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AI and cloud drive digital lab transformation as lab informatics market to hit $8.7bn by 2029

The global laboratory software market is experiencing rapid growth through LIMS and ELN integration, with cloud-based solutions leading deployments in 2024. AI, synthetic biology, and IoT adoption are reshaping how laboratories manage data and conduct research across pharmaceuticals, biotechnology, and clinical diagnostics sectors, writes Rob Roe

The global laboratory informatics market is experiencing a period of growth due to the use of digital transformation and AI, as well as the rising use of data management tools to support these technologies. The global market growth also benefits from potential expansion in emerging countries and into new markets, such as the cannabis industry.

The laboratory software market primarily includes laboratory information management systems (LIMS), electronic lab notebooks (ELN), and other solutions designed to streamline laboratory workflows, improve data accuracy, and ensure compliance with a range of industry regulations.

The laboratory software market has experienced significant growth due to increasing laboratory automation, the rising adoption of cloud-based solutions, and the need for regulatory compliance across industries. This market encompasses a variety of sectors, including pharmaceuticals, biotechnology, clinical diagnostics, food and beverage, environmental testing, and research institutions. With advancements in AI and the internet of things (IoT), laboratory software solutions are becoming more sophisticated, enabling predictive analytics, real-time monitoring, and seamless integration with laboratory instruments. MarketsandResearch (M&R) reports the global laboratory informatics market at $5.3bn in 2024[1], while Precedence Research predicts it will be $3.95bn in 2025[2]. Both research companies predict the market will grow over the next few years, with M&R reporting it will reach $8.7bn in 2029 and Precedence predicting $5.22bn by 2034.

> “One of the most prominent changes over the next five to 10 years will be the continued convergence of LIMS and ELNs into unified, all-in-one platforms”

The discrepancy between these predictions stems from M&R predicting significant growth in the cannabis testing market segment. Both companies note that growth is being driven by several contributing factors, such as increasing investments in research and development, a shift toward sustainable laboratory practices, and the ongoing transition from paper-based systems to digital technologies.

That digital transformation makes LIMS a key contributor to this significant revenue growth. The demand for centralised data management, workflow automation, and regulatory compliance has made LIMS an essential tool across industries globally. As laboratories strive for Good Laboratory Practices (GLP) and high-quality data standards, LIMS adoption continues to rise.

The life sciences and pharma industries are at the forefront of digital transformation among lab-based industries. However, they lag behind banking, telecom, retail, and other industries in digital maturity. A McKinsey analysis from 2016[3] identified a multitude of factors that make life sciences companies slow to adopt digital and analytics (DnA) innovations, including not fully understanding healthcare practitioners’ (HCPs) decision journeys, challenges linking DnA to the broader business and difficulty maintaining an efficient operating model. Demand has been fueled by the growing emphasis on molecular diagnostics, increasing outsourcing by pharmaceutical companies, and the need for integrated laboratory systems. The sector is also

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driven by stringent regulatory guidelines, the expansion of biobanks, and the rising adoption of technologically advanced informatics solutions. It adds up to a complex picture that is fast moving.

AI impacts laboratory informatics by streamlining data storage, analysis, and retrieval. AI-powered algorithms enhance accuracy, reduce human error, and improve research efficiency. The integration of AI enables laboratories to process vast amounts of data for precise diagnostics, treatment planning, and scientific discovery.

Delivery models are also evolving, with cloud-based solutions reportedly making up the largest number of installed deployments in 2024[1] . Cloud technology offers remote access to massive data storage, reducing hardware dependency and enhancing operational flexibility. The 2022 State of Digital Lab Transformation in Biopharma Report from Tetra Science found that 74% of biopharma organisations are replatforming their scientific data to the cloud to enable scale, resilience, and faster time to market[4]. However, the future of laboratory informatics may be on-premise, in-house deployments, which are predicted to gain traction in new deployments in 2024[1]. This could be due to organisations seeking greater control over their laboratory informatics systems and their data in the future.

The LIMS and ELN market

The laboratory information management systems (LIMS) and electronic lab notebooks (ELN) market is experiencing growth, driven by the increasing need for efficient data management and enhanced laboratory operations. A notable trend is the convergence of LIMS and ELN functionalities into unified platforms, providing comprehensive solutions that streamline workflows and improve data accessibility. This integration facilitates seamless data exchange, enhances collaboration among researchers and supports compliance with a range of regulatory standards.

Integrating IoT devices with LIMS and ELN systems is also gaining momentum. IoT-enabled laboratory instruments can automatically capture and transmit data to these systems, reducing manual entry errors and providing real-time monitoring of laboratory environments.

