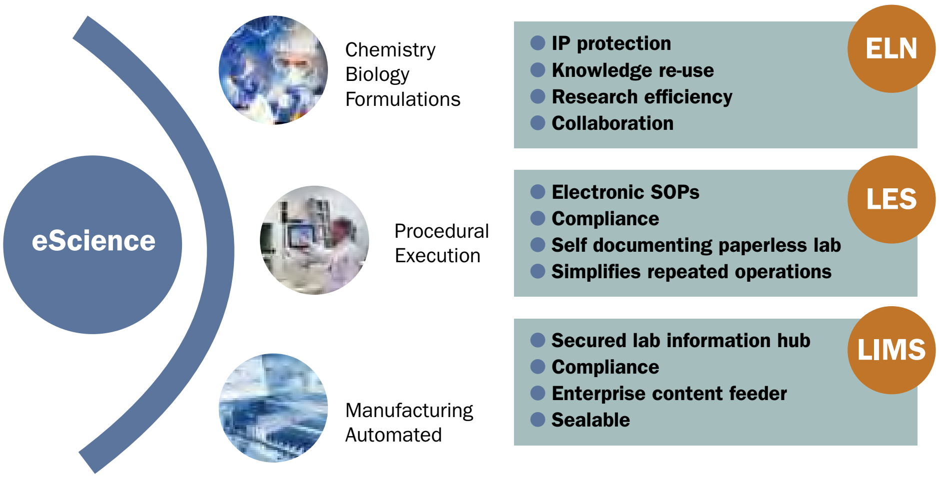
It is amazing how mainstream modern cars have adopted modern GPS and wireless technologies. Connection of any smartphone from almost any brand can be integrated in virtually any car around the world. There's no need to be an IT professor to connect these devices; no need to be a computer expert to test and operate these (complex) devices, no need to buy expensive software updates

'It is known that audit trails are a secure resource to maintain a record of activity'

or applications to enjoy music, to take the shortest route to your favourite location, or to dial any phone number via voice recognition process with your audio system.

So why is it that our scientific industry – instead of adoring these great out-of-the-box, cheap technologies – is finding ways to avoid using or ignoring them completely? A recent survey showed that new graduates are not familiar with the term RS232 at all. While many instrument suppliers still refer to this RS232 standard in their technical documentation, the new generation has no clue what that means.

Industry 4.0 IoLT Potential for Laboratories	
Real-time Data Capture	Self-documenting process to include metadata and content in single process
Predictive maintenance	Predict equipment failures before they happen, and systematically prevent them
Remote monitoring	Remote monitoring solutions collect live data from assets, and use that data to trigger automatic alerts and operational actions based on current conditions, such as remote diagnostics and maintenance requests
Deep learning data analytics	Ability to include and mine (external) big-data in R&D projects
Instrument interaction	Auto registers material and equipment that you are using –for instance, predict reagent consumption and initiate action when reagent is low with supplier
Customer/Consumer experience	Will provide contextualised and personalised C2C experience. Focus on customer experience, including physical safety and security
Enables multi technology validation	Ability to automatically compare test results from multiple technologies on a large scale
Automate to transform	Integrate with existing lab applications and explore to re-use existing dead-data silos
Location tracking	Biometrically knows who you are. Automates user authentication process and reduces keystrokes. Simplifies application experience



The role of lab data management software

Explaining that an USB port is the modern replacement of such a serial port, and that Bluetooth is the wireless equivalent, opened their eyes! It is crucial that we prepare our laboratories, and instrument suppliers such as Mettler-Toledo and Sartorius are extending their offerings with new ways both to integrate their instruments and to support wireless technologies.

DATA ANALYTICS IS UNDERESTIMATED

Implementing scientific statistical and advanced data analytics may have a significant positive impact on how laboratories may operate in the future.

The data-analytics revolution is reaching the scientific community faster than many of us might think. New 'easier to use software' – with significantly increased better algorithms, including self-learning capabilities – will result in a new mind-set to implement these mathematical processes.

But are we prepared? What do we need to do? Proven in other industries, data analytics has the potential to transform how companies organise, operate and manage science, and create value faster, with more confidence. The perception that laboratories are a necessary 'evil', and perceived as cost centres, may change dramatically. The complexity of applying robust scientific methodologies outside the laboratory, and the increased importance of robotics to support Industry 4.0 strategies, are in the fast-track tornado.

The scientist is no longer in the laboratory, but integrated in the overall quality process. A good example is the use of analytical technologies outside the laboratory. Examples include PAT (process analytical techniques) such as NIR and UPLC. Water's Empower CDS systems are deployed in several development and manufacturing processes! The domain knowledge in the laboratory will be crucial to making this happen on a larger scale.[16] Implementing machine learning (M2M) is an easier way to assist tech transfer processes has the potential to accelerate how laboratories may deliver value in the future; many legacy laboratory processes will have to be reassessed.

Finally, predicting the shelf lifetime of a stability study may accelerate development or validation of drugs. Analysis of covariance (ANCOVA) can be employed, where time is considered the covariate, to test the differences in slopes and intercepts of the regression lines among batches. This may result in an early detection for a stability failure and reduces laboratory testing.

'Cross-industry best practices can be used to create start-to-finish knowledge management repositories'

Analysis of covariance is used to test the main and interaction effects of categorical variables on a continuous dependent variable, controlling for the effects of selected other continuous variables, which co-vary with the dependent. The control variables are called the 'covariates'. This process meets FDA/ICH guidelines for stability analysis using ANCOVA.

CONCLUSION

Data intensive science is becoming mainstream, and new technology will change the dynamics of how scientists will work together. Healthcare, banking and the consumer industry have all adopted paperless and electronic data integration approaches, which means that many technologies are now mainstream and available at our disposal. This is an exciting time, as cross-industry best practices can be used to create start-to-finish knowledge management repositories, and enable cross-functional collaboration between internal information silos to transform scientific information into actionable insights.

Peter Boogaard is an independent laboratory informatics consultant and founder of Industrial Lab Automation, which provides services to address harmonisation, integration, and consolidation of business processes in development and manufacturing. Industrial Lab Automation launched the Paperless Lab Academy, for which *Scientific Computing World* is media sponsor. Taking place on 4 and 5 April in Barcelona, the 2017 event focuses on how to transform scientific information into actionable insights in R&D and QA/QC laboratories in pharmaceutical, biotechnology, consumer goods, and chemical industries. The interactive congress offers actionable insights on how to adopt a new mind-set in daily work. The academy includes 20 hands-on workshops, many practical presentations, a networking reception, conference dinner, and live demonstrations from more than 20 leading vendors.
www.paperlesslabacademy.com

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