Laboratory Informatics Guide 2021

Understanding the needs of the laboratory

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EDITORIAL AND ADMINISTRATIVE TEAM
Managing Editor: Tim Gillett (editor.scw@europascience.com)
Editor: Robert Roe (robert.roe@europascience.com)
Feature Writer: Sophia Ktori
Circulation/readership enquiries: subs@europascience.com

ADVERTISING TEAM
Advertising Sales Manager: Mike Nelson (mike.nelson@europascience.com)
Tel: +44 (0) 1223 221039 Fax +44 (0) 1223 213385

DESIGN TEAM
Production manager: David Houghton (david.houghton@europascience.com)
Senior graphic designer: Zöe Andrews (zoe.andrews@europascience.com)

CORPORATE TEAM
Managing director: Warren Clark
Web: www.scientific-computing.com

It is clear that Covid-19 has had a significant impact on laboratory operations. Even for laboratories that are not working directly on Covid-19 testing, drug and vaccine development, restrictions on laboratory space and access to equipment are putting a significant burden on scientists.

Thankfully, laboratory informatics software tools can shoulder some of that burden by providing a platform for remote access, automation of laboratory operations or by providing access to data and tools for collaboration to keep scientists working productively.

This issue of the Laboratory Informatics Guide aims to highlight the working practices of researchers, and highlight technologies and tools that can help overcome the challenges that scientists face in the laboratory. We start with an in-depth look at the work that has been going on around the world to fight against the pandemic on page 4.

We've a series of vendor predictions for the year ahead beginning on page 10. Thie features experts from several informatics software providers discussing the role of automation, cloud-based systems, remote access tools, and other technologies that can ensure laboratory productivity, despite reduced access for many users.

Starting on pages 16 and 20 are two interviews with research leaders. The first features the European Bioinformatics Institute and the second takes a look at the Wellcome Sanger Institute. The interviews share some of the work that has been conducted on Covid-19 and the importance of open science in fighting the pandemic.

Digital transformation in the laboratory is the focus on page 22, as Sophia Ktori talks to informatics software providers about the technologies and tools scientists can use to advance lab operations.

On page 28 we consider how advances in computer vision, combined with AI computing, are helping pathologists more accurately identify subtypes of cancer. And finally, Thermo Fisher's Darren Barrington-Light details the importance of cloud-based solutions on page 30.

Covid-19 changes the laboratory landscape

Demand for testing and requirements for remote working tools drive changes in the laboratory

The pandemic has defined the development of laboratory software and technologies, as collaboration and remote working tools become requirements to a productive laboratory.

It has increased demand for laboratory services in areas such as testing, genomics studies and vaccine and drug development. However these demands must be met with restrictions on laboratory space and more demanding project timelines.

To facilitate this research and scale-up testing capabilities, laboratory scientists are using laboratory information management system (LIMS) and electronic laboratory notebook (ELN) software to help manage collaborative work, and promote reduced-capacity working environments in the laboratory.

Patrick Rose, digital science product manager at Thermo Fisher Scientific, notes that there has been a pivot in the tools used in laboratories due to Covid-19. 'The labs are starting work leaner, they are having to collaborate with other partners, other contract research organisations [CROs] to help battle the pandemic and find the vaccine.

> **"The tooling and solutions, like the LIMS that we offer, become more pivotal and critical"**

'What we are seeing is an increased need to work remotely due to alternating days, slimmer shifts trying to minimise the time people are in there together. But, they still need to work on their results, gather and share data and collaborate,' added Rose. 'So the

tooling and solutions, like the LIMS that we offer, become more pivotal and critical. It is being able to see what other users have done – potentially what they may have done in the last shift, what you need to do for the next shift.'

Tools facilitate remote working

LIMS or ELN systems can help to minimise the time scientists have to spend in the lab, as mobile alerts or other features can help notify scientists when their experiments will be finishing. Streamlining data sharing and access also helps facilitate agile decision making, and lets scientists access data and analyse or work on data from home.

Several LIMS and ELN vendors are now equipping their software with pre-configured workloads to help scientists get set up with key laboratory operations. This reduces the amount of setup and administrative work that needs to be done by scientists, which should lead to increased productivity.

Lauren Taylor, digital science solutions manager at Thermo Fisher Scientific, said: 'Some of those workflows we have already pre-configured to get customers up and running as quickly as possible. In terms of the integration of instrumentation, for example, you may have specimens in the lab that you want to sequence, that information needs to be put onto the sequencer so that you know which samples you are sequencing, and that information can be relayed back to the correct sample.

'The integration really is automating the push of information to the sequencers, so that you are not copying and pasting or uploading and downloading files manually.'

Using AI in the fight against Covid-19

AI tools are becoming increasingly useful to laboratory scientists. A partnership announced between Elsevier and ExactCure provides a software platform collaboration to develop and offer to hospitals – without charge – drug-specific exposure models for 20 already approved medicines that are being tested as potential treatments for Covid-19.

Each drug-specific model, generated using ExactCure's AI-driven simulation platform, will help to predict a drug molecule's pharmacokinetic properties in each individual patient, according to their age, sex, whether they have other diseases – comorbidities – and other factors, and thereby give guidance to clinicians on likely optimum dosing.

> "We put automated software processes in place to help capture testing data: that may be challenging because you are out in the field somewhere"

Development of the drug exposure models will leverage data held in thousands of drug-related documents in Elsevier's PharmaPendium drug data resource, which contains decades of searchable FDA and EMA regulatory approval and related documents on the drugs.

Olivier Barberan, director of translational medical solutions at Elsevier explains: 'We will provide ExactCure with information held in PharmaPendium that spans more than 50 drug-specific parameters, including PK and pharmacodynamic data, safety data, adverse events and drug-drug interaction records, together with data on drug efficacy. This may encompass many thousands of reports, for example, there were in excess of 13,000 records just for the antiviral drug ritonavir, which is one of the drugs under consideration for Covid-19 therapy.'

ExactCure is exploiting the PharmaPendium data and its own AI tools to build a simulation-based digital companion – a digital twin application for smartphones that patients would use to help make sure that they use medicines safely, and at an appropriate dose and frequency, 'whether that be an OTC painkiller, or an antiviral medicine,' Fabien Astic, ExactCure co-founder, said. 'This can help to prevent underdosing, overdosing, and to prevent drug-drug interactions or adverse events relating to the individual's health status, or even genetic profile.

'The AI-based software derives the personalised guidance according to key patient-specific characteristics such as weight, age, gender, renal and liver function, smoking status and genetic background. Importantly, it could also feedback information to the prescribing physician, so that they will know how well the patient is sticking to their drug schedule,' Astic suggested.

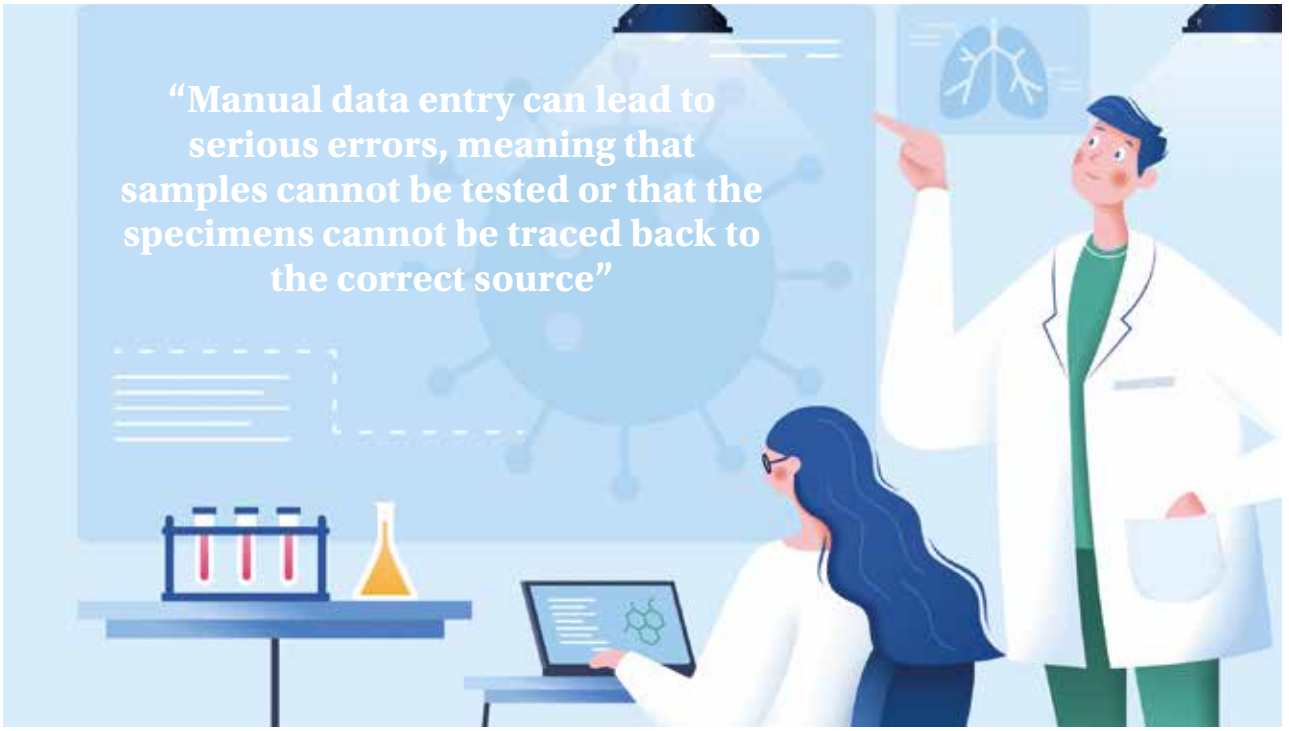
'Our first model, for paracetamol, could help dramatically reduce overuse of the drug and even prevent overdose-related deaths.' 'We signed a partnership with Vidal, a key player of medical information in France, to integrate our technology into their Vidal Sentinel platform designed for hospitals. They call our API [Application Programming Interface] and the pharmacist or doctor can run personalised simulations until they reach what they estimate to be the best posology for a given patient,' added Astic.

