LABORATORY INFORMATICS GUIDE 2018

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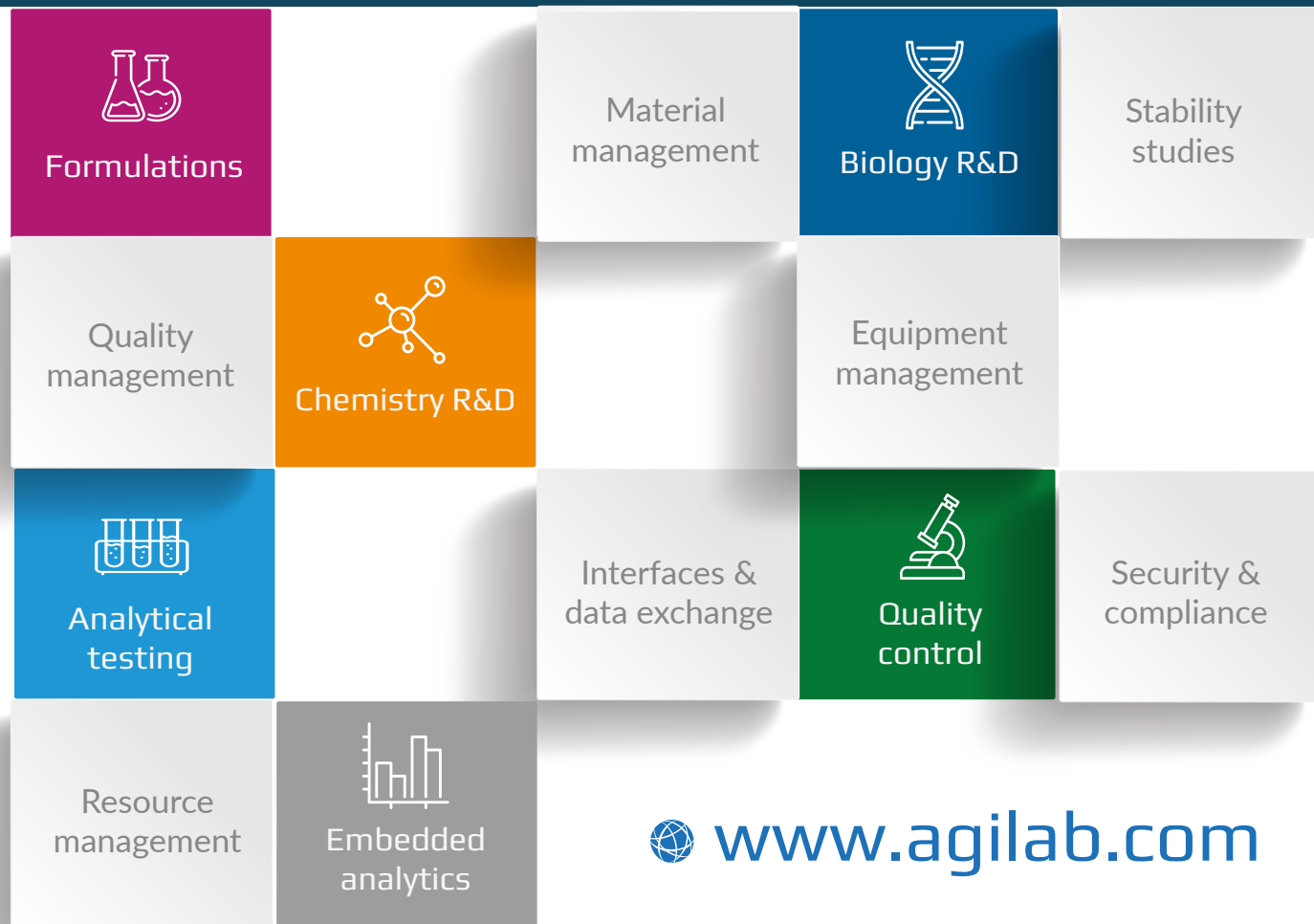
WELCOME

Over the few years that Europa Science has been producing the *Laboratory Informatics Guide*, one constant has been the fact that the informatics industry does not stand still for long.

On page 4 of this publication, we look at the effect that artificial intelligence (AI) technology is having on healthcare research, and the huge potential it has to shape the future. Combining traditional laboratory informatics processes with AI technology could open up huge potential to advance research and provide faster and more specialised treatments to patients. The technology can be used to approximate human cognition of complex medical data freeing researchers to work on other areas of the work and accelerating research or helping a physician to get to an accurate diagnosis in less time.

It is clear that this is a time of real disruption in informatics, as we find on page 8. While some laboratories still cling to traditional processes and paper-based workflows, there is huge potential for a new world of integrated technologies that can enable new research or increase a laboratory's throughput or capability for collaboration.

Many of these technologies have been around for some time but are now becoming a reality through a convergence between availability of applications, data, IoT technologies and AI/machine learning capabilities – all tied together through cloud computing. There are lessons that can be learnt from informatics providers and their users who are making use of these technologies to disrupt traditional laboratory processes.

One page 12 key industry leaders back up this assertion with their views on the last 12 months, as well as making predictions for the next couple of years in laboratory informatics – and analysing the driving factors for change or innovation in the laboratory.

There's a round-up of some of the key news stories of the last 12 months, while we have a comprehensive list of suppliers… making the *Laboratory Informatics Guide* the must-have publication for 2018!

Robert Roe
Editor

AI RESHAPES THE FUTURE OF MEDICINE

Robert Roe explores the use of AI technology in healthcare and medicinal research

AI technology has already made a big impact in many areas of computing, including enterprise and academic applications, but increasingly it is now being applied to healthcare research due to its huge potential.

Combining traditional laboratory informatics processes with AI technology could open up huge potential to advance research and provide faster and more specialised treatments to patients. The technology can be used to approximate human cognition of complex medical data, freeing researchers to work on other areas of the work and accelerating research, or helping a physician to get to an accurate diagnosis in less time.

AI technology is now being applied to many aspects of healthcare. This ranges from assisting patients and clinicians, cataloguing laboratory results, generating abstracts for scientific papers, precision medicine, accelerating research into drug discovery and helping experts to better understand disease and injuries. To create AI requires a lot of computational power, as neural networks or training algorithms require huge amounts of data to teach the AI to perform a task with a high degree of accuracy.

If AI and machine learning techniques are combined with the large amounts of medical research and data from LIMS and ELN systems, AI networks can be used to help advance research and free researchers from mundane tasks.

LEADING THE CHARGE

IBM has been deploying its IBM Watson cognitive computing system in research centres and hospitals for a number of years but now these collaborations are beginning to produce results that can benefit patients and doctors. IBM has partnered with New York-based Memorial Sloan Kettering Cancer Center to train Watson Oncology to interpret cancer patients' clinical information and identify individualised, evidence-based treatment options.

As Watson Oncology's teacher, Memorial Sloan Kettering (MSK) Cancer Center is trying to create a powerful resource that will help inform treatment decisions for those who may not have access to a specialty centre such as MSK.

It is hoped that this collaboration will decrease the time it takes for the latest research and evidence to influence clinical practice across the broader oncology community, help physicians synthesise available information, and improve patient care.

MSK cares for more than 130,000 people with cancer each year. It will use this patient data alongside specialised oncologists with unique expertise and integrating the latest published research – to teach Watson how to identify and treat cancer. The success of the MSK IBM collaboration has led to the development of a genomic service using data from MSK through a collaboration between IBM and Quest Diagnostics.

The project aims to use IBM Watson's core capabilities reading natural language, evaluating cases with evolving machine-learned models, and rapidly processing large volumes of data to address the challenges facing oncologists today.

IBM and Quest Diagnostics first launched the new service in October 2016 to assist researchers in advancing precision medicine through the combination of cognitive computing with genomic tumour sequencing.

Memorial Sloan Kettering will supplement Watson's corpus of scientific data with OncoKB, a precision oncology knowledge base, to help inform individual treatment options for cancer patients.

'We now know that genetic alterations are

'Through this collaboration, oncologists will have access to MSK's expertly curated information about the effects and treatment implications of specific cancer gene alterations. This has the power to scale expertise and help improve patient care'

responsible for many cancers, but it remains challenging for most clinicians to deliver on the promise of precision medicine, since it requires specialised expertise and a time-consuming interpretation of massive amounts of data,' said Paul Sabbatini, deputy physician-in-chief for clinical research at MSK. 'Through this collaboration, oncologists will have access to MSK's

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that researchers around the world have access to information about oncogenic effects and treatment implications of thousands of unique variants at their fingertips.

MAKING SCIENCE EASIER TO PUBLISH

Another use for AI technology is language processing and this has been applied to creation of abstracts for scientific journal articles. sciNote – the creators of a free open source electronic lab notebook (ELN) of the same name – has incorporated AI into its ELN software.

The sciNote Manuscript Writer add-on allows researchers to generate a draft of a scientific manuscript using data stored by the user on its platform and relevant references. With the add-on users can simplify the process of preparing scientific manuscripts, giving them more time to focus on research.