Combined with a set of advances in AI and blockchain technology, these developments are driving laboratory software solutions to become more sophisticated, enabling predictive analytics, real-time monitoring, and seamless integration with laboratory instruments. Different industries have distinct requirements for laboratory software, of course. Pharmaceutical and biotechnology companies, for instance, require software that supports research and development, sample tracking and compliance with stringent GLP and FDA regulations.

Clinical and diagnostic laboratories prioritise software that facilitates patient sample tracking, integrates with electronic health records (EHR) and adheres to strict data security guidelines such as HIPAA. Environmental testing labs and the food and beverage industry often seek solutions to ensure quality control, regulatory compliance, and streamlined reporting. On the other hand, academic and research institutions require flexible and collaborative tools that support data sharing and project management.

Planning for the future of lab informatics

The laboratory informatics market is expected to undergo significant transformations over the next five to 10 years, driven by advancements in AI, automation, cloud computing, and data integration technologies.

One of the most prominent changes will be the continued convergence of LIMS and ELNs into unified, all-in-one


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> “Laboratories will increasingly adopt software-as-a-service (SaaS) models, making informatics solutions more accessible to small and mid-sized labs”

platforms. This integration will improve workflow efficiency, enhance regulatory compliance, and provide seamless data interoperability across research and clinical environments. The shift toward cloud-based solutions will accelerate, enabling remote access, real-time collaboration, and scalability while reducing IT infrastructure costs. Laboratories will increasingly adopt software-as-a-service (SaaS) models, making informatics solutions more accessible to small and mid-sized labs.

AI and machine learning will become more embedded in laboratory informatics, enabling predictive analytics, automated data interpretation, and enhanced decision-making. AI-driven algorithms will improve quality control, optimise workflows, and accelerate drug discovery by analysing large datasets more efficiently. Additionally, automation and robotics will reduce manual processes, increasing accuracy and reproducibility in experimental workflows.

Pushing for far greater data transparency

Regulatory compliance and data standardisation will become more critical as laboratory informatics solutions must align with stricter guidelines such as Good Laboratory Practices (GLP), Good Manufacturing Practices (GMP), and 21 CFR Part 11 for electronic records. As regulatory bodies push for far greater data transparency and security, vendors must enhance their software’s compliance features.

The next decade will see a shift toward more intelligent, automated, and highly integrated laboratory environments where digital transformation drives efficiency, accuracy, and collaboration. Adopting AI, cloud-based solutions, and IoT, will redefine laboratories’ operations, enabling faster scientific breakthroughs and better decision-making.

How emerging technologies will transform lab research

Emerging technologies, particularly in computational tools and advanced biotechnologies, will profoundly transform laboratory markets over the next decade. As computational tools such as AI and ML continue to evolve, they will drastically improve the efficiency and scope of laboratory research, particularly in data analysis, decision-making, and automation. AI and ML algorithms are already being utilised in a range of laboratory applications, from automating routine tasks to identifying complex patterns in large data sets. In the future, these technologies will not only automate experimental design and data collection, but also enable laboratories to generate previously impossible or time-consuming insights. For example, AI-driven predictive modelling will allow researchers to forecast experimental outcomes or detect subtle changes in experimental conditions that may otherwise go unnoticed. ML will also enhance personalised medicine by enabling more accurate analysis of patient data to develop tailored therapies.

Synthetic biology is emerging as a game-changing field with significant potential to impact laboratory research and the broader biotech industry. Synthetic biology combines engineering principles with biology to design and build new biological parts, systems, or organisms with novel functions. This field will drastically reduce the time and cost of experimentation in labs. Using genetic engineering and CRISPR technologies, researchers can more precisely manipulate genomes, accelerating drug development, disease modelling, and personalised therapies. In addition, synthetic biology will be key to the future of biomanufacturing, allowing for the efficient production of bio-based products, from fuels to pharmaceuticals, directly in laboratory settings.

Together, AI, ML, synthetic biology, and genetic engineering are transforming how labs approach research and development. Computational tools will allow for faster, more informed decision-making, while biological advancements will enable the creation of more accurate models and more effective therapeutics. Moreover, these technologies will enable laboratories to explore new areas of innovation, such as biocomputing and bioinformatics, and bring about breakthroughs in areas such as precision medicine, gene therapy, and regenerative medicine. The integration of these technologies will not only enhance the speed and scope of scientific discovery but will also make laboratory research more cost-effective, reducing barriers to entry for emerging start-ups and institutions in the field.