Digital companion apps could also be utilised by the pharma industry to support clinical drug trials and potentially speed time to market, while reducing attrition at the trials stage.

Dosing optimisation for Covid-19

Certara launched the Covid-19 Pharmacology Resource Center in April, an online resource giving scientists around the world access to simulation and modelling tools to aid the design of clinical trials and optimise dosing regimes for candidate drugs such as hydroxychloroquine, and lopinavir/ritonavir, against Sars-CoV-2. Funded by the Bill and Melinda Gates Foundation, and supporting global collaboration in the drive to develop new treatments for Covid-19, the centre offers researchers a workbench of in-silico modelling tools, integrated with existing and emerging data.

The centre offers an accessible outreach of the expertise that Certara provides in the global Covid-19 Therapeutics Accelerator, which has been set up with an initial $125m in funding from the Gates Foundation, Wellcome and Mastercard, through



which the World Health Organization, governments, healthcare providers and industry are collaborating to speed the development of therapeutics to treat Covid-19 or prevent Sars-CoV-2 infection.

Craig Rayner, president, integrated drug development at Certara explains: ‘Certara is providing expertise in translational and clinical pharmacology, quantitative science and regulatory strategy to support critical stage decisions, clinical trials design and dosing optimisation for Covid-19.

‘For a virus like Sars-CoV-2, for example, Certara researchers invest significant efforts in bringing the biology and math together to help improve decision making for new therapeutics. One can now evaluate how the virus enters cells, how it interacts and replicates, what the immune system is doing in response, via sophisticated quantitative pharmacology frameworks and predictive tools and then simulate new situations,’ he suggested.

‘We can take huge amounts of data from preclinical models, in vitro testing and clinical experience, as a fundamental foundation on which to use math engines to model what will happen in different trial scenarios, start to simulate clinical trials accurately, and then add data derived from new trials back into the model, and validate in-silico learning,’ said Rayner.

Certara’s Simcyp Simulator has been developed as a suite of modules that simulate drug pharmacokinetics (PK) that can predict and describe how the body affects the drug-drug absorption, distribution, metabolism and excretion (ADME), and how PK may be altered by formulation, patient variables such as age, gender or genotypic information, or concomitantly administered medications.

The Simcyp Simulator links laboratory data to in vivo ADME data and when integrated with and extended to pharmacodynamic (PD) information (how the drug effects the body) such as biomarkers or clinical efficacy and safety, is a powerful tool to support dosing decision-making in new trials.

Keith Nieforth, senior director of Certara’s software division, said: ‘Designing and running clinical trials for any drug or vaccine is hugely expensive and time consuming, so there is a great need to boost efficiency, and improve the likelihood of success.

‘The Certara tools can also model drug activity at particular sites of action, and look at the physicochemical properties of that molecule in the context of other molecules with similar structure and activity, to make predictions on whether the drug will reach target tissues, such as the lung, if we consider Sars-CoV-2,’ Nieforth said.

‘In the case of Covid-19 drug development, the Certara models integrate simulations of drug pharmacokinetics and pharmacodynamics, alongside virus interaction with the host and symptoms.

‘You can then link those models together and that enables you to simulate what you think might happen in clinical trials. Ultimately, modelling and simulation can reduce the number of patients, or trial arms required, as well as evaluate the influence of other design factors on trial outcomes, and so improve the probability of success,’ added Nieforth.

Advancing viral testing

With the world’s focus on the pandemic, LIMS providers are working to develop solutions tailored to assist in the testing and management of virus samples. By streamlining processes, increasing connectivity and reducing manual data entry samples can be tested more efficiently and more accurately.

Edward Krasovec, director of clinical solutions at LabWare explains: ‘Manual data entry can lead to serious errors, meaning that samples cannot be tested or that the specimens cannot be traced back to the correct source. When dealing with healthcare, this means potentially very sick patients missing out on results from their tests.’

John Gabathuler, director of industrial and environmental at LabWare, also highlighted the importance of removing errors from manual data entry processes. ‘They are processes that have not been there previously. They have had to set these processes up, and therefore they are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going through them for the first time, or they are not as tried and tested, so the chances of systems not getting the right information can exacerbate problems. With the current situation you want to be as accurate as you possibly can, as fast as you possibly can, because people's lives depend on it.

'We are trying to help by putting automated software processes in place to help capture the testing data: that may be challenging because you are out in the field,' added Gabathuler.

Labware developed the Portable Disease Surveillance Lab kit in partnership with Tangen Biosciences. They recently announced a partnership for LabWare to distribute Tangen's GeneSpark device as part of the kit in response to the pandemic.

The kit connects to the LabWare LIMS software portal to capture patient demographic and clinical information, document field collection of respiratory swabs for Covid-19 testing, attaining the sample, and rapidly disseminate this data to public health agencies.

Beyond Covid-19, Tangen is making a Flu/Covid-19 Panel that can detect Flu A, Flu B and Covid-19 simultaneously from one patient sample in a single processing run, so that patients with flu-like symptoms will know whether they have flu or Covid-19, or neither.

Richard Birkmeyer, president and CEO at Tangen, said: 'The pandemic is tragic for many families. Everyone at Tangen Biosciences has been working long hours to have our sensitive Covid-19 assay on the market. More importantly, we believe the combined Covid-19 and Flu A/B test will be a critical surveillance tool for respiratory illness management. In addition to the Covid-19 test, we are also developing a sepsis panel and an antimicrobial-resistant panel, and are currently looking for strategic partners for both.'

The firms are aiming to continue this partnership to include multi-target testing. The combination of Tangen's rapid, highly sensitive and point-of-care molecular diagnostics and LabWare's real-time data reporting LIMS software should enable public health systems to react quickly in terms of quarantine guidelines, patient tracing, hotspot monitoring and infection surveillance.

Maintaining interoperability

Covid-19 demands that laboratories adopt new practices and workflows quickly, but when new technologies are created and deployed quickly interoperability can become a challenge. As Labware's Krasovec points out, the company's strategy has been to recognise that no single organisation can do it all – collaboration with the right partners is crucial.

With data analytics and AI applications becoming increasingly widespread, new data sources and ways of analysing data are now available. AI and data analytics also asks questions of existing data. Has legacy data been stored in a way that allows it to be easily reused in the future? If that is not the case, then an organisation must clean and order that data before integrating AI into their workflows.

Interoperability between software systems, different workflows and the various outputs that these processes create, are key to providing a stable platform for laboratory data.

As LIMS providers collect and store data for laboratories, it is crucial they play a role in working with specialised software partners to ensure interoperability. 'It's not just about having an instrument that can do the test. That is just one part of the process. If you cannot get that test where it needs to go, to the healthcare provider, patient, or public health authorities, then it is a wasted effort,' noted Krasovec. 'Not to mention that the people you are testing are out there, potentially not knowing they are infected, and they continue to infect others.

Gabathuler added: 'That is why we have this enterprise laboratory platform, because there are a lot of parts to it and they can all act up in a nice cohesive joined-up way to help in lots of different areas. You have got a functional platform and then everything can be leveraged from that going forward.'

Rapid adoption of new technologies requires LIMS providers to be agile in ensuring interoperability with software partners. This enables them to provide the infrastructure or platform that can not only interact with instruments and laboratory equipment, but also data analytics or AI software frameworks.

'There is a rapid adoption of new technologies in the healthcare laboratory in terms of a genetic-based testing platform which has spawned this order of magnitude difference in the amount of data that is created – that data has to be managed,' said Krasovec. 'Quite often it involves specialised technologies to interpret that data.'

'As a LIMS provider, we are not a domain expert in analysing genetic data. It is important we are able to get data that may be captured from an instrument and interact with the software specialised to do that interpretation of these gigabytes of data that can be generated by sequencing processes,' Krasovec added. 'That is obviously very important, because no one system is the be all and end all, and they need to coexist and share information with other systems.

'We manage the workflow process and there may be data analytics that goes along with it that could be done by specialised software. Then we are responsible for distributing the final report to whoever it needs to go to. We have a role in the process. It is important that we are able to interact with the other systems as well,' said Krasovec. ■

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Laboratory technology changes

Informatics experts share their views on the future of the laboratory and how things might change due to the added pressure of Covid-19

What do you think will be the biggest change in the laboratory?

Richard Milne VP and general manager of digital science at Thermo Fisher:

One of the things that 2020 has done is it has created a tipping point in the laboratory. People will find they need to reconfigure lab space and the configurations of labs. But we are also seeing higher demand to make the lab available.

How can people work from outside the facility? How can people access data when they are not inside the laboratory? How can they collaborate when they cannot travel as easily as they did? How can they control their experiments and run their lab without being inside it?