'At this point we are using it to create the draft of a scientific paper. This is the first electronic lab notebook to use AI in this

'At this point we are using it to create the draft of a scientific paper. This is the first electronic lab notebook to use AI in this way'

way,' commented Dr Klemen Zupancic, CEO of sciNote. 'The main benefit is saving time for researchers. Writing a scientific paper is not only tedious but it is also time consuming.

'According to our research, researchers can spend on average 72 hours writing a scientific paper, and a lot of that time is just putting the data together and re-formatting that data. That is one area where we feel that AI can do a really good job,' added Zupancic.

Recognising the importance of timely publication of scientific findings, Scinote created the add-on to significantly reduce the time taken to prepare initial content. The software draws upon data contained within the ELN and references that are accessible in open access journals, to provide a structured draft for the author to then edit and develop further.

Zupancic said: 'While the competition within the scientific community to publish articles in high-ranking journals is constantly on the rise, it is also vital that valuable research data are published, and therefore accessible, at the earliest possible time. sciNote's ELN is already

expertly curated information about the effects and treatment implications of specific cancer gene alterations. This has the power to scale expertise and help improve patient care.'

The new service involves laboratory sequencing and analysis of a tumour's genomic makeup, to help reveal mutations that can be associated with targeted therapies and clinical trials.

Watson then compares those mutations against relevant medical literature, clinical studies, and carefully annotated rules created by leading oncologists, including those from MSK. Watson for Genomics ingests approximately 10,000 scientific articles and 100 new clinical trials every month.

Bolstering the amount of data Watson

can use, MSK will provide OncoKB to help Watson uncover treatment options that could target the specific genetic abnormalities that are causing the growth of the cancer. Comparison of literature that may take medical experts weeks to prepare can now be completed in significantly less time using Watson.

OncoKB was developed and is maintained through MSK's Marie-Josée and Henry R. Kravis Center for Molecular Oncology, in partnership with Quest. It includes annotation for almost 3,000 unique variants in 418 cancer-associated genes and in 40 different tumour types, including descriptions of the effects of specific mutations, as well as therapeutic implications.

The project is publicly accessible, meaning

➤ used by over 20,000 scientists to store and manage scientific data. The announcement of this new AI add-on has the potential to transform the article writing process and empower these scientists, while establishing sciNote as a leader in the industry.'

Zupancic explained that the impetus to add these new AI-based capabilities to the sciNote ELN came from the experience of trying to create scientific papers in an increasingly competitive environment: 'We started as researchers, the company owners and company founders are all researchers with ample experience in writing scientific papers, so we knew that this process could be improved. Then there was a couple of news stories in the past few years where people had made hoaxes by writing fake scientific papers using software, and that sort of thing.

'This led us to the realisation that science and scientific publications [use a] structured enough language for software to be able to grasp it. This is where we found that advances in AI have done amazing work,' Zupancic continued. 'It is hard to get AI

'The main benefit is saving time for researchers. Writing a scientific paper is not only tedious but it is also time consuming'

to write a poem, but when the text that it needs to output is very well defined and 'standardised', then the job for AI is much easier. That was one of the things that drove us to explore the use of AI for this particular challenge.'

sciNote LLC is now inviting scientists interested in the Manuscript Writer add-on to visit the website, create an account in sciNote and provide feedback, to optimise AI capability and overall user experience.

One of the more interesting aspects of AI development is that the accuracy, and ultimately how useful the software is to its user community, is based on the number of people using the system and the quality of the data used to train the system.

'It depends on many factors, not only on your area of work but also how you record the data, how detailed, in what kind of format. All of these factors have an impact on how useful the end result will be for you,' said Zupancic. 'It is too early to tell, but it seems to work best with life sciences. That being said, an important part of this AI life cycle is the learning phase. AI learns how

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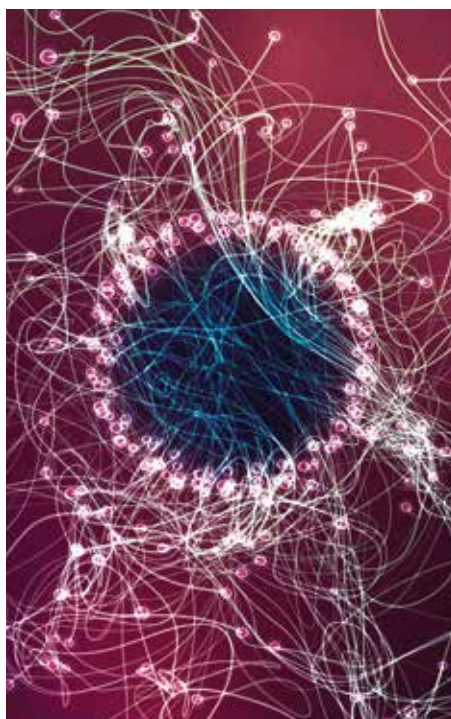
people perceive what it outputs and what changes they make, so we have high hopes that AI will get better and smarter over time.'

Zupancic also stated that the team behind the manuscript writer add-on hope it may be possible to expand the capabilities to generate patent or grant applications. 'That is the vision but how fast and how well it learns is quite difficult to estimate at this point. What AI is really good at is searching publicly available information and seeing how that relates to what you have done, and how your research fits into the boarder spectrum of scientific progress.'

AI DIAGNOSIS

One example of the research enabled through AI is Poland-based Future Processing, a member of NVIDIA's Inception programme.

The company is working to simplify the use of these tools, making the diagnosis process more affordable, accessible and accurate. Its medical imaging solutions business segment works closely with medical imaging experts, research institutions and clinics around the world to develop software that can process and analyse images.

One area of focus is dynamic contrast enhanced imaging and the analysis of computed tomography (CT) images. The company's research in this area could lead to the increased utility of CT scans in the

detection and diagnosis of lung cancer. To diagnose the disease, physicians rely on the segmentation of lesions on the lungs, using a combination of PET and CT scans. These determine the functional properties of a lesion, as well as its anatomical structure and characteristics. Lung cancer causes one in five cancer-related deaths worldwide – taking about 1.6 million lives a year – with high rates of mortality. In England more than one third of cases are diagnosed after presenting as an emergency, by which time the vast majority are already at a late stage. With the hopes of advancing the fight against lung cancer, Future Processing is working on a system that will eliminate the need for the combination of PET and CT scans. Instead, doctors would be able to make diagnoses based exclusively from CT scans.

Using convolutional neural networks, the team has shown that diagnoses from CT scans alone can be made efficient and accurate.

'Before, the segmentation of active lesions required co-registering PET and CT sequences in a time-consuming procedure,' explains Dr Jakub Nalepa, senior research scientist at Future Processing. 'In fact, we have just presented a paper where, using CNNs with CT scans, we demonstrated segmentation of a single image within minutes – and this can be accelerated further.'

This acceleration in segmentation speeds is powered by NVIDIA Tesla GPU accelerators and could make a huge difference for both doctors and patients. By automatically segmenting the lesions, radiologists can save precious time and measure lesion progress. It would also be a boon for medical sites without access to PET scanners, as they could care for their patients directly, using only a CT scanner. This is more cost-effective for medical sites, with a CT scan costing from $1,200 to $3,200, whereas a PET scan costs on average $3,000 to $6,000.

Nalepa and his team have shown that their approach reduces the rate of false positives, when studying lung data without active lesions, from 90.14 to 6.6 per cent.

In addition, to further increase the accuracy of this technique, in the future Nalepa and her team hope to apply this technology to different forms of cancer, which could make a huge difference for both doctors and patients. ●

AGE OF DISRUPTION

Robert Roe looks back over the year at technology and processes driving trends in the laboratory

While some laboratories still cling to traditional processes and paper-based workflows, there is huge potential for a new world of integrated technologies that can enable new research or increase a laboratory's throughput or capability for collaboration.

Many of these technologies have been around for some time but are now becoming a reality through a convergence between availability of applications, data, IoT technologies and AI/machine learning capabilities, all tied together through cloud computing.

While technology is not one-size-fits-all in the laboratory, there are lessons that can be learnt from informatics providers and their users who are making use of these technologies to disrupt traditional laboratory processes.

Integration is a theme that has been running throughout many different labs over the past 10 years, but in the past this focused on creating ties between instruments and LIMS/ELN systems or connecting labs with collaborating organisations.

Today integration now refers to the creation of smart laboratories, but, also, creating comprehensive software collaborations, tying disparate data streams for translational research or enabling new drugs or diagnostics and the use of AI and machine learning with life science research.

Experts in many disciplines from life sciences, to chemistry or statistics have come to broadly similar conclusions – that integration is the key to overcoming future barriers to innovation.

Integration can help break down barriers between disciplines integrating knowledge from different domains; it can be used to increase an organisation's capability for collaboration or to receive data directly from the field through the use of IoT devices.

Even at the most basic level, integrating laboratory instruments and LIMS or ELN

'It is not individual tools that will revolutionise science; it is all of these tools that are available working together, integrating and talking to each other'

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systems helps to reduce errors in data collection and processing.