These emerging computational tools and advances in biotechnology will reshape laboratory markets by enabling faster innovation, improving accuracy and precision, and expanding the scope of possible research and treatments from more effective diagnostics to customised genetic therapies. **LIG**

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Go beyond data standards to better integrate LIMS

It's not lab data standards that create the value, says Burkhard Schaefer, it's the workflows and the use cases they enable

Burkhard Schaefer has been an active member of the laboratory informatics community for more than 25 years. He started his career working on instrument control and data standards at Los Alamos National Laboratory, and later at the National Institute of Standards and Technology. He co-founded BSSN Software, is the AnIML standard's lead architect, and is a SiLA Consortium board member. Burkhard Schaefer is currently the Managing Director of Splashlake.

At Pittcon this year, Schaefer will run a short course – Scientific Data Management and Instrument Integration – to provide a comprehensive overview of scientific data management and instrument integration with LIMS and ELN systems.

Burkhard Schaefer, the Managing Director of Splashlake

You have been engaged in the development of laboratory standards for several years. How have standards evolved during this time?

Schaefer: In the past, it's been about standards being front and centre. People were talking a lot about which standard you should be using, and it was getting political, whereas now, it's a question of what's the problem I'm trying to solve and what's the right tool to solve it? So, in retrospect, those discussions today feel like, what's better, a hammer or a screwdriver? Well, it depends. If you have a nail, you're better off with a hammer. If you have a screw, then your screwdriver will probably be more helpful, but in the end, they help you fulfil the same end goal. Your end goal is not hammers and screwdrivers, but to hang that picture of your family on the wall. You want to think about the picture, the family, the present memories, etc. You don't want to think about hammers and screwdrivers. And it's really the same thing with standards.

It's not the standards that create the value; it's the workflows and the use cases they enable. That's why people are doing it, and that's also what has caused a lot of friction in adopting standards: people were not talking about the beautiful pictures that you could now hang much more quickly. They were comparing tools.

So, what does that mean for the end user, the bench scientist or the laboratory manager?

Schaefer: Now, it's much more application-driven. What do you want

to achieve, and how can you get there? Standards can be a valuable tool in your toolbox that you can use to get certain things done, but you need much more. For example, when you are talking about an open data format, well, that data format is nice, but do you want to store it on a USB stick? Do you want to put it on your hard drive? Do you want to email it to a colleague? That's not what you would do in an everyday situation. You would need a system to store that data, which would need specific features and capabilities, and we were only talking about the format.

So, in the past, we had a JPEG versus PNG conversation, and we did not have a Photoshop conversation. So now we are having that conversation in terms of what the tools have to look like to increase productivity, improve data integrity, and create value in the lab, and there are a couple of things that make that rather challenging.

We already know about the fragmented landscape with all the different vendors and the different data formats. Now, we see people using more and more measurement and processing technologies together. You might have a robotic arm that handles the samples. That sample goes into a plate reader, which is later injected into a mass spectrometer. You've got several different instruments. They each represent a silo because they are different measurement techniques.

I can't use my mass spec instrument software to look at the plate reader data, and I can't use my plate reader software to look at the mass spec data. However, in the eyes of the scientists, they belong to the same experiment. How do I get them on the same screen?

It's helpful to normalise the data from those two instrument families into one common format. How do you get that in front of the scientist? How do you also then make that data ready for reuse when it comes to data analytics, when you're considering providing that data to the plethora of AI tools now available? We all depend on that solid data foundation and tools that allow us to do something with that data.

So that's why the standards debate has evolved from our perspective, and that has made a significant change. Now, when we're talking about the use cases, we find that people adopt the use case, and then they ask, 'Well, how did you do that? How do you get the plate reader data together with the mass spec data?' We will explain how that works, but we don't go out first and say, 'You should be using that standard'. The right way to think about the challenge is 'How do I solve this tricky use case?' The standard is working under the hood and enabling stuff, but that is all the scientists need to think about regarding the standards.

How can organisations better integrate the different data sources in a laboratory?

Schaefer: The middle layer is something that, historically, people had to build themselves, or they would hire third-party consultancies to create a bespoke solution for them. We thought, no, you know that this is just not sustainable, and it doesn't scale. So how about we come up with a set of repeatable patterns and try to productise this so that you can get these types of integrations as an off-the-shelf piece that knows how to access the data for that particular instrument and another piece that knows how to get it to where it needs to go.

You have a flow of data to the LIMS, ELN, AI tool, or wherever the data needs to go. However, it is important not to create a unidirectional data flow from the instrument to those systems, but to make it bi-directional. If the LIMS knows that I have the following tests to run, that list of tests can go to the instrument so that the instrument is pre-configured to run them, to build the sequences and things like that.

That's where we've been focusing in the past two years: to build that middle piece in a reusable way. So we've got a scalable approach that works with these patterns, and then we have something that complements the standards. Because the standards they define, these are the communication protocols. So whether you want to use SiLA or whether you want to use a web service, or whether you want to use MQTT, depending on the type of instruments, different ones work best, and we speak to those. But then, simultaneously, you've got the different data formats.