A lot of those drivers that we are seeing in all aspects of society at the moment are going to continue to persevere. We are finding that there is a very significant increase in people wanting to see technology shoulder some of the burden and assist in the changing parameters of the workspace. We are seeing it in every industry and every walk of life, but it is also being clearly illustrated in the laboratory.

We are doing a lot of work around cloud-based computing platforms, collaboration environments, data moment and data storage. There is a lot of work going on at the moment around connected instruments and how data can flow more easily.

Stephen Hayward, Biovia technical marketing manager:

Transformation of the user experience with the inclusion of advanced techniques. For example, voice recognition, where a use case would be dictating observations and results utilising scientific awareness in the recording process.

Transfer to cloud-based systems, driven by corporate IT policy changes – this enables more remote access, which is becoming critical in times of a pandemic

AI – truly leveraging all existing knowledge from the lab to better guide future work. Finally, augmented reality technology which can transform lab process execution – visualising additional contextual information, or alerts about sample status and pending tasks.

Many lab technicians are considered 'essential workers', so they have continued working during a pandemic. But the way of working has changed. Teams working in the lab are now split into smaller groups that are working in shifts to minimise contact while covering the workload. This makes efficient and flexible laboratory scheduling critical.

"We are doing a lot of work around cloud-based computing platforms, collaboration environments, data moment and data storage"

Additionally, all tasks that are not related to physical activities in the lab are now performed remotely. Therefore, it is important to be able to work with experimental data away from the lab while retaining contextual data for decision making, which is typically supported by cloud solutions.

How has Covid-19 changed how the scientific ecosystem works together?

Arvind Kothandaraman, general manager diagnostics, PerkinElmer: A major takeaway from Covid-19 has been that every second matters when it comes to a response. In order to be more nimble and agile, labs require tools with high levels of sensitivity and reliability in order to detect disease, develop therapeutics and discover preventive measures that can be taken before there is an opportunity for a surge to begin. Early detection and diagnostics are vital for labs, as screening becomes the new normal.

We will also see a shift towards molecular testing and surveillance in general over the next year or two. Covid-19 necessitated this shift, and labs have realised that they must be equipped with life science and diagnostic tools to better manage the spread of infectious diseases now and in the future. While we hope to never experience a pandemic of this magnitude again, it is in our best interest for labs to proactively conduct surveillance to better manage the potential risk.

Collaboration among scientists is the backbone of labs. The fight against Covid-19 has been prioritised across the globe, and this has accelerated how all organisations work in a united effort to ultimately serve the public. In that sense, pharmaceutical and biotech, which are conventionally considered competitors, have joined together to work towards the same goal.

Information sharing will help

ensure the abundance of testing kits and therapeutics for everyone and everywhere. The collaboration has been unprecedented, and we'll see this approach continue in many ways moving forward.

Dr Barry Bunin, CEO of Collaborative Drug Discovery (CDD):
While the concept of remote working is nothing new, the Covid-19 pandemic has created a new reality where many scientists are forced to spend less time in the lab and instead work from alternate locations. One of the main challenges that comes with this is data availability – do you have access to your data outside of the lab? How do you share data with colleagues and collaborate when everyone is physically separated? And if you do share your data, how do you make sure there is adequate access control to prevent unauthorised access? These are important considerations, in particular in deadline-driven projects where achieving specific research milestones is critical for the success of the organisation.

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In fact, we have written a white paper on the subject of remote data access, and interested readers can find it on the *Scientific Computing World* website.

What are the biggest challenges that lab users face?

Stephen Hayward, Biovia:
Higher project throughput with the same number of staff requires efficient tools for handling data, observations and result analysis. Distributed labs means that all data must be available to all team members in real time.

Although most labs have electronic solutions in place, they are very rarely integrated and users are forced to transfer data and results manually between systems, which is time-consuming and error-prone. Only flexible, integrated solutions across sites and collaborating partners can fulfill such requirements.

No competitive lab can work without digital support for process automation, data capture, sample management, data sharing and analysis. Most laboratories in the life sciences space have already implemented digital solutions for compliance and efficiency reasons.

'We are observing that laboratories in other process industries, as well as discrete industries, have started to implement electronic tools too, but are still in a less digitised and connected state. We expect that this will continue to increase as the benefits of efficiency, better innovation, decision making and faster time-to-market are too compelling.

> "Teams working in the lab are now split into smaller groups that are working in shifts to minimise contact"

Disconnected systems, rigid applications and lack of sufficient support from corporate IT in labs is making it difficult for organisations to deploy new technology. Only a transformative approach will enable labs to move to a truly digital lab that also allows them to leverage new technologies. This transformative approach is typically supported by scientifically-aware collaborative business platforms.

Oscar Kox, CEO at iVention:
We started with cloud from day one and we said 'we want automatic upgrades' we do not do custom software. And if we do some custom software it will be taken up into the core product, so that we can still do the automatic upgrades.

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We have now developed the automated OQ scripts [IQ/OQ Validation Protocol] and system to enable the automated execution of these scripts. When we release software and you do it agile, every two weeks, it is impossible to have everyone testing the software manually.

For other providers, it can take months to upgrade and even longer to complete the validation. We do not want to see upgrades taking longer than days. We will validate, put the OQ scripts in a document and even add some screenshots. The system will try to login in Chrome or Edge and this is how we do it. It generates a complete report.

We are still doing really well in implementations because we can work with people using Teams meetings to do configurations together, because we are in the cloud. From an implementation standpoint it is massive, because some people who cannot work right now as they cannot go to the office, they can test software, when normally they would do that next to their day jobs.

The second thing is that if you look at the old-fashioned implementations from the more conventional providers, you need a VPN connection and then there are still Excel files that are stored on your PC in the office. This means you cannot get to all of your data. The old-fashioned implementations with the client on the PC in the office means that you cannot access that when you are working from home.

What role do automation and integration technologies play in overcoming laboratory challenges?

Richard Milne, Thermo Fisher:

We are looking increasingly at how you can connect devices to look at their operating parameters and confirm that they are online and within range.

We want to be able to do that from a mobile phone at a safe distance to ensure that your experiments are running, regardless of where you may be.

We are doing a lot of work with our laboratory automation team at the moment. One of our most recent, big and impactful solutions that we released into the market was the Amplitude solution, which is the high-volume Covid-19 testing solution that is being used across the world at the moment.

There is significant integration between our laboratory automation and our digital science team to make sure that [Amplitude] is working with minimal touch, minimal operator system.

> "A major takeaway from Covid-19 has been that every second matters when it comes to a response"

Trish Meek, director of marketing at Thermo Fisher:

One of the key things we are seeing when we talk about connectivity and lab automation and ensuring that organisations are leveraging their data effectively, is the value of the scientist.

For years people were filling in the gaps, with a lack of automation the scientists would fill the gap and do that work. I think there is a recognition from organisations that the scientists are their greatest asset, and any way that they can automate and integrate data and the workflow means that scientists can be more effective and focus on the science itself.

When we talk about integration with our customers, there are a few different pieces. There are the partnerships they have between organisations, the integration with outsourcing and so we work with our customers to facilitate the integration between Contract Research Organisations (CROs) and Contract Development and Manufacturing Organisations (CDMOs) that they are working with, as well as within their own organisation.

Our pharma services group is implementing our capabilities to manage their [customer] CDMO operations across 25 sites. This has enabled us to partner with them as a customer ,but also as a part of Thermo Fisher to find the ideal state as they talk about their scientific ecosystem, and how they take it from where they are today.

Richard Milne, Thermo Fisher:

We recognise that a lot of organisations have legacy investments in software applications and many of those can be deeply embedded in their processes. Rather than looking at this as a revolution where you disrupt the existing situation. We are looking at it more as how do you integrate into that, and therefore protect the investments that people have made in other software tools but provide integration across those, so people can get an easier customer experience and also the value of the integration from the different toolsets.

I don't think Covid-19 is causing it. This is just my perspective, I am basing this on my own conversations with customers, but my feeling is that Covid-19 is the catalyst for this change. It would have happened anyway, but slowly and more sporadically.

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Open science drives bioinformatics research

The European Bioinformatics Institute is developing tools and infrastructure to promote open science and provide programmatic access to biological data

Today the European Bioinformatics Institute (EBI) maintains the world's most comprehensive range of freely available and up-to-date molecular data resources. It provides 307 petabytes of raw data storage for bioinformatics data and receives more than 62 million web requests per day.

The focus on open science and delivering infrastructure to support scientists' access to scientific data is at the heart of EBI's mission to support bioinformatics research. The first steps to creating bioinformatics data resources so that scientists and researchers could share sequence data in Europe were in 1980, with the creation of the EMBL Nucleotide Sequence Data Library (now EMBL Bank, part of the European Nucleotide Archive). The archive was established in 1980 at European Molecular Biology Laboratory (EMBL) in Heidelberg, Germany.

Johanna McEntyre associate director of EMBL-EBI services, senior scientist and head of literature services, said: 'EBI was started more than 25 years ago now with a remit to provide data resources for life sciences. The original resource, the EMBL data library, housed nucleotide sequences for research. Sequencing technologies were taking off. They had moved out of being a research project in themselves, to something that more and more people were doing.

'There was a requirement for a database to keep these things, because there is a lot of value in comparing sequences from different organisms.'

This initial EMBL data library grew

and scientists realised other resources were being created that would also be of great value if they could be shared with the wider community. What began as a straightforward task of abstracting information from scientific literature soon grew to a major database, with researchers submitting data directly.