Klemen Zupancic, CEO of sciNote, commented: 'It is not individual tools that will revolutionise science; it is all of these tools that are available working together, integrating and talking to each other. We need to step together as a community, promote collaboration and help each other for better science. IoT is coming in the labs and with that comes automation, traceability, transparency and reproducibility.

'It is important that we, as a community, adopt this mindset of using technology to our advantage and recognise the benefits it can bring.'

COLLABORATION THROUGH INTEGRATION

The failure of a candidate drug can cost millions of dollars in wasted research – for this reason many chemists are now turning to software that not only provides modelling or predictive capabilities but multi-parameter optimisation that can aid decision making, leading to more efficient use of resources.

For every successful compound, thousands of potential drugs fail, so it is of the utmost importance that compounds are carefully selected. Some of this risk comes from knowing which compound or series of compounds to choose for a project but, as Optibrium's CEO and company director Matthew Segall explains, uncertainty in the data – if not well managed – can lead to wasted resources.

'There are a lot of different end-points measured or calculated and many different compounds or chemistries a project will explore – but a point we emphasise, that we believe is underused, is uncertainty in data – very significant uncertainty,' said Segall.

This combination of complex parameters

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for a drug development project – the uncertainty in data, and the huge list of potential candidate drugs – were primary factors that drove Optibrium's decision to develop 'decision analysis methods to help people navigate through a very complex landscape of data,' said Segall. 'The goal is to prioritise compounds and to understand the structure activity relationships that are driving activity and other properties within the chemistry.

'Everyone knows the value of downstream failure. If you pick the wrong chemistry and push it forward, you can end up with these incredibly costly late-stage failures.' But Segall stresses this is a hidden cost, which is how many potential drugs have been missed, due particularly to the uncertainty in the data.'

This lack of understanding around uncertainty can lead scientists to make decisions that are not supported by the data that is available.

As drug development projects become increasingly complicated with multiple parameters that need to be optimised, this uncertainty can be an acute stumbling block, or, as Segall explains, it can be used to a chemist's advantage.

Drug development relies on a scientist's

'We develop a lot of technology in-house, but as a company we recognise that no one entity can develop all that is cutting edge in every area of computational chemistry and cheminformatics'

ability to manage hugely complex streams of data on any number of compounds of interest to a particular project. To keep up with all of this data and make effective decisions requires the use of sophisticated software that can alleviate some of the pressure from drug development projects.

However, some companies recognise their expertise lies in a particular area and so work to ensure complementary software packages can work together, so users have the choice to pick and choose software right for them.

'We develop a lot of technology in-house, but as a company we recognise that no one entity can develop all that is cutting-edge in every area of computational chemistry and cheminformatics,' stated Segall. 'We actively seek partners that are leaders in their space to bring the technology into their software environment and make the interaction as seamless as possible for the end-user.'

It is this acceptance that many specialist tools are required, which helps to create an environment where several highly specialised software packages can be used together to create an effective platform for drug development.

'We have partnerships with Collaborative Drug Discovery (CDD), The Edge and Certara. Their platforms are being used for ELN or storage of databases to gather, reduce and store data for drug discovery projects. We work with them to ensure that our software works seamlessly with theirs,' said Segall.

To maximise this integration, Optibrium aims to provide integration with their software and that of partner's organisations, removing the need to manually correct data formats, data exportation and formatting. 'That is a big part of our philosophy, as well as being very agnostic to where people will get their data – we want to make that process as easy as possible,' said Segall.

PRECISION DIAGNOSTICS
Precision tumour diagnostics firm Helomics established a clinical CRO operation at the start of 2017, and now offers pharmaceutical, biotech and diagnostic clients a range of services for clinical and

➤ translational research, spanning biochemical profiling, genomics, proteomics and cell biology. 'It's an extra revenue stream on top of our clinical diagnostics business, and allows us to leverage our proprietary patient-derived tumour models to help develop new therapies,' noted Mark Collins, vice president of innovation and strategy.

Integrating these technologies requires significant data infrastructure. There are now many diagnostic firms providing specialised services beyond the scope of the traditional CRO's remit.

'Modern clinical trials are highly data-driven. You are selecting cancer patients based on biomarker profiles,' said Collins. These types of specialised biomarker panels, including the patient-derived tumour assays offered by Helomics, in turn require highly flexible informatics systems that can manage, process and analyse complex data.

Helomics is overcoming this challenge by making use of its proprietary regulatory-compliant D-CHIP (dynamic clinical health insight platform) bioinformatics platform, launched in April, which applies machine learning to data from multi-omic studies in the database for insight about how patients are likely respond to drugs. Helomics has also employed Abbott Informatics' STARLIMS for the last six years as its clinical diagnostics LIMS, and is now deploying STARLIMS to drive its CRO business.

While flexibility is key, you don't want a LIMS so complicated it becomes impossible to maintain. 'That sort of 'lifeboat' software – which has every kind of functionality for every kind of eventuality – becomes a beast to maintain,' Collins said. 'Sometimes a more focused solution can work better.'

'We want to be able to set up and configure new projects within days, not weeks, and have role-based permissions that guarantee client data security and meet regulatory guidelines and rules we are subject to, such as CLIA. As a boutique CROs, we need software that is project centric to manage diverse and often complex workflows for individual clients, which is very different to the sample-centric structure of a traditional LIMS. You want to be able to keep all your project data together, and easily accessible, and available to the

'You also need seamless integration with instruments and other software, and a test ordering, scheduling and reporting system that can handle multiple types of workflow'

sponsor, in the correct format, in just about real time,' commented Robert Montgomery, Helomics manager of IT and LIMS.

PULLING IT ALL TOGETHER

Managing data is not a new concept for LIMS and ELN users but today's predictive or translational research projects require specific infrastructure that can effectively manage data on a scale not seen before.

Next-generation sequencing or predictive modelling requires more than just storing data, as seemingly disparate data streams need to be analysed together in order to provide true value to the user.

'For predictive testing based on next-generation sequencing you need to have a database that can map patients' histories, possibly in context with those of their families, including children, siblings, parents and grandparents,' explained Lisa-Jean Clifford, CEO at Psyche Systems.

'Sophisticated algorithms are used to analyse all of this information and identify the best course of treatment going forward. It's a huge ask for a laboratory information system (LIS) to be able to handle and coordinate experimental/analytical and complex data workflows and reporting requirements,' added Clifford.

Molecular diagnostic assays enable anatomic pathology laboratories to combine clinical and anatomic pathology diagnostics with a suite of molecular analyses. This enables speciality diagnostic laboratories to emerge that focus on just one, or a few, types of highly complex assays and technologies, such as next-generation sequencing, or predictive modelling.

But whatever their specialisation, all diagnostic laboratories will have some key fundamental requirements in common, Clifford noted. 'Underpinning every LIS will be a discrete database that lets you mine and compare disparate data, so that you can derive maximum value from that data.

'You also need seamless integration with instruments and other software, and a test ordering, scheduling and reporting system that can handle multiple types of workflow. A key requirement is the ability to integrate in a bidirectional manner between applications, and between instruments and applications, as well as output human-readable data. And on top of that, your data flow must be managed and communicated in a compliant, automated fashion,' Clifford concluded. ●

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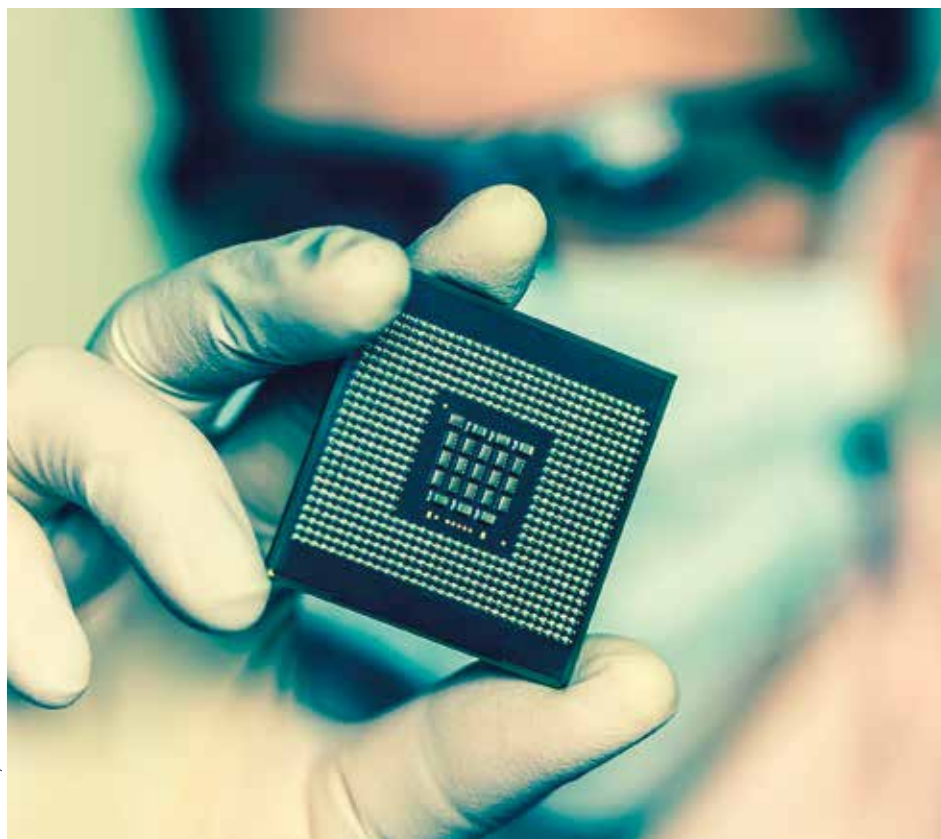
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THE FUTURE OF LABORATORY INFORMATICS

Robert Roe discusses potentially disruptive technologies and their impact on the laboratory informatics market

WHAT HAS CHANGED IN LABORATORY INFORMATICS SOFTWARE OVER THE LAST 12 MONTHS?