If it's analytical data, AnIML works well. But for microscopy data, you wouldn't use AnIML you're best using DICOM, or SVS; they are well established and work, so why replace them? It's thinking more about those use cases and then making that middle tier work with a curated set of standards and formats that allow the scientist to bring this solution into a lab.

Standards are open, and everyone can implement solutions themselves.

> "People were talking a lot about which standard you should be using, and it was getting political, whereas now, it's a question of what's the problem I'm trying to solve and what's the right tool to solve it?"

And if they want to do it in-house, they can. Historically, people have written all of that stuff in-house or had it written by third parties. But that creates challenges; we are seeing that people now ask 'If something goes wrong, who can I call for support? Who will fill in my cyber security audit questionnaire and who will take responsibility for operating this in a compliant environment?'

It's got to be a combination. There are the open standards, which we contribute to a lot, but then there is the tooling bit that allows you to use the standards where appropriate. You can also go proprietary if you want, but that sits in that middle piece that allows for that integration to work seamlessly, and that's what we've been working on in the past two years.

I really love this work because it's complementary. People have the choice of what they want to do. It's an open ecosystem, and we can accelerate the adoption of that ecosystem by making it trivial even for small companies to adopt. So, in some cases, we're working with small biotechs; it's a dozen people who otherwise could never afford to build this themselves, who don't have the expertise or resources and can now go-live within a month. And that's wonderful to see because, then, you're getting all of that work that we've done previously on the standardisation and you can get that to work in the labs and make people happy. That's how we look at it. **LIG**

Building better organoids: how bioinformatics drives innovation in lab models

Postdoctoral researcher Iguaracy Pinheiro de Sousa is using bioinformatics to develop better organoids, miniaturised 3D tissue cultures designed to mimic the structure and function of organs

Postdoctoral researcher Iguaracy Pinheiro de Sousa is using bioinformatics to support the development of better organoids. Working at EBI in the Petsalaki research group, Pinheiro de Sousa uses single-cell transcriptomics data to understand how different types of cells interact and communicate to form a tissue. One of the applications of his work is the development of organoids – miniaturised 3D tissue cultures, derived from stem cells, and designed to mimic the structure and function of organs.

EMBL

Iguaracy Pinheiro de Sousa, Postdoctoral Fellow at EMBL's European Bioinformatics Institute (EMBL-EBI)

Can you tell us about your background in biomedical science and how it led to your current research focus?

Pinheiro de Sousa: I chose biomedical science mainly for research purposes. When choosing my Bachelor's course after high school, I was wavering between medical school, biomedicine, and biology. Medical school was too clinic-focused, while biology was too broad. I found biomedicine to be a middle ground and became specifically interested in human genetics.

I pursued a Master's in genetics and molecular biology, working on a small study focused on pharmacogenetics in a hypertensive cohort from the Amazonian population, exploring how their genetic background influenced a particular hypertensive drug treatment. This led me to continue working on cardiovascular disease and eventually move to the Heart Institute in São Paulo.

Why transition from wet lab experiments to computational bioinformatics?

Pinheiro de Sousa: I met questions that required a more holistic approach, which was often limited by wet lab experiments and time-consuming methods. Bioinformatics allowed me to address these questions faster and with a broader perspective. The growing availability of public data facilitated this. However, the transition wasn't easy. I tried many online courses, but the turning point was having a bioinformatics project. Through its Next Generation Scientist program, I was selected for an internship at Novartis, in Basel, Switzerland. For three months away from the bench, I focused on developing computational skills in RNA-seq and ChIP-seq data analysis. Engaging in a bioinformatics project was key to enabling my transition. My PhD research on cardiovascular disease was helpful,

especially in interpreting computational results and extracting insights from big data. It helps translates findings into strategies for building better cardiac organoids; 3D miniaturised, cell-based in vitro models designed to mimic the structure and function of organs.

How are you using bioinformatics and single-cell transcriptomics data to improve the development of organoids?

Pinheiro de Sousa: I am using single-cell transcriptomics data to predict interactions between different cell types in heart tissue. By integrating databases based on known protein-protein interactions and prior knowledge of which proteins act as receptors and ligands, we can predict how cells communicate based on the gene expression levels of a receptor in one cell type and a ligand in another. This approach provides insights into higher-order cell-cell communication within a tissue, helping to identify the most relevant cells to co-culture with cardiac cells, thereby enhancing organoid complexity. Initiatives like the Human Cell Atlas (HCA) project, which aims to map all human cell types, provided the heart cell atlas data that made this work possible. Bioinformatics plays a key role by leveraging this data for biomedical applications. Current organoid models