In 1992, EMBL Council voted to establish the EMBL-European Bioinformatics Institute (EMBL-EBI) and locate it on the Wellcome Trust Genome Campus in Hinxton, UK, where it would be in close proximity to the Wellcome Sanger Institute. In September 1994, EMBL-EBI was established in the UK.

'EBI was created almost 27 years ago. The institute grew from just a few pioneers at that time to an 800-strong institute today,' noted McEntyre.

EBI's mission is split into five distinct areas: computational research; supporting industry use of bioinformatics data; providing training on the use of these resources; hosting the Elixir hub; and supporting scientific services and resources such as the European Nucleotide Archive (previously the EMBL Data Library).

Open access infrastructure supports Covid-19 research

Another aspect related to this open access data is research paper preprints, which have been very valuable for sharing data during the pandemic. A preprint allows researchers to share results with the scientific community in advance of peer review, making data available much faster than was previously possible.

'Another very recent thing that we have done is a project based on Covid-19 preprints,' said McEntyre. 'Instead of being behind closed doors

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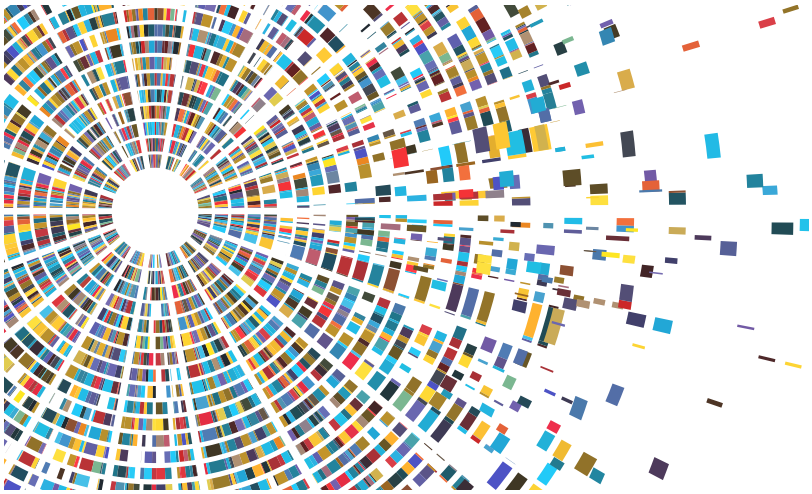


you just post your finished manuscript to a preprint server. When you do that, what happens is a very light screening process. That means that your results are available in 48 hours of submitting it, as opposed to months.

'During the pandemic pre-prints have been very important in very quickly sharing results. The model is that it doesn't avoid peer review, it's just that peer review happens after the fact,' McEntyre added.

Need for open access research data

Today EBI has a huge collection of tools and data resources, including Europe PMC, a full-text database of research articles and abstracts that are openly available for everyone to read, with a subset of those available for reuse.

'The point of running this database is because funders of life science research in the UK needed some infrastructure to support their open-access policies. Very simplistically put, their policies will say something along the lines of "we expect all our researchers to publish the outcomes of their research openly",' said McEntyre. 'That will often specify that these papers should have a CC-BY licence, a licence that allows people to reuse that work without having to request permission – this can be very important for machine learning and AI,'

As the data volumes and types of resources increased, some of the organisations funding research were trying to find a way to make results openly available. 'A lot of research funders, not just EBI, needed a repository to support that open access policy. They invented what was called UK PMC at the time, which has also now grown to include 30 funders across Europe, and so it is called Europe PMC,' said McEntyre.

Europe PMC is a global, free, biomedical literature repository, providing access to worldwide life sciences articles, preprints, micropublications, books, patents and clinical guidelines. The resource currently contains more than 36 million abstracts and more than five million full-text articles. A subset of the full-text information corpus is the open access literature that can be downloaded and used from the FTP site, for example for text-mining research.

'This database was originally created to support those open access policies introduced by research funders, but it does lots of other things as well. One of the most important things is to provide bulk downloads and APIs for programmatic access to the content,' said McEntyre.

'The second very important thing is linking to the data. When someone deposits data into one of our databases, it is usually because they have generated the data in the course of doing some experiments, and typically those experiments will be written up in the form of a research paper. You want to link the data to the literature for the biological context, and you want to link from the paper to the data, to show the provenance of the research results,' McEntyre said.

'This means that you can look at the data behind the paper and see for yourself whether it supports the assertions that have been made in the research paper. That linking between the literature and the data is very important in both directions.'

Open access to the data generally improves the reproducibility of the

> "Open science is a great equaliser"

science, as more people can see the outputs and access the contextual data that supports the research paper. However, linking the data is also very important for research, and trust in that research.

'Coming from the data point of view, you might argue that linking to the data is less important, but where that really comes into its own is where people have developed algorithms to search through the data,' stressed McEntyre. 'I think, and many other people think, that linking to the data is very important, because you need to have as big a collection as possible of open access literature for people to invent new ways of doing things. For example searching or browsing literature.'

In order for AI and machine learning to be possible, data needs to be made available, and in a way that allows scientists to generate huge datasets. Creating a large database of open data enables researches to access data from several different sources that have all been stored and made available for reuse.

If data is not managed in the correct way, these types of activities are made much harder, as individuals would need to seek out that data manually from several different sources. This data may be stored using different formats, making data cleansing and pre-processing necessary. 'Managing in the correct way means open data, it also means storing in formats that can readily be consumed by machines and humans, and having the appropriate amount of metadata,' said McEntyre.

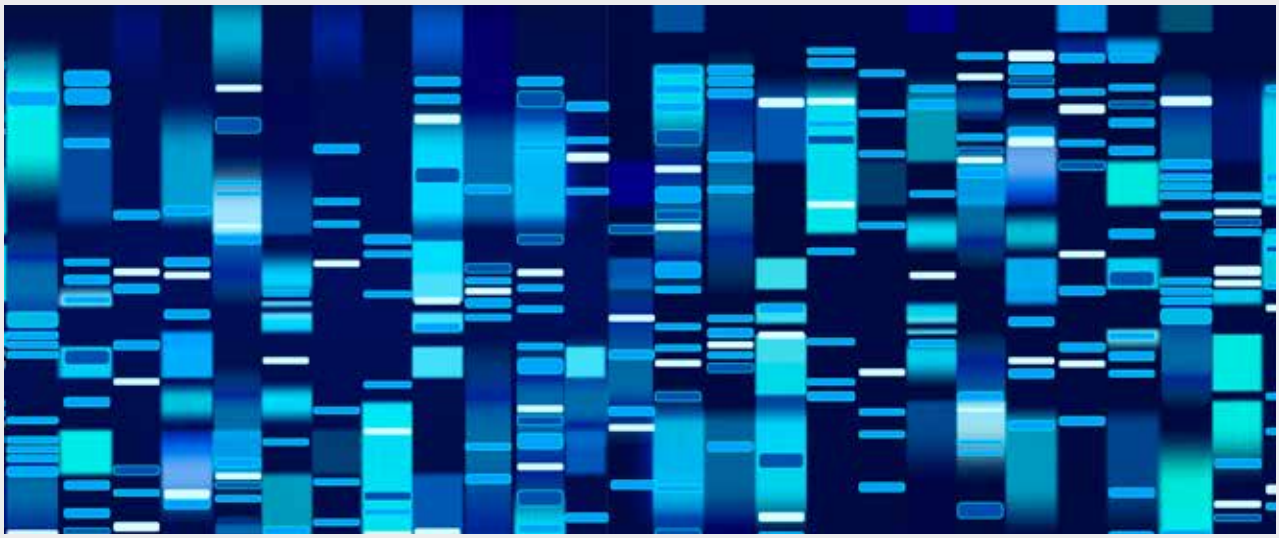
Open science infrastructure can open up new ways of conducting research and interrogating data, but ultimately the driving factor of open access research is to drive scientific discovery by sharing insights with other researchers.

'Open science is a great equaliser. It is far more likely that someone in a developing country is going to have an internet connection, than access to a library of scientific data.

'It opens up research to everybody in the world,' said McEntyre. ■

The leading-edge of genomics research

Wellcome Sanger Institute's Julia Wilson tells Robert Roe about the research centre's role and impact on the wider scientific community



The Wellcome Sanger Institute aims to tackle some of the most difficult challenges in genomic research. This demands science at scale alongside a creative approach to research that pushes the boundaries of scientific understanding.

Sanger's scientific niche is in large-scale, high-throughput biology, often incorporating systematic genome-wide screens. These are enabled by major data generation platforms in DNA sequencing, and genetics with an accompanying large IT platform supporting computational data analysis.

An overarching theme of the centre's science is genome variation; naturally occurring and engineered, inherited and somatic; explored in human beings, pathogenic micro-organisms, human cells and mice.

The Wellcome Sanger Institute Associate director Julia Wilson describes the history of the institute, which highlights the research goals at Sanger which adapt and evolve over time to constantly push the boundaries of scientists' understanding of genomics.

'The history, in a nutshell, was that Sanger was established to sequence that first human genome. That took ten years and cost millions of pounds to get that one first human genome sequenced,' said Wilson. 'We needed to then be able to understand the information in the human genome, map it to health and disease, so scientists can compare between populations.

'Since then, Sanger has been studying the biology of genomes – the DNA code. Everything we do at the Sanger Institute involves understanding genome sequences and applying them to improve human health or increase the understanding of the living world,' added Wilson. 'Our mission is to advance understanding of biology and to improve health. Everything we do is about genomics so that runs through all of our science.'