Laurence Painell, vice president, product management and marketing at IDBS: The cloud is becoming the norm for laboratory informatics software. Informatics providers must now have a cloud and SaaS strategy or they will not be considered in selection processes, and nearly all of the new players in the market are providing their technology as SaaS only.

Integration is an area that has really moved on this year – and you can see why: integration is the foundation of automation and is the gateway to more efficiency gains

instead of just providing a single, specific and defined answer.

Daniela Jansen, director of product marketing at Dassault Systèmes: Software and hardware vendors are moving towards a platform offering, but in most cases it is a closed, proprietary platform. Platforms can provide data continuity and traceability, and support decision making across the product lifecycle.

A platform allows for a substantially different architectural setup: small dedicated agile applications can be plugged into the platform in a modular fashion; services like reporting or instrument interfacing can

> ### 'Integration is an area that has really moved on this year – and you can see why: integration is the foundation of automation and is the gateway to more efficiency gains and insights'

be used by the different applications. This approach avoids overlap and redundancy of capabilities, improving the user experience and work efficiency. It also lowers the cost of ownership.

In addition, the enablement of cloud-based technologies and solutions is increasing. The increased adoption of cloud technology is based on both, the natural progression from legacy systems, as well as the need to transform laboratory operations. Many legacy systems are about to run out of support, so organisations are looking for replacements. Due to technological advancements, organisations have the opportunity to not only move to a newer system but to also take a new approach towards their laboratory informatics landscape.

They can move away from rigid monolithic systems that often come along with duplication in capabilities, to a platform-based approach with modular applications and common services allowing them to transform the way labs are working today. Many of the new solutions are allowing them to adapt the scale, cost and capabilities of their deployment to their current needs. In times of ongoing merger, acquisitions and divestments, this is a compelling value proposition.

Klemen Zupancic, CEO of sciNote: Software solutions are becoming more and more user-friendly, data is moving to the

cloud and the number of startups in the field of laboratory informatics is on the rise.

There is an emphasis on the user friendliness, i.e. ease of use of the software. User interfaces and overall user experience is improving with the aim to enable the users to understand the software and seamlessly integrate it in their work. The need for affordable software that adapts to a laboratory's way of work and is compatible with other platforms used today is being recognised. There are many great companies working towards that goal and we are excited to see what will happen in the following years, with the rise of Internet of Things and similar concepts.

We see that cloud providers and cloud based software is gaining recognition as well. The major benefits of it are: encrypted data storage, high level data safety and security, automatic upgrades with virtually zero downtime. The amounts of valuable digital research data are on the rise and the risks of losing the data due to lab accidents or technical issues that labs may face can be solved by storing the data on the cloud. We all rely on cloud solutions in our everyday life and we see that this trend is entering the scientific world as well.

We are also glad to see many different startups and innovative platforms rising up and working towards empowering the scientists in many different ways, whether it is data management, team collaboration, compliance, data analysis, data visualisation, virtual and augmented reality and more.

Since our main focus is in the field of electronic lab notebooks, sciNote team conducted and published one of the largest studies on user perception of electronic lab notebooks (ELNs) software. The study focuses on user perception of ELNs, market trends and market barriers. The paper gives a detailed insight not only in which direction the ELN market is moving, but also why ELN adoption is so slow.

LOOKING TO THE FUTURE, WHAT TECHNOLOGIES OR CHANGES TO WORKFLOW AND PROCESS WILL CAUSE THE BIGGEST CHANGE TO THE LABORATORY IN THE NEXT YEAR OR TWO?

Painell: Although it has been a hot topic for a long time, we need to improve the availability of insight across the research, development, manufacturing and clinical cycle by integrating and moving data

and insights. Organisations can't truly benefit from open APIs, data lakes and IoT without integration. So, from software platforms through to the management and monitoring of instruments themselves, businesses have become more aware than ever before about their need to integrate and leverage technology to do so.

We have also seen a big change in what big data really means in this industry. This is not just about velocity and volume – that is a given – it is about how to leverage all that data effectively. AI and semantic enrichment means that, increasingly, analysis is becoming more about providing insight, context and exploration of data

➤ backwards and forwards in an automated and meaningful way – translational research. This is the area where all technologies converge, by creating, linking and providing data and insight at the right place and time to impact the decision making processes in each area.

Jansen: Systems consolidation and convergence will provide laboratory users with a new experience and transformation in efficiency. Traditional systems will start being replaced by more agile user-friendly cloud-based lab informatics applications, based on a holistic open platform approach.

Organisations will start leveraging the Internet of Things (IoT) in the laboratory. This will provide them with more data – delivering more data and more insight as well as more reliable data of higher quality and integrity.

IoT will allow users to work more efficiently in the lab, as it will remove many time consuming non-value adding steps from the workflows as the 'things' are not only limited to lab equipment, but can also include wearable devices, google glasses, biometric bracelets, motion sensors, location beacons etc. At the same time, it will improve data integrity and quality as data transfer from and to the devices is automated. And through the introduction

'Software and hardware vendors are moving towards a platform offering, but in most cases it is a closed, proprietary platform'

(more) sensors labs will be able to generate more data faster that can improve and accelerate decision making.

The adoption of IoT technology depends largely on the maturity of the organisation and the industry, as well as the kind of laboratory. While some companies are only now replacing paper in the lab and digitalise their processes, other companies have already evaluated and adopted IoT. Generally speaking, the research labs of innovative life science organisations are spearheading the crowd and leveraging the technology today, while other industries and regulated labs still might take years to step into the 'lab of the future'.

Zupancic: We definitely see the benefit for the scientists in the future integrations between the platforms that are used in labs today. This correlates with the concept of IoT. For example, Gilson inc and sciNote are working on introducing the IoT platform, which would enable scientists to do various things such as: setting up your experiments in sciNote electronic lab notebook, adding

the lab instruments you use, connecting your pipettes to track your progress etc.

It is not individual tools that will revolutionise science, it is all of these tools that are available working together, integrating and talking to each other. sciNote is only a piece of the puzzle and we need to step together as a community, promote collaboration and help each other for better science. IoT is coming in the labs and with that comes automation, traceability, transparency and reproducibility.

It is important that we, as a community, adopt this mindset of using technology to our advantage and recognise the benefits it can bring. Another interesting aspect is the introduction of artificial intelligence and machine learning – software that can understand the need of the scientist and can be a helpful tool.

IN YOUR OPINION, WHAT ARE THE DRIVING FACTORS FOR CHANGE OR INNOVATION IN THE LABORATORY?

Painell: The need to increase efficiency and throughput in order to bring a step change in the time and cost of bringing new products and therapies to market is the primary driver. Linked to this is the diminishing returns of the old manual ➤
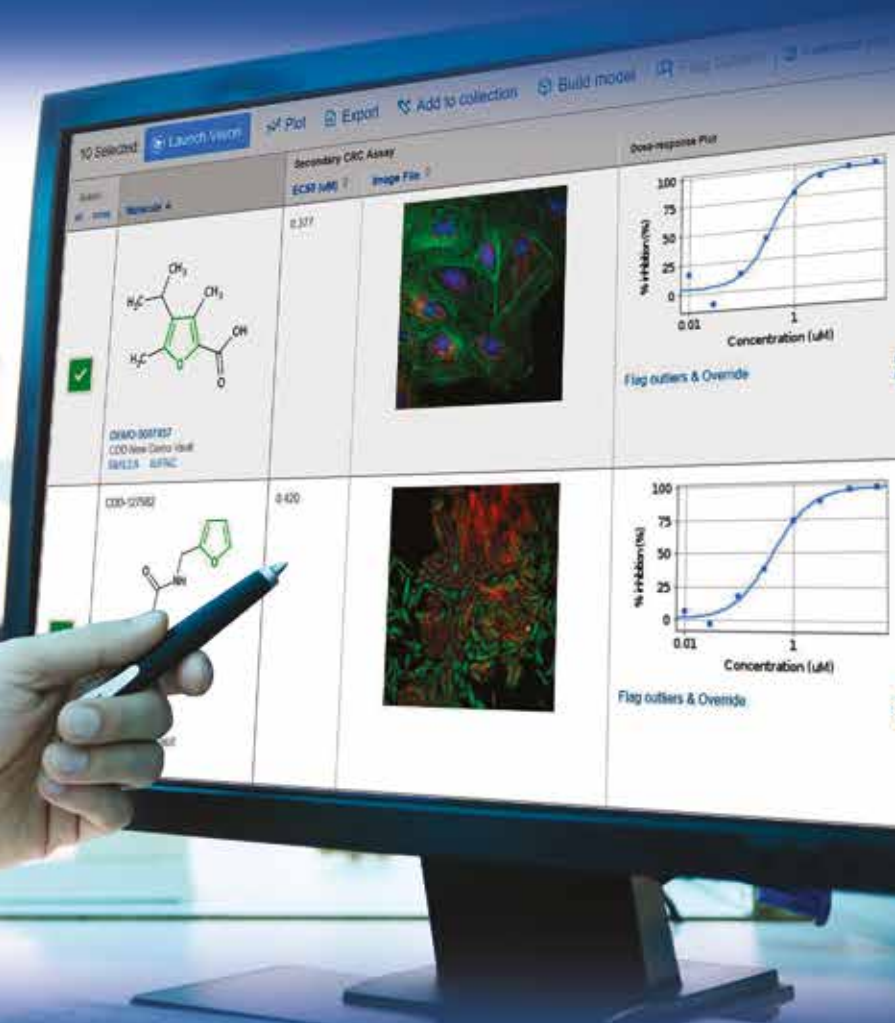
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approaches and the intrinsic need to automate and innovate for a competitive advantage.

Finally, the sheer volume of data to wade through needs different automated approaches beyond what a human can manage, and this requires new technology.

Jansen: In conversations with our customers, we have identified time-to-market being the ultimate driver for change.

Personalised health and the desire for more precision therapies is changing the way how they are developed. Knowledge capitalisation is basic for leveraging of new and existing knowledge in the lab and next-gen manufacturing, with moving from large batches towards continuous manufacturing having a deep impact on the analytical instruments and methods used, as well as on the related data analytics. And total quality management efforts are attempting to make compliance and quality an asset, instead of a cost.

Laboratory informatics need to allow users to work not only in a more efficient and cost-effective way, while remaining compliant, they also need to provide the flexibility to adapt to completely new ways of working. They need to be able to deliver contextualised data in real-time for faster decision making. Machine learning

'It is not individual tools that will revolutionise science, it is all of these tools that are available working together, integrating and talking to each other'

technology does not need to be adapted, it just needs to be used in the right way. It is more about identifying the right data and providing the data in the right format to be leveraged. Data needs to be standardised and contextualised for meaningful outcomes. Dassault Systèmes does provide the tools today, and in order to help our customers to leverage their data, we are actively engaged in data standardisation projects of consortia like Allotrope, of Pistoia Alliance.

Zupancic: Labs need to cope with the ever-increasing amounts of digital data generated while conducting research. Keeping track of data, preventing data loss and data management, in general, are the major factors that influence labs' need to adopt digital solutions. sciNote's aim is to help out with that and contribute to the more reproducible science.

There is also an increasing need to collaborate. Research that results in high-ranking scientific publications is in most

cases conducted by various teams working together from different locations, and even in different languages. Platforms that enable seamless team collaboration within an institution, and with external partners, can play an important role as well.

sciNote electronic lab notebook, for example, besides helping labs organise work on projects, enables teams to collaborate and share comments and use the same protocols within protocol repositories.

ARE THERE ANY ADDITIONS OR IMPROVEMENTS REQUESTED BY YOUR USERS?

Painell: The main area our customers are interested in is the integrations space and the ability to provide data out of the system, then pull derivative data and analysis back in at the point of use. This is linked to all the cloud-based technologies such as IoT, AI, semantics and automation that can impact this process. To help, many of our legacy customers are deciding to move to our cloud platform, to ensure their technology is future-proofed, enabling them to move capital from maintaining systems to driving innovation.

Jansen: A focus for many organisations is to provide their users with intuitive, user-friendly interfaces. This increases the user adoption and makes operations more efficient. We also see an increasing demand in cloud-based technology and solutions. The ability to integrate is a key request and an open platform is often considered as the right approach to achieve this. This will replace costly bespoke point-to-point integrations and at the same time provides the ability to integrate existing and legacy systems into the lab informatics landscape.

Zupancic: Currently AI is working on open access articles. The biggest desire expressed by our users, besides smaller improvements in the user experience, was to include non-open-access research articles in the literature. We are receiving valuable feedback from the users and are taking into account their opinion to improve the manuscript further, to become an even better, helpful tool for the scientists.

The aim is to shorten the time to gather data and start writing the manuscript. We would really like to point out we are open to discussions, open to receive opinions and feedback and would like to invite all interested scientists to test the Manuscript Writer and share feedback, ideas, concerns and comments with our team. ●

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SYNERGY BETWEEN MAN AND MACHINE

The failure of a candidate drug can cost millions – so many chemists are turning to software that provides modelling capabilities and multi-parameter optimisation

Drug development is a huge business, as successfully trialled drugs can generate billions of dollars in revenue. But, for every successful compound, thousands of potential drugs fail. Software has been used to compliment and accelerate drug design for several years, but this still leaves chemists with complex and risky decisions to make when selecting potential compounds.

Some of this risk comes from knowing which compound or series of compounds to choose for a project but, as Optibrium's CEO and company director Matthew Segall explains, uncertainty in the data – if not well managed – can lead to wasted resources.

'There are a lot of different end-points measured or calculated and many different compounds or chemistries a project will explore – but a point we emphasise, that we believe is underused, is uncertainty in data – very significant uncertainty,' said Segall.

This combination of complex parameters for a drug development project – the uncertainty in data, and the huge list of potential candidate drugs – were primary factors that drove Optibrium's decision to develop 'decision analysis methods to help people navigate through a very complex landscape of data,' said Segall. 'The goal is to prioritise compounds and to understand the structure activity relationships that are driving activity and other properties within the chemistry.

'Everyone knows the value of downstream failure. If you pick the wrong chemistry and push it forward, you can end up with these incredibly costly late-stage failures.'

But Segall stresses this is a hidden cost, which is how many potential drugs have been missed, due particularly to the uncertainty in the data.' This lack of understanding around uncertainty can lead scientists to make decisions that are not supported by the data that is available.

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MULTI-PARAMETER OPTIMISATION

As drug development projects become increasingly complicated with multiple parameters that need to be optimised, this uncertainty can be an acute stumbling block, or, as Segall explains, it can be used to a chemist's advantage.

'What is really unique about the approach that we use, is that we explicitly propagate the effect of that uncertainty through to the decision that is being made. We have published numerous papers on this. One of the things

'This uncertainty can be an acute stumbling block'

that we observed in a paper published in *Drug Discovery Today* around 2012 was the cognitive biases involved in decision making.

'This is something that has been well explored by experimental psychologists that everyone, including scientists, find it very difficult to make decisions on complex data

when there is a lot of risk and uncertainty involved. Helping people recognise and use uncertainty appropriately is very important and unique to what we do,' said Segall.

COMPLEMENTARY SOFTWARE

Drug development relies on a scientist's ability to manage hugely complex streams of data on any number of compounds of interest to a particular project. To keep up with all of this data and make effective decisions requires the use of sophisticated software that can alleviate some pressure from drug development projects.

However, some companies recognise their expertise lies in a particular area, and so work to ensure complementary software packages can work together, so users have the choice to pick and choose software right for them.

'We develop a lot of technology in-house, but as a company we recognise that no one entity can develop all that is cutting edge in every area of computational chemistry and cheminformatics,' stated Segall. 'We actively

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Tyler Olson/Shutterstock.com

seek partners that are leaders in their space, to bring the technology into their software environment and make the interaction as seamless as possible for the end user.'

It is this acceptance and willingness to use the best tools, that creates an environment where several highly specialised software packages can be used together, to create an effective platform for drug development.

'We have partnerships with Collaborative Drug Discovery (CDD), The Edge and Certara. Their platforms are being used for ELN or storage of databases to gather, reduce and store data for drug discovery projects. We work with them to ensure that our software works seamlessly with theirs,' said Segall.

To maximise this integration, Optibrium aims to provide integration with their software and that of partner's organisations, removing a need to correct data formats, data exportation and formatting. 'That is a big part of our philosophy, as well being very agnostic to where people will get their data – we want to make that process as easy as possible,' said Segall.

VISUALISATION IS NOT ENOUGH
Managing all this data requires sophisticated data visualisation tools that can more intuitively display complicated data that is produced or collated throughout drug development projects. While many companies have their way of visualising data, Optibrium has decided to employ a card system that allows users to quickly group compounds with similar properties. However, Segall stressed that it is

not just the visualisation tools themselves, but the combination of visualisation in tandem with support for decision making and data analysis that creates the most benefit for users.

'If you think about five parameters you might be interested in, you could have a three-dimensional scatter plot: X, Y, Z. You end up with these incredibly complex 3D plots that look really great, but frankly, when you do this with real data it is very hard to make a decision – even before you take the uncertainty into account,' said Segall.

This is further complicated by the level of expertise of the user, as increasingly these projects include non-computational experts that may have little experience with this kind of data analysis. 'Often it is a medicinal chemist or biologist making decisions about this data and using the tools,' said Segall. 'Having some very complex software windows buttons or even asking scientists to work from the command line is just not good enough these days.'

This reality requires that software developers streamline software for non-domain experts that want to access the data but do not necessarily have the programming skills or expert chemical knowledge that a computational chemist would possess.

'Very often you may run a complex algorithm that clusters compounds together or analyses "match pairs" or "activity cliffs" to understand the structure activity relationships in a chemical series. Most of these methods produce a great big table of numbers. Poring over that table and trying to understand what they are telling you about the structural modifications, or impact

on properties and so on, is very challenging.'

'We pioneered a visualisation tool we call 'Card View – and, as the name suggests, it represents each compound on a card that is arranged on an infinite desktop that provides a very nice way to show the relationships between compounds,' said Segall.

He explained that, in many cases, a chemist is interested not in a single compound, but a series that they can take forward. 'This algorithm tries to group compounds that represent a series, and the card view represents each of these series or clusters of compounds as a stack of cards.

'The output of these complex algorithms can be represented in this environment more visually, so key patterns just jump out at you. This could be a small change in structure that drives a big change in activity – clearly, this is something scientists need to understand in order to be able to take the next step in designing new compounds,' said Segall.

Optibrium has designed its software to be as easy to use a possible, so data can be interpreted as intuitively as possible. 'This allows you to apply these methods, and it allows users to understand what those methods

'This reality requires that software developers streamline software for non-domain experts'

are telling you about your data very quickly. This is absolutely key to the effective use of these technologies,' said Segall.

However, it is not yet time to step back and let the computer take over. 'The problem with these algorithms is they never completely agree with a chemist's view of what a chemical series might be,' Segall added.

A crucial point is that software must work with the expert; it may be beneficial to use a clustering algorithm to help define a particular series but it is important an expert can still use their experience to fine-tune software predictions and refine the overall results.

'There are always artefacts of the algorithm that do not agree with a chemist's eye', stated Segall. 'In our system you can see the output but then you see two clusters that are very similar, in the chemist's opinion part of the same series, you can simply pick it up and drop one on top of the other and the software will show you the updated analysis.'

In an increasingly competitive and complex industry, it is this synergy between expert and machine that will be crucial to future drug discovery projects. ●

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DATA LAKES AND CLOUD COMPUTING

Data types used are advancing from the simple text formats of old, writes Paul Denny-Gouldson

For research and development organisations, the rise of instrument and process automation is leading to a phenomenal increase in the amount, variety and complexity of scientific data that is gathered. All this data needs to be made available so it can be integrated into projects and new scientific approaches, both now and in the future. The requirement to be useable has been growing over the past decade and is reaching a critical point.

Instrument data is driving new science and, as organisations move to large image-based and high-density data structures to support their work e.g. phenotypic screening, the data types used are advancing from the simple text formats of old. To ensure these new data types are (re)useable in R&D and are consumable by existing and emerging technologies such as Artificial Intelligence (AI) and machine learning, the data has to be accessible, clean and adequately tagged with metadata. These high value 'data lakes' can become silted up and quickly turn into swamps if data is not properly tagged with all relevant contextual information – projects, tested molecules, results, downstream use, conclusions, derived data, related data etc.

Designing and keeping data lakes in good health requires constant work and effort, but cloud computing strategies like new storage (S3) and adaptive indexing technologies (NOSQL, Triples) will help. While some people think of data lakes, or even data, as a static picture after it has been captured, in reality, data needs to be continually enriched and augmented with learnings. Often, informatics organisations consider the data as the record – and in some cases, it is – but it does not have to be cast in stone and 'stored'. Intellectual property (IP) records can be captured and stored in other systems – while the working data is stored in other data structures and 'put to work'.

'Designing and keeping data lakes in good health requires constant work and effort'

Enrichment is a hot topic in the pharma informatics domain. We have seen the emergence of many tools that all essentially do the same thing: make data more consumable or discoverable by scientists and computers. Semantic enrichment or natural language processing has been around for many years and has shown good benefits particularly in the healthcare domain, where it is used to extract and normalise data from clinical trials.

In Pharma R&D, the enrichment approach is gaining traction with the prevalence of new technologies and commercial offerings. Ontological, taxonomical and semantic tagging are set to become mainstream as the technology and application integration becomes easier and vendors deploy their tools in the cloud.

A corporate data lake must be defined and viewed as the place to go to find, search, interrogate and aggregate data – making it easier for data scientists to investigate and build data sets for their work. Find and search are two separate concepts here – one is where you know what you are looking for – the other is when you don't know what you are looking for – and want to explore the data.

A data lake must be integrated into all systems that are part of the data lifecycle, crudely: creation, capture, analysis and reporting, so that all aspects of the R&D data landscape can be consumed and leveraged, re-indexed and continually enriched. A data lake should not be viewed as a regulatory or intellectual property (IP) store – it needs to be a living ecosystem of data and indices that adapts to the needs of the science and business.

Pharma is looking to shift to a situation where it can be much more data-driven. But first, data must be discoverable for scientists, data scientists and the applications they use. These data jockeys need access to vast quantities of highly curated data to do their jobs – and data lakes are likely the best answer.

AI and other tools like deep learning, augmented intelligence and machine learning all need a similar set of inputs to data scientists – lots of well annotated data. Adding more tags and metadata to a set of data is something that sits at the heart of what a true data lake should be – and the impact could be far reaching. The data volumes are huge and this leads to a couple of issues. Where should this data be stored? And how can it be made searchable? This is where the cloud helps.

Whilst searching is often discussed in a macro sense – Google-type searching for example – the questions that scientists want to answer are not always 'keyword' or phrase based. Scientific questions are far more intricate and need more than just typical text indices: they require fact-based searching and relationship-based searching too.

This requirement means data must be treated as a living organism and structured in a way that can handle tricky questions. This means each of the 'index' types need to be aware of each other so you can jump concepts, while also remaining easily updatable for when new data types are introduced.

This is not easy, but rapid progress is being made through the deployment and use of cloud storage, semantic enrichment, alternate data structures, data provisioning, data ingestion, analysis tools and AI. All these technologies have a part to play and their level of use depends on the questions being asked of the data. The cloud is the best way to leverage these technologies in a cost effective and consumable manner – vendors just need to make sure their applications are prepared. ●

Paul Denny-Gouldson is VP, Strategic Solutions, at IDBS

TALES FROM THE LAB

Tim Gillett rounds up some of the top stories of late 2017

IDBS acquired by Danaher

IDBS, a provider of scientific informatics platforms and software, announced in November that it had been acquired by the Danaher corporation.

IDBS joined Danaher's Life Sciences platform, which includes such businesses as SCIEX, Phenomenex, Beckman Coulter Life Sciences, Pall, Leica Microsystems and Molecular Devices.

'IDBS' informatics solutions integrate insights derived using scientific instruments from various vendors and from many different disciplines, enabling better and faster scientific and business decisions, ultimately affording patients faster and better therapies. IDBS opens a new generation of vendor agnostic information-based digital services for Danaher and makes the digital lab a reality' said Rainer Blair, Danaher executive vice president.

IDBS will help provide the foundation for a portfolio of life sciences informatics and knowledge management solutions that will accelerate the speed of discovering, developing and producing new drugs and therapies.

'Danaher is a global science and technology innovator and shares our purpose of helping customers solve complex challenges and improving quality of life around the world. Their trusted brands hold unparalleled leadership positions in diagnostics, life sciences, dental, environmental and applied solutions' said Neil Kipling, founder and CEO at IDBS.

'By linking the IDBS knowledge management platform with their comprehensive instrument coverage, it will create a "data spine" that connects instruments, creating opportunities for new information-based services and the realisation of the digital lab of the future. We have found what I believe to be the right home for our business, and it is incredibly exciting to know that IDBS will form the foundation of Danaher's new life science informatics business,' Kipling added.

Heidelberg University Hospital joins oncology programme

Thermo Fisher Scientific signed an agreement with the Institute of Pathology Heidelberg (IPH) to establish its Centre of Molecular Pathology at Heidelberg University Hospital as the newest member of the Next Generation Sequencing Companion Dx Center of Excellence Program (COEP).

The initiative focuses on forging strategic collaborations with European organisations that can lead studies using Thermo Fisher's Oncomine portfolio of research panels, destined for development as companion diagnostics to accelerate oncology research.

Working in collaboration with pharmaceutical partners and Thermo Fisher, the IPH Center of Molecular Pathology, headed by Dr Albrecht Stenzinger, will conduct studies and trials under the leadership of Professor Peter Schirmacher, director of the Institute of Pathology, Heidelberg University Hospital.

'The initiative focuses on forging strategic collaborations with European-based organisations'

'Molecular pathology is a multidimensional and rapidly evolving field where high-level expertise ranging from genetics to trial design and close collaborations are the key for innovation that ultimately benefits patients,' Stenzinger said. 'Liquid biopsies, genetic biomarkers guiding immunotherapy approaches and clinically exploitable genetic themes that are shared by many cancer types, such as DNA repair deficiency, are currently the most exciting and promising areas for diagnostic applications and will keep us busy in assay development, daily diagnostics and clinical trials.'

The Institute is also the site of Germany's

Heidelberg University Hospital

largest tissue biobank, featuring a sophisticated laboratory information management system that has incorporated Thermo Fisher's Ion Torrent bioinformatics software. Coupled with its biomarker development and translational diagnostics programme, the IPH is uniquely positioned as an ideal Thermo Fisher partner to develop NGS-based diagnostics.

Heidelberg University Hospital is one of the largest medical centres in Europe, with its campus shared with the German Cancer Research Center. It is characterised by its pursuit of developing innovative methods in diagnosis and treatment, while its clinical research arm has long been an early adopter of leading technology.

'With an ever increasing number of drugs coming to market, scalable detection of clinically relevant biomarkers that enable targeted therapies and the use of agents modulating the immune system will be the key for successful implementation of precision oncology,' said Joydeep Goswami, president of clinical next-generation sequencing and oncology for Thermo Fisher Scientific. 'We are committed to companion diagnostic development and will continue on this path with leading global organisations.'

Medley Genomics and Transformative AI receive awards

In October, two startup companies were recognised by the Pistoia Alliance for their work accelerating research into precision cancer therapies and advancing deep learning in healthcare.

The Pistoia Alliance, a global, not-for-profit alliance that works to lower barriers to innovation in life sciences research and development, has announced the winners of its 2017 President's Startup Challenge: Medley Genomics and Transformative AI.

The grand prize winner, selected by a panel of seven industry judges, is Medley Genomics. The audience vote winner, chosen by The Pistoia Alliance's members, is Transformative AI.

The two startups were chosen from five finalists, shortlisted from 20 challenge entries from the US, Europe and India, following a live 'Shark Tank' pitching event at The Pistoia Alliance's 2017 member conference in Boston. Both Medley Genomics and Transformative AI will receive an award of $20,000 and six months of one-to-one mentorship from a Pistoia Alliance member; in addition to one year's access to Elsevier's

R&D Solutions portfolio, and to Clarivate Analytics' life-science assets. All five finalists receive a $5,000 award and one year's free membership to The Pistoia Alliance.

'I congratulate Medley Genomics and Transformative AI on their wins – two dynamic startups in the field of data analytics, deep learning and AI. Both teams pitched innovative solutions that will

'Medley Genomics is a US startup dedicated to addressing the challenges of genomic heterogeneity'

ultimately lead to better patient outcomes, through the pioneering application of advanced technology,' commented Dr Steve Arlington, president of the Pistoia Alliance.

'All five finalists of this year's President's Challenge are examples of the exciting, inventive mindset that is a vital feature of the life sciences sector. As pharmaceutical and healthcare companies struggle to make use of the deluge of data flooding the industry, startups such as these will be critical in helping to unlock the value of data that leads

to breakthrough discoveries and precision therapies for patients,' added Arlington.

Medley Genomics is a US startup dedicated to addressing the challenges of genomic heterogeneity in the diagnosis and treatment of complex diseases – with an initial focus on cancer. Through advanced data analytics of molecular sequencing data, Medley Genomics seeks to better inform initial therapeutic decisions, including combination therapies, resulting in significant benefit in patient outcomes.

Transformative AI is a UK startup that uses cutting-edge artificial intelligence and novel analysis techniques also employed at CERN, the European Organisation for Nuclear Research. The team's mission is to transform the treatment of serious medical conditions by collecting and translating clinical data into real-time, predictive assessments that will guide the actions of patients and healthcare providers.

The President's Startup Challenge is an annual award that rewards the companies that are transforming life sciences and healthcare.

Certara reports shows VK modelling could provide faster, safer route to more effective anti-viral drugs

Certara, a specialist in model-informed drug development, announced in September that it has developed a report on viral kinetic (VK) modelling to accelerate research into drug-resistant strains of influenza. The review was published in *Current Pharmacology Reports*.

As the number of drug-resistant influenza strains grows, researchers are searching for better ways to develop safer, more effective anti-viral drugs. 'This paper describes how mathematical models, and especially viral kinetic models, can increase researchers' knowledge of influenza biology and antiviral pharmacology,' said co-author Professor Carl Kirkpatrick, director of the Centre of Medicine Use and Safety (CMUS) at Monash University, Melbourne, Australia.

'For example, population-based

viral kinetic models can identify sources of variation between and within individuals, helping explain why some influenza patients become sicker than others,' said Professor Kirkpatrick.

The United States Centers for Disease Control and Prevention estimates influenza has caused between 9.2 million and 35.6 million illnesses, 140,000 to 710,000 hospitalisations, and 12,000 to 56,000 deaths annually since 2010.

These viral kinetic models have been used to support the dose optimisation of neuraminidase inhibitors and also the clinical development of monoclonal antibodies that are currently being investigated as potential influenza therapies.

Viral kinetic models use mathematical equations to describe the changes in viral load with time in an infected patient.

They can provide valuable information about the cell infection rate, viral production rate and viral clearance rate.

'By combining viral kinetic models with PK/PD models, researchers can quantify drug effects based on their mechanism of action and evaluate in silico the efficacy of specific drug combinations. Together, these models can be used to explore how antiviral drugs reduce influenza symptoms and viral load,' said lead author, and Certara executive director for consulting services, Mark Lovern.

'PK/PD models are also starting to be coupled to epidemiological and health economic models to assess the effectiveness of public health treatment strategies. Epidemiologic models can quantify changes in susceptible, exposed, infected and recovered

patients during an outbreak, and assess the ease with which an infectious disease can be transmitted among them,' added Suzanne Minton, PhD, Certara scientific communications manager and co-author.

'Health economic models then determine the relative change in quality-adjusted life-years based on the predicted number of infected patients. We anticipate that this pharmacology-to-payer framework will inform decisions regarding managing existing and emerging pathogens on a global scale,' said Patrick Smith, PharmD, chief scientific officer at Certara Strategic Consulting Services and co-author.

The paper, Applications of Influenza Viral Kinetic Modeling in Drug Development, can be found at https://link.springer.com/article/10.1007/s40495-017-0104-3.

TAKING AIM AT LIMS SOFTWARE

Robert Roe looks at the use of precision medicine and its potential impact on laboratory informatics software

The evolution of laboratory practices is driving new workflows and opportunities for research. Combining modern laboratory informatics infrastructure with genomic data that is properly collected and catalogued can enable laboratories to engage in precision medicine.

The concept of precision medicine and personalised medicine have been around for some time but it is the convergence of cheap genetic screening and the availability of modern LIMS infrastructure which enables data to be properly collected, stored and shared is opening up opportunities for precision medicine projects that were not possible previously.

WHAT IS PRECISION MEDICINE?

Precision medicine refers to the tailoring of medical treatment to the individual characteristics of each patient. It does not mean the creation of drugs or medical devices that are unique to a patient, but rather the ability to classify individuals into subpopulations that differ in their susceptibility to a particular disease, in the biology or prognosis of those diseases they may develop, or in their response to a specific treatment.

The concept of personalised or precision medicine is not new but has required computational and data resources to match the requirements of such projects. It is necessary to build up large databases of genomic data that can then be used to develop an understanding of how specific treatments might be used to fight disease.

Four years ago Dr Margaret Hamburg, Commissioner of Food and Drugs for the FDA, noted that 'In just the last two years, the FDA approved four cancer drugs for use in patients whose tumours have specific genetic characteristics that are identified

'Clinicians have long observed that patients with similar symptoms may have different illnesses, with different causes; and similarly, that medical interventions may work well in some patients with a disease but not in others with apparently the same disease'

by a companion diagnostic test. Last year, FDA approved a new therapy for use in certain cystic fibrosis patients with a specific genetic mutation. Earlier this year, three-dimensional printing was used to create a biodegradable tracheal splint for treating a critically-ill infant,' stated Hamburg.

'Clinicians have long observed that patients with similar symptoms may have different illnesses, with different causes; and similarly, that medical interventions may work well in some patients with a disease but not in others with apparently the same disease. What is new is that advances in

a wide range of fields from genomics to medical imaging to regenerative medicine, along with increased computational power and the advent of mobile and wireless capability and other technologies, are allowing patients to be treated and monitored more precisely and effectively, and in ways that better meet their individual needs,' added Hamburg.

PRECISION MEDICINE INITIATIVE

While precision medicine has been slowly gathering pace, the development of this paradigm was accelerated by the US government by President Barak Obama, who announced the Precision Medicine Initiative in his 2015 State of the Union address.

During the address, President Obama announced that he was launching the initiative with a $215 million investment from the President's 2016 Budget.

The Initiative is a research programme set up to drive the development of precision medicine projects involving the National

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The Precision Medicine Initiative has both short-term and long-term goals. The short-term goals involve expanding precision medicine in the area of cancer research. Researchers at the National Cancer Institute (NCI) hope to use an increased knowledge of the genetics and biology of cancer to find new, more effective treatments for various forms of this disease.

The long-term goals of the initiative focus on bringing precision medicine to all areas of health and healthcare on a large scale. To accomplish this goal the NIH launched a study – known as the All of Us Research Program – which plans to profile genetic data of at least one million volunteers from around the United States.

Participants will provide genetic data, biological samples, and other information about their health. To encourage open data sharing, participants will be able to access their health information, as well as research that uses their data during the study.

Researchers will use these data to study a large range of diseases, with the goals of better predicting disease risk, understanding how diseases occur and finding improved diagnosis and treatment strategies.

LEVERAGING INFORMATICS INFRASTRUCTURE FOR PRECISION MEDICINE

As interest in precision medicine grows, informatics companies are beginning to develop or adapt laboratory informatics software so that it can be used to gather, store and analyse data for precision medicine projects.

Core Informatics and PerkinElmer have both developed solutions specifically for the collection and processing of genomic or next generation sequencing (NGS) data and these systems can be leveraged by users that want to start developing precision medicine research. As with other areas of laboratory informatics, choosing the right LIMS can keep your lab running smoothly but selecting technology that is not up to the job can reduce the efficiency of the laboratory staff.

Core is relying on the flexibility of its LIMS to add the ability to add new tests, reagents and instruments. Core also points out that if labs decide to transition to diagnostics from research, the LIMS would need to adapt there too, by

supporting validation or other procedures.

Core is now offering NGS researchers its platform as a service (PaaS), which offers an app based marketplace with several apps aimed at genomics workflows. The genomics solution is comprised of modular applications available in the marketplace. The applications can be put together, without any custom code, in an order which fits the workflow in your lab.

The idea here is that the Platform for Science can be tailored and adapted to the way the lab works. Allowing users to capture and track NGS data easily and accurately.

Chrisanne Wnek, genomics application specialist at Core Informatics: stated in

KuLouKu/Shutterstock

'Some tests are detecting a single gene associated with disease and others look for multiple genes associated with a disease'

a blog post for the firm: 'Personalised medicine relies heavily on the use of genetic biomarkers. Genetic biomarkers can be used to indicate a disease state or a normal biological state, and they can be measured accurately and the results can be reproduced.

'There are many labs that perform this type of genetic testing. Most of the labs developed tests found in a CLIA lab are used for some form of personalised medicine. There are tests that can detect genetic variants associated with a single nucleotide base change, these are called SNPs (Single Nucleotide Polymorphism). Some tests are detecting a single gene associated with disease and others look for multiple genes associated with a disease,' stated Wnek.

'So, how do we find these genes associated with disease? Gene sequencing. Gene sequencing from traditional Sanger or Next Generation Sequencing (NGS) methods gives

us the ability to uncover the SNPs, the single genes, and the multiple genes associated with disease and can put researchers on the right track to finding a therapeutic to treat it,' Wnek concluded.

PerkinElmer has also developed a platform for precision medicine workflows called 'Signals for Translational'. PerkinElmer released a white paper earlier this year that detailed the cost effectiveness of this system, when compared to other frameworks for precision medicine.

The white paper notes that while the goal of translational is to develop the right treatment, for the right patient, at the right time, the reality of supporting these processes, in practice, requires significant effort.

Precision medicine or translational research requires software that can integrate, access, analyse, and visualise wide and disparate datasets, within and across firewalls, to bring new scientific discoveries to patients as quickly as possible.

'By hosting data in the cloud and provisioning access for the scientists, PerkinElmer's Signals for Translational addresses these requirements at a significantly reduced cost compared to the tranSMART platform and custom built-for-purpose solutions, states the white paper.

PerkinElmer claims that using their system is less than half the cost of a custom deployment and a third of tranSMART installation cost.

There are several areas where these savings are made, including licensing software, purchasing hardware and web services and loading and managing data within the system. PerkinElmer state that their software reduces overall costs by significantly speeding up the time to load data – it is approximately half that of tranSMART.

As laboratories adapt to make use of precision medicine technology, it is likely that the number of software solutions will continue to increase, but as data is central to the ability to efficiently conduct research using precision medicine, it is likely that these cost factors will become increasingly important.

As noted earlier, there are already plans to create cohorts of more than 1,000,000 patients. Being able to access and search through all of this genomic data will require informatics infrastructure that has been specially designed for use in precision medicine. ●
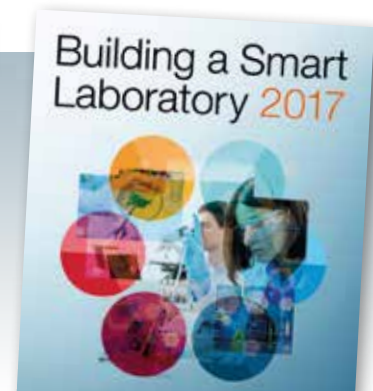
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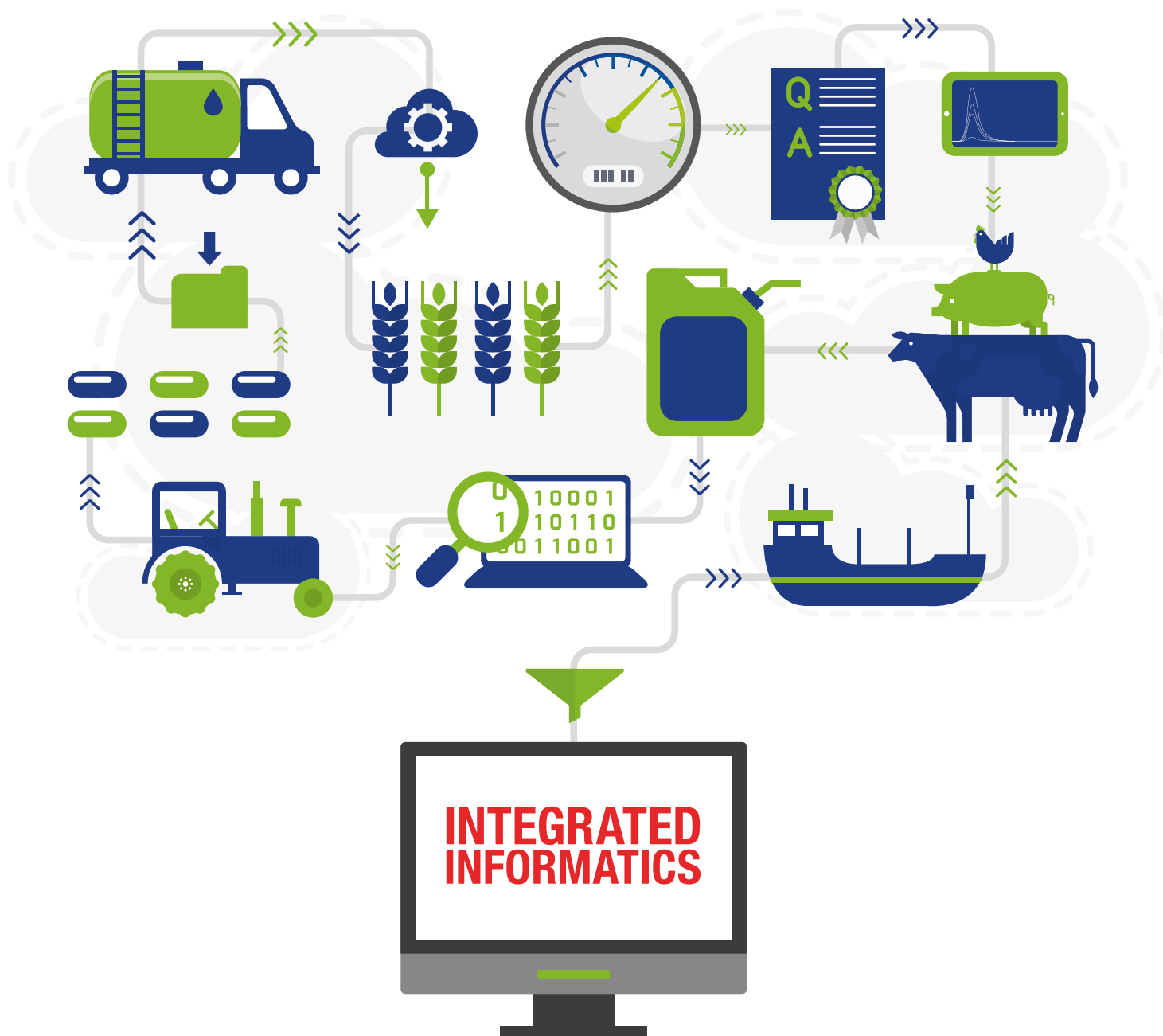
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