> "When the rest of the world can do what we do, then we need to change direction – we should always be breaking new ground"

Pushing the boundaries

One of the mandates or hallmarks of scientific research at Sanger is the constraint drive to break new ground. Pushing the boundaries of understanding in genomics requires that the focus must frequently shift, as the understanding of a certain topic becomes more ubiquitous.

'When the rest of the world can do what we do, then we need to change direction – we should always be breaking new ground in genomics,'

said Wilson. 'That means we are at the leading edge of technologies but also thinking about where genomics can take us. In that sense, it is quite a fundamental research organisation.'

The current research programmes at Sanger are split into five distinct fields; cancer, ageing and somatic mutation, cellular genetics, human genetics, parasites and microbes and the Tree of Life.

All of these projects are research at scale, producing vast amounts of data which must be analysed. 'We have got an enormous fleet of data generation – particularly DNA sequencing machines that generate vast amounts of data that needs to be interrogated and interpreted to generate findings,' added Wilson.

Two of the largest projects being run are the Human Cell Atlas (HCA) and the Tree of Life. The Cellular Genetics' Programme jointly leads the HCA global consortium alongside the Broad Institute. The HCA vision is to create comprehensive reference maps of all human cells – the 37 trillion fundamental units of life – as a basis for understanding human health and diagnosing, monitoring and treating disease.

The Tree of Life investigates the diversity of complex organisms (eukaryotes) through sequencing and cellular technologies. Sanger generates and uses high-quality genome sequences to explore the evolution of life, provide the raw materials for new biotechnology and deliver tools and understanding for biodiversity conservation. This project aims to sequence approximately 66,000 Eukaryotic organisms.

However while these 'juggernaut' projects may take five to ten years to complete, 'the programmes adapt and change to find new challenges and break new ground in genomics. Some have evolved. The cancer programme was previously focused purely on looking at genes associated with cancer,' said Wilson

'Now everybody can do that and as it has been implemented into genomic medicine, we no longer need to make the associations between genes and cancer. The programme evolved to look at the ageing process and the links between cancer and ageing, and to take a deeper dive at what we call mutational signatures.

'That is an example of where the programme has evolved, because to remain at the leading edge we have had to pivot and change direction. There have been many examples of this over the organisations history.

'We get funded in five year tranches, so we can take on projects that may last five years, ten years or beyond. We can take on those riskier projects,' added Wilson. 'There is always that push to adapt and evolve and take on some of the biggest scientific challenges. It is a mixture of the technology and the ambition and evolution to remain right at the cutting edge.'

> **"There is always that push to adapt and evolve. Take on some of the biggest scientific challenges"**

However these large-scale projects do not come without their own challenges. For Sanger this can mean working to develop new methods or tools that can support genomics at an unprecedented scale.


Julia Wilson

'Another hallmark of Sanger science is that because we are a core-funded institute, we invest in this vast scientific infrastructure. We have got one of the largest fleets of DNA sequencing machines, definitely the largest in Europe but one of the largest concentrations of that technology in the world. We have to be applying it to projects that only we can do – like sequencing all of life in the UK, or looking at 37 trillion cells in the human body,' said Wilson.

'A huge amount of our budget goes on kit and consumables, but also teams of real deep-domain technical experts that run these pipelines. We have got expert, skilled technical staff running the DNA pipelines. Some of these are trained at PhD level and beyond but they are driven by working in team science to deliver something that is greater than the sum of the parts,' added Wilson.

Open science

Another hallmark of Sanger science is that the tools, software, data and other resources at Sanger are made freely available to the scientific community.

This means that other organisations can pick up these resources and carry on the work, taking it in interesting directions as Sanger shifts focus.

'Everything we produce is made freely available to the scientific community with the expectation that we want others to take that data and those tools and build on our discoveries. We cannot follow all of the leads from the data that we generate, so we want that data to be used by others,' said Wilson.

She also noted that this focus on open science was adopted at the start of the Sanger Institute. 'This happened at the very outset, when genomics was a new thing and our founding director John Sulston was working on that first genome at the time. It was mandated this data should be released in real-time for humanity to benefit,' added Wilson.

'International parties who contributed to that first genome signed up to these principles and historically it used to be released each day. There was a ticker tape above reception and the genomic data would go across as it would come off the machine. Obviously we cannot do that any more because the data has increased by so much, but genomics was founded on open data.

Wilson stressed that this drive for open data is necessary in genomics research, because a single genome is of very little use. 'If they are all locked up in individual labs, then none can benefit from this,' Wilson said.

'It is a principle of Wellcome funding as well. Wellcome, as a funder, has been so influential, and that ethos of open science has filtered through Sanger since it has been open,' Wilson said. ■

Julia Wilson is associate director at Wellcome Sanger Institute

Digital drive laboratory transformation

Sophia Ktori considers how software can transform the laboratory

'Choosing a system that offers flexible configuration to match specific teams' needs is key to digital transformation,' says Sharon Williams, Interactive Software's product director. The UK-based firm works with universities and pharma to configure its Achiever Medical LIMS, designed for managing complex workflows.

It's important to look at the operational requirements of any potential user, and to understand what they already have in place to manage their workflows, and where, or what their deficits are, Williams noted. 'We go into labs, see how they operate, and try to understand their end-to-end processes. We need to see what they are struggling with – they may be still relying on spreadsheets that get emailed between people with little or no security, for example – and then we can highlight those deficits.'

It's 'gap analysis,' at a high level, she continued, which is more than just trying to reduce or remove the need for manual data input. 'Once we understand where they are now, and what their aims are, we can then demonstrate how we can fill the gaps and build in value, security and efficiency. Not infrequently, implementation of a new platform might also highlight processes that may have been partially buried. 'We've had customers come to us and say that they need to establish an SOP for a process that they only realised they were carrying out when they automated the workflow,' said Williams.

Understand the ultimate endgame and you can work backwards from there, suggests Williams. 'People tend to get tied up with looking at the software platforms that are on the market, rather than starting with what they want to achieve and how they

want to get there. Realistically we can't change the world in one go. Our aim is to try to break the problem down and look at what is going to have the greatest impact. Then we can start from there and work outwards.'

Is a LIMS always necessary?

Organisations may also try to shoehorn their existing processes into mismatched legacy software, either through configuration, customisation or upgrades. 'This may seem like the logical option, but if the software isn't designed to do the job, then the outcome may be disappointing, and costly,' Williams stated.

'You have to be realistic about what your existing software can do, and acknowledge when it may be better all round to look for something that is more fit for that purpose.'

In fact, companies are quick to assume that they will need an expensive, complex LIMS platform whereas it's not always a given that a LIMS will be necessary, she continued.

'If you are only dealing with a couple of hundred samples and there is no complexity associated with the data associated with those samples, or what you are doing with them, then commercial sample tracking software may be sufficient to help you manage samples. They are reasonably priced, and would do the job for you.'

Interactive Software works with those organisations that do have the scale or complexity of workflow to require an informatics infrastructure founded on a LIMS for sample management. For organisations working in areas that involve accessing patient data and samples, the implications for security, and permissions for individual users, are uppermost, and so the concept of digital transformation may be highly reliant on security,' she noted. The ability to set authorisations and access permissions at the individual user level is therefore critical.

Journey from any starting point

Of course, every laboratory or lab-based organisation will have its own vision for short- and long-term digital transformation, according to where they already are on their digital journey.

Some organisation's labs and businesses have taken steps to become paperless, but, Gabi Koberg, senior regional sales manager, EMEA, at Abbott Informatics, feels it is not uncommon for organisations to be reliant on paper and/or Excel, especially when it comes to performing lab procedures, for example, sample preparation.

> "It will always be more difficult to implement for the R&D Labs, just because the work that's being done is typically less routine"

'We see that even in 2020 there are still companies that haven't yet implemented fundamental IT software solutions, such as an enterprise resource planning (ERP) platform.'

For these organisations, in particular, but also for those that might be much further down the digital road, it is critical to be realistic about immediate goals. A good starting point, according to Andreas Schüler, technical solution design manager EMEA at Abbott Informatics, could be looking for opportunities to implement software that will offer quick and immediate benefits.

'For example, using mobile technologies and associated software for functions – such as environmental sampling or sample preparation for testing – where there is no ready access to a PC, can have immediate time and error-saving benefits.'

The ubiquitous nature of barcoding has now made this a relatively simple form of digitalisation to implement, suggested Schüler. 'It won't necessitate high overheads, and the relevant software and equipment – everyone these days is familiar with a touchscreen-enabled tablet, or mobile – is easily integrated into daily working practices.'

RFID tagging technology also offers an opportunity to completely automate inventory. 'Stock management can become a self-documenting process, with the benefit that you always are aware of where any given piece of inventory is, and how much of any inventory you still have. Not only that, but feasibly the system will automatically generate a PO to order new inventory, once a threshold level has been reached,' added Schüler.

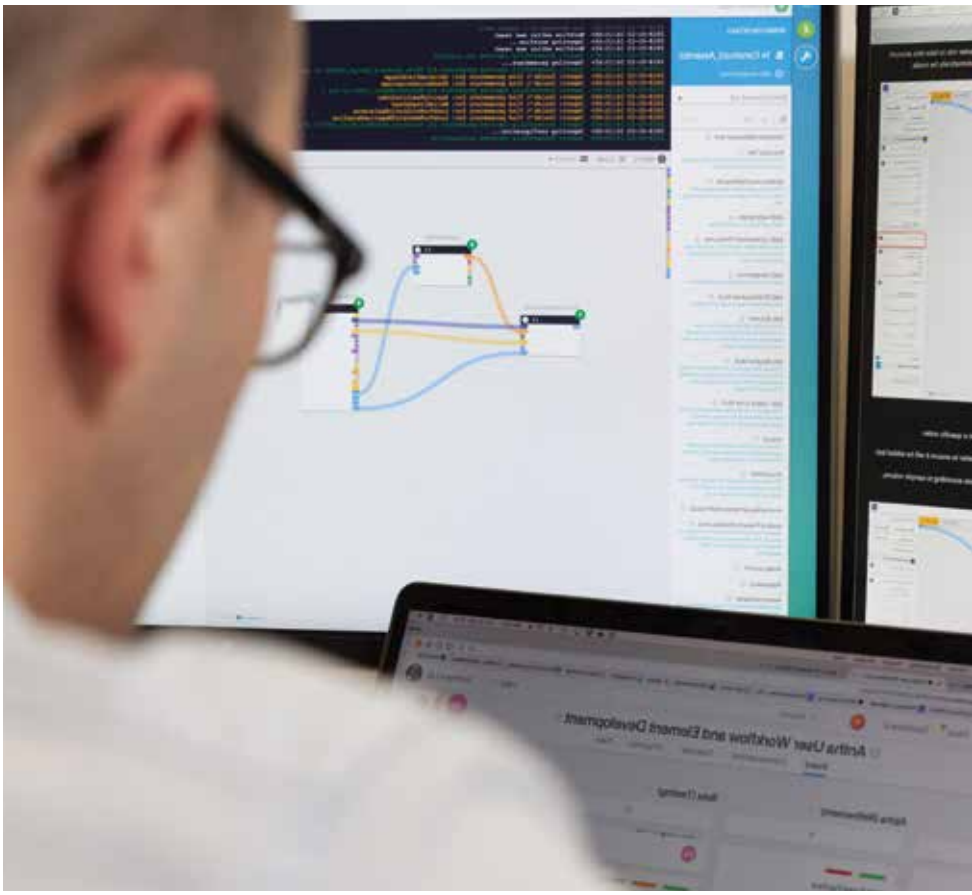
Consider user acceptance

'For any organisation considering advanced technologies, the human element is a major consideration,' Schüler continued. If we think about implementing relatively well-known digital systems, whether that be barcode scanning, or transitioning from other paper-based workflows to tablet-based systems, it's likely that the end-user will only have to learn how to use a new touchscreen digital interface for data recording and access. 'For this type of digital system, the threshold for user acceptance probably isn't that great,' Schüler suggested. 'Plus, users can see the immediate benefits of not having to record their data manually, scan it into a system, and then archive that paper original. Instead, they immediately have their data digitally stored and easily accessible.

'Progress to the concept of using more complex technologies, whether that be sophisticated voice control, or augmented reality, and there may well be more human resistance, both with respect to learning how to use the technology itself, but also with the potential that such systems may watch, listen, record and report on their every move throughout the day.'

In this environment, end-to-end automation is just more complicated, Schüler noted. 'It will always be more difficult to implement for the R&D Labs, just because the work that's being done is typically less routine. The more routine your work is, the easier it is to optimise and make it more efficient digitally.'

> "It's more feasible to layer on things such as machine learning, because you have laid the foundations of really robust, rich datasets, which have incredibly detailed metadata"



Digitisation and automation is a key goal also for the R&D lab, Koberg continued. 'Implementing advanced technologies, such as predictive modelling, could allow labs to reduce the number of experiments they are carrying out, and save on both resources and time. Such technologies can feasibly aid in the design of experiments that provide more insight, which would reduce development time, and ultimately speed time-to-market for new products.'

The ability to reuse data is really important for maximising insight from historical experiments. 'One key priority is to reduce the amount of unstructured data, and so put as much data and metadata as possible into a structured format that can be easily accessed and mined in the future,' added Koberg.

Data standards

Thinking about data utility naturally leads to the concept of data standards. Schüler said: 'You want to make sure that the data you are capturing will still be accessible for data mining long after the system that created it has been retired.

One focus of product development at Abbott Informatics is to enable labs to progress their digital transformation and enable that end-goal of a seamless, end-to-end automation and digital data handling, Koberg noted. The firm maintains that its StarLIMS integrated solution has long been at the forefront of LIMS-based platforms that are designed to facilitate interfacing and integration of typical laboratory and other enterprise hardware and software platforms.

Speeding drug development

Ultimately, digitisation in the pharma or biotech lab will help to speed the identification of new targets and the development of drugs, vaccines or gene therapies, suggested Markus Gershater, co-founder and CSO at UK-based Synthace. Embracing smart software that can automate the complexity associated with experimental design and execution will take the benefits of digitisation in the lab beyond automating how (and what) data can be directly obtained from analytical instrumentation, and its management and analysis.

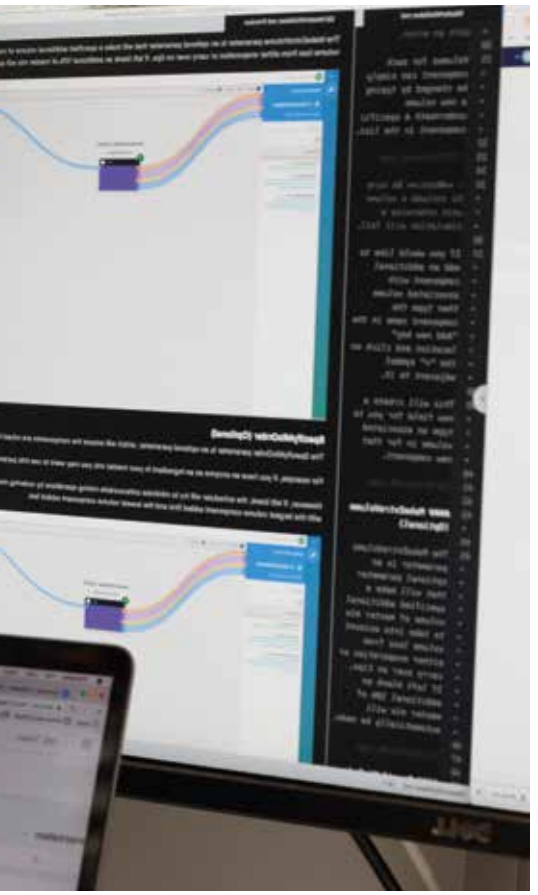
Synthace is developing a new generation of software tools that will effectively speed up how scientists can design and carry out experiments that will help to answer highly complex biological questions. By doing this it should be possible to maximise the depth and utility of data that can be derived from those experiments, and the associated metadata that can map every step of the experimental execution. 'It's a concept of digital augmentation that we call 'computer-aided biology,' Gershater noted.

The aim is to harness software that can close the gaps in digitisation and automation gaps in the R&D cycle. 'This cycle typically starts with a hypothesis or question, against which an experiment is designed,' he explained. 'The experiment is then executed, the resulting data is collated, recorded and reported, and data analysis can then be carried out. That analysis subsequently informs the design of the next experiment.'

There has been a lot of focus on automating how results data are handled, managed and in what formats, with a view to maximising value from that data, which will then aid in its analysis to help make next-step decisions, he explained.

However, the design, planning and execution of those experiments is still very much a human process. 'Scientists today will commonly use tools such as Excel to help them work out their experimental plans,' and electronic lab notebooks (ELNs) are used to record their processes, SOPs and results, Gershater said. 'These tools are digital aids to design,' but they don't automate the detailed experimental planning.

In reality, planning experiments is a hugely complicated task, he



suggested. 'Powerful experimentation is a requirement for trying to address biological complexity, but it can also be very difficult to carry out by hand. Each experiment can take a huge amount of very meticulous planning, and running experiments may involve 14-hour days of complex manual pipetting steps.

'So, if experiments are limited at the planning or execution stage, it doesn't matter how much of the rest of the lab is digitised, there will always be limits in terms of experimental feasibility.'

"Antha can be interfaced with ELNs, LIMS and other emerging digital tools to generate a potentially gapless end-to-end workflow"

Taking the limits of experimental design

The vision for the future is to enable scientists to design and run whatever experiments are required to address biological complexity, without these human limits, he continued. Without such constraints, scientists should be able to generate more sophisticated datasets, because the design of the experiment has been set up to optimise the value of each run, and automation can carry out these complex designs.

'If you then are able to generate datasets that are very well structured for addressing the hypotheses that you just looked to address, you can have very sophisticated analysis on the top of those sophisticated datasets. And that's when it will be more feasible to layer on things such as machine learning, because you have laid the foundations of really robust, rich datasets, which have incredibly detailed metadata. This depth of metadata completes that experimental map, to maximise context, which provides the foundation for then building machine learning on top,' stated Gershater.

Synthace's flagship cloud-hosted platform Antha allows scientists to plan complex experimental protocols, execute the workflows – through direct interface with liquid handling robotics – and then associate and integrate resulting data and every point of metadata back to the experimental source.

'Our software maps out exactly what has to be done to fulfil a particular experimental design,' Gershater said. 'It works out every single liquid handling action that's needed, and then drives the robot to carry out the experimental steps as defined. So that means you know exactly what's happened throughout the entire experiment.' In effect, the software generates a kind of 'experiment digital twin,' which is then executed in the lab, he suggested. 'Integrate this capability with complex data handling and management, and you get much closer to the vision of seamless digitisation. With this as an ultimate goal, Antha can be interfaced with ELNs, LIMS and other emerging digital tools to generate a potentially gapless end-to-end workflow.'

Having started life as a biology company focused on addressing biological complexity in process development, Synthace initially developed the Antha software to help its own labs execute the type of science that otherwise wouldn't have been possible. 'We realised that the platform would have much more impact if we pushed it out across all of biology, instead of keeping it in house,' Gershater explained.

The firm started marketing the first iteration of the Antha software in 2017, and the most recent version can interface with most state-of-the-art laboratory robotic systems. 'Importantly, we have our own laboratories,' Gershater noted, and so the platform continues to be developed through experience with real-world experimental scenarios and setups.

The firm has close working relationships with its clients, which include major pharma and biotech companies – such as Merck & Co in the US, and Oxford BioMedica in the UK – and with some of the major liquid handling robotics and other hardware providers. Synthace also continues close research links with Microsoft Research.

Completing the circle

Synthace clients are demonstrating the utility of the Antha platform to improve how complex lab experiments are designed, set up and executed, Gershater noted. 'Oxford BioMedica, for example, has really embraced the concept of digitising that complete experimental loop, and is using our platform for execution, and for collation of data, and are collaborating with Microsoft Research to add artificial intelligence on top of that collated data, in order to loop back round again to experimental design.'

Ultimately the aim is to enable a completely interconnected digital laboratory ecosystem, and while Synthace is currently working with clients on specific applications, the aim is to roll out comprehensive digital solutions for broader applications.

Citing Oxford BioMedica as an example, Gershater explained how the Synthace software can have a tangible impact on the value of experiments. 'What's really encouraging is when you see signs that scientists are using our tool to do the kind of science that they otherwise just wouldn't be able to consider. Computer-aided biology is how people could work in the future, and represents an ecosystem of different tools we think will be required for truly digitised lab working.' ■

Do you need a chemical and biological registration system?

Registration systems can be useful IT tools in the arsenal of labs that are looking to streamline their workflows. As the name suggests, these software systems are designed to help track the different chemical or biological entities used for experiments, as well as ones created in the lab as intellectual property.

A core function of registration systems is the ability to generate (or mirror) unique identifiers that unambiguously identifies each entity and batch combination. Among other functionality, these systems support the ability to capture information on complex chemical and biological molecules, including details about their structure, various physical and chemical properties, and assay testing data.

Broadly speaking, entities that can be registered fall into two categories:

1. chemical molecules
2. biological entities

Some registration systems specialise in handling one category, while others, such as CDD Vault by Collaborative Drug Discovery, are designed to accommodate both.

Chemical Registration includes tools for entering individual compounds and groups of compounds, searching for compounds by structure, and for assigning unique identifiers for each compound that comes into the lab. These systems include functionality for establishing and showing relationships between individual compounds and families of compounds, and for linking compounds to associated screening data in the lab. Moreover, registration systems are a step up from some chemical databases, which simply store the molecule without some of the more fine details about stereochemistry or associated protocol data.

> "These systems support the ability to capture information on complex chemical and biological molecules"

Biological registration offers functionality that lets users define, register, query, and report on biological entities including proteins, enzymes, antibodies, DNA, RNA, cell lines, plasmids, proteins, siRNAs, and protein-drug conjugates. It also includes tools for managing relationships between biological entities, collecting details on individual entities such as protein expression information, and generating chemical representations of entities where possible.

Benefits of registration systems

Findability – perhaps the most important reason for registering entities is also the most obvious, findability. Being able to find what's needed for a given test at any point saves time, and results in less frustration for researchers. Labs can have hundreds or thousands of molecules and/or biologicals in stock at any time. These include reagents, as well as entities made for testing as the core part of an organisation's intellectual property portfolio.

Uniqueness – a related and equally important consideration, for labs that work with chemical compounds or biologicals, is being able to track important details about an entity (lots, salts, etc) that are related to uniqueness and a cause for ambiguity or duplication errors. Registration systems can flag when researchers are unwittingly duplicating entries or screening different forms of the same entity. These systems can distinguish between entities with similar structures, sub-structures or sequences.

Tracking – another reason to register your entities using a registration system is their ability to store chemical and biological entities for future tracking. Researchers can run queries for entities and see full details about the structures, including information on stereochemistry or similar sequences.

Compliance – labs need to comply with government regulations. A good registration system can help ensure there are no surprises at lab inspections or audits. Since the information is in a single, central location, reports can be made quickly, accounting for all present entities.

Comparison with LIMS and ELN

Laboratory Informatics Management System (LIMS) and Electronic Laboratory Notebook (ELN) are related laboratory informatics tools that can have overlapping functionalities with registration systems. While LIMS typically follow pre-defined generalised workflows defined at the level of lab management, ELNs tend to be more personalised and flexible to change by individual researchers.

This distinction makes sense in the context of regulated environments, where LIMS are needed to support the tightly regimented workflows and structured data required in these spaces. With their more fluid nature, ELNs may be better suited for research and discovery environments, where changing workflows and unstructured data are more of the norm.

In contrast, registration systems are more similar to LIMS in their structuredness, but focus more on organising structures and activities at the chemical/biological entity level, rather than the sample level.

However, the lines between all these systems are increasingly fluid. For example, CDD Vault offers fully integrated registration system and ELN, as well as entity-tracking features typically expected of LIMS. When evaluating various solutions, researchers should look beyond the name to find a system that matches the needs of a particular lab.

Across industries, chemical and biological registration systems add significant value to R&D teams working with large numbers of chemical and biological entities and associated data. Implementing CDD Vault as part of a larger suite of research informatics tools can improve your operational efficiency, reduce risks of human error, save time and ensure the integrity and legacy of your work. ■

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SCIENTIFIC COMPUTING WORLD

Looking at cancer

Robert Roe discovers from Dan Ruderman, assistant professor of research medicine at the Ellison Institute USC, how advances in computer vision and AI computing are helping pathologists identify cancers more accurately – leading to better treatments

'80 years on pathologists still rely on their eyes to diagnose,' says Dan Ruderman, who together with his colleagues at the Ellison Institute have been using large-scale AI simulations, run in partnership with Oracle, using the Oracle Cloud Infrastructure.

'Pathologists use their eyes to make these decisions so whether they have gone from a microscope to now looking at digital images that have been scanned in from slides, they are still looking at them with their eyes and making those decisions,' Ruderman said.

Their research uses pre-existing Hematoxylin and eosin stains (H&E stains) to identify cancer subtypes by training neural networks.

'Every patient around the world who goes through surgery and has a pathologist examine specimens has an H&E stain done to find out what the diagnosis of this patient is,' said Ruderman. 'This means that it costs zero dollars, because the test has already been done.

'What is surprising about that is given the amazing advances we have had in computer vision for things like self-driving cars and certain modalities in medical imaging, we are not using the advanced capabilities of computers to help in these diagnoses to make better decisions for patient care.'

Using computers to assist in diagnosis

Today the fields of visual pathology and AI and machine learning are being employed to solve particularly challenging questions in the diagnosis of cancer subtypes. This is an important step in the effective treatment of cancer, because it means that patients can potentially receive the correct treatment faster and without having unwanted side effects from drugs that may be ineffective.

> "They are still looking at them with their eyes and making those decisions given the amazing advances we have had in computer vision"

'The big question in clinical care is who is going to respond to which

therapy. Once a diagnosis has been made, what subtype of, in my case cancer, is it, which determines the therapies a patient gets.'

There are several existing molecular markers that can help identify potential treatments but while 'they are good, they are not good enough,' argues Ruderman. 'For example, if there is a mutation in a patient's melanoma to the BRAF gene, they would be given Zelburaf to treat them. But despite having this molecular marker, only around half of those patients are going to respond to that drug,' added Ruderman. 'What is common to all of these is that patients are going to have to suffer the side effects of these therapies but not achieve any benefit.

The question that researchers at the Ellison Institute began to ask was: 'can AI help to make better decisions in these cases to predict, not just which patients have these markers, but which patients will respond?'

The initial research looked at hormone receptor-positive breast cancer. Traditionally this is done with a $300 immunohistochemistry test, if a sample is found to be estrogen receptor-positive (ER+) then approximately 60 per cent of patients respond to endocrine therapy such as Tamoxifen.

'Fundamentally these two cancers look the same under the microscope. If you ask a pathologist to designate just by eye from this kind of scan – is it an ER+ or ER- tumour? They generally would not be able to do it,' said Ruderman. 'There are certain subtypes, such as lobular cancers, where the cells all arrange in lines which could be identified as ER+ cancer, but that is a fairly rare subtype.

'Can we use AI and all the wonderful advances in computer vision to "read the tea leaves" and find things that are too subtle for our eyes to discern?'

The slides are digitised and then broken down into different measurable variables, such as the size of nuclei, orientation etc which is fed into a deep (more than five layers) neural network.

Testing on non-trained samples enabled researchers to create an ROC curve, which is a graphical plot that illustrates the diagnostic ability of a binary classifier system. The initial area under the curve (AOC) was 0.72.

While initial results were promising, several iterations of the network and advances in organisation, compression and fingerprint technologies have meant that the accuracy of prediction using the H&E stain has risen dramatically. AUC in the later tests was found to be 0.89, which provides a much better standard for diagnosis.

> "What is common to all of these therapies, is that patients are going to have to suffer side effects but not achieve any benefit"

Running on the Oracle Cloud Infrastructure, researchers at the Ellison Institute are using bare-metal GPU instances to run and train deep convolutional neural networks. They are also making use of Oracle Autonomous Database to store a lot of their training and inference data. 'We have tens of millions of rows in these database tables. Then on the shared file system, we have the whole slide images. Terabytes of data from all of these slides that have data captured,' said Ruderman.

The hope is to take multiple slides and produce a 3D model which could provide much greater accuracy, as the amount of data contained in each patient sample would increase dramatically.

Looking to the future

Ruderman also hopes that the work done here and at other research centres looking at different cancer types or other diagnoses can help to develop the frameworks for wider research into this combination of medicine, AI and computer vision.

'We can take that exact same slide that has already been created and extract more information out of it. This information can tell a clinician that they may benefit from hormonal therapy. That is valuable because those pills are cheap, for example,' said Ruderman. 'It is information already held in the slides they have in their hands. You just need to get it digitised and into a computer so they can make the analysis.'

This data could be collected at the point, or it could be mailed off and scanned at another location. However, Ruderman stressed that this should not be seen as a replacement for traditional methods, rather it should be used to supplement and improve doctors ability to diagnose.

'For every cancer, there is an alphabet soup of these kinds of mutations or tests you can do to subclassify these cancer-specific mutations according to what therapies they will respond to. If you look at the publications in digital pathology people are working on lung cancer, bowel cancer, prostate cancer and others,' said Ruderman.

'They are not exactly asking the same questions that we are asking but people are now digitising those samples and running deep convolutional neural networks on them.'

In this new age of AI and deep learning, Ruderman stressed that there is no magic bullet to develop the perfect model. 'We are still in the age where it is know-how, trial and error and an art form. The more computing power you have the more room you have to experiment and try different architectures simultaneously' said Ruderman.

This is a key part of the collaboration between the Ellison Institute and Oracle, as the computing power provided by the latter allows researchers to try different model parameters to explore the ways that the model can be improved.

'People are now getting things to work at a certain level and they publish their architecture. You might look at the number of layers and try to emulate it ,or build from that existing process or protocol developed previously.

'That is where having a lot of computing resources, that we have with our collaboration with Oracle, is really helpful, because it allows us to explore these things. The short answer is, there is no formula, go out for yourself and try stuff,' said Ruderman.

'You take something that works, start there and then tweak it. That is the world we are in right now. As computing power becomes more accessible, that means we can experiment more,' Ruderman concluded. ■

Dan Ruderman is assistant professor of research medicine at the Keck School of Medicine, and the Lawrence J Ellison Institute for Transformative Medicine, at the University of Southern California

Safeguarding quality, empowering collaboration

Thermo Fisher Scientific's Darren Barrington-Light highlights the need for standards as data volumes increase

Across all areas of the life sciences, the volume of data handled by analytical laboratories has massively expanded. Thanks to improvements in the capacity and speed of technologies such as liquid chromatography (LC), gas chromatography (GC) and mass spectrometry (MS), research organisations are generating data on an unprecedented scale.

At the same time, ongoing advances in bioinformatics tools, as well as data storage and computational processing power, mean scientists can now derive more insight from a greater number of samples, faster than ever before.

The expansion in the volume and complexity of laboratory data has occurred alongside the growing normalisation of outsourcing and strategic collaboration in the life science sector, which involves the sharing of data on a global scale.

Simultaneously, regulatory authorities have put additional focus on the accuracy, consistency and traceability of this information to protect the safety of consumers and end-users. As such, it has become more important for organisations to have the right digital tools in place to collect, store, manage and share laboratory data. But with aspects of information management challenging for even the smallest of laboratories, how can enterprise-level organisations, with teams working across several sites, optimise their digital systems to minimise inefficiencies and achieve the highest standards of data integrity?

The challenge of managing data securely and efficiently

For enterprise organisations with laboratories situated across multiple countries and even continents, commercial success depends on the seamless and secure flow of information between teams. With international supply chains, regional outsourcing partners and global centres of excellence, organisations must act as one – there's no room for fragmented thinking when it comes to winning the competitive advantage.

The limitations of adopting a fragmented approach to data management are perhaps most apparent at the interface between systems. While individual platforms might allow laboratories to perform specific functions successfully, considerable manual effort is required when it comes to applying or sharing this data downstream, including the transcription of data, conversion of file formats or navigation of complex folder systems.

Not only are these efforts slow and inefficient, but they also increase the potential for human error, putting the accuracy of data in jeopardy. Moreover, if multiple copies of the same dataset are stored on individual local systems, sharing the most up-to-date version between teams can cause confusion and waste valuable time and resources, if discrepancies must be investigated and resolved. Each of these issues can delay decisions, costing businesses valuable time and undermining organisational agility.

Additional challenges associated with poorly integrated data management systems centre around compliance. With information stored on local computer terminals – in some cases protected by a single user account used by the entire team – there is a greater risk of unauthorised or undocumented access.

Encountering these challenges in just a single laboratory can be a major headache. When you multiply these issues across an enterprise-level organisation, they become a serious threat to operational functionality.

Cloud-based CDS solutions: Simplifying data sharing and collaboration

Fortunately, modern cloud-based chromatography data system (CDS) software solutions are helping enterprise-level businesses to overcome the challenges of disparate information management through integrating people, technologies and workflows in a single system. By storing chromatography and MS data centrally in the cloud, these systems eliminate friction caused by using multiple systems, allowing instant, secure sharing and access of information from any location. With a single source of truth, all authorised individuals have seamless access to the data they need, helping teams spend more time on the tasks that add real value in workflows.

Furthermore, some of the latest

CDS solutions are highly compatible with instruments from a wide range of vendors, enabling teams to collaborate with whatever their legacy instruments. This enhanced flexibility also gives companies the freedom to invest in the best technologies available to them, unrestricted by vendor constraints, enabling full workflow scalability as business needs change.

Upholding enhanced standards of data integrity and compliance

In addition to streamlining workflows and making collaboration more efficient, cloud-based enterprise software is helping companies of all shapes and sizes safeguard the accuracy and integrity of their laboratory data. By applying a single, flexible solution across the organisation, businesses can standardise the way information is collected, processed and analysed, supporting more consistent and reliable outcomes.

Human-introduced errors are a major source of frustration in the analytical laboratory, potentially causing out-of-specification data, the need to re-run samples and, if working in a regulated environment, additional documentation for regulatory authorities. This challenge can be particularly acute for laboratories with multiple chromatography and MS control systems, or workflows requiring extensive manual steps for data processing or instrument set-up.

Cloud-based data management systems are making data more controllable with the latest CDS solutions delivering a level of information security that's a world away from the spreadsheet and paper-based workflows of the past. The flexible user management and secure access control features found in platforms like Thermo Scientific Chromeleon CDS, for example, allow individuals to be assigned unique view and edit privileges, ensuring individuals can only access and/or make changes to the information they are entitled to. This capability is supplemented by electronic signatures, assuring compliance with 21 CFR Part 11 requirements for the seamless implementation of paperless environments.

Also, by securely logging all user interactions with the system in a detailed audit trail, organisations can access an unambiguous source of truth with which to demonstrate full regulatory compliance. Thanks to the powerful audit trail search functionality and version management tools in the latest CDS packages, recalling specific events or investigating non-compliant behaviour is also quick and easy.

> **"Storing chromatography and MS data centrally in the cloud, eliminates friction caused by using multiple systems, allowing instant, secure sharing and access of information from any location"**

Assuring data integrity and boosting efficiency in biopharma

Given the benefits of bringing together teams, instruments and processes, enterprise-level organisations operating across the life science sector are increasingly leveraging new CDS software to streamline their workflows and better protect the integrity of their data.

One such organisation is a global, multi-site biotechnology company focused on drug discovery and development.

With sites around the world, the business needed an efficient solution that would seamlessly integrate users from across quality control, analytical development, and R&D laboratories. The platform had to simplify and empower collaboration, while maintaining robust data quality standards in their fast-paced regulated laboratories. After considering their options, the company chose to implement Chromeleon CDS, with data storage provided by Amazon Web Services, and Amazon AppStream set up to manage the applications.

The biotechnology company worked closely with application specialists at Thermo Fisher Scientific, who developed a cloud-based system architecture that ensured all data could be securely stored off-site, while fully meeting the needs of non-regulatory and regulatory compliant teams. The platform's flexibility meant the system could be implemented 'out-of-the-box', and its broad customisability allowed for the solution to be perfectly tailored to meet the company's needs across different business units.

Following a quick and hassle-free implementation, the CDS enabled the QC team to access their LC systems remotely via a browser, integrating more than 100 personnel across multiple teams at different sites.

One of the biggest advantages of the new system for the QC team was the ability to eliminate computer terminals from the laboratory itself, freeing up valuable workspace to expand analytical capacity. As well as making the company's laboratories more productive, this also strengthened their ability to uphold the highest standards of data integrity by reducing uncontrolled access to data across multiple workstations. Based on the inherent scalability afforded by the cloud-based platform, the company was able to expand its operations with minimal disruption, adding new LC systems as required.

Above all, the new cloud-based CDS software increased organisational flexibility, performance and productivity, while reducing IT operation and maintenance costs compared with on-site data storage.

As the volume of chromatography and MS data expands, fragmented approaches to information management are putting effective collaboration, operational efficiency and data integrity at risk. Thanks to the latest cloud-based CDS solutions, enterprise organisations are integrating their digital systems to achieve high-quality, compliant results.■

Darren Barrington-Light is senior product marketing manager, eCDS, Thermo Fisher Scientific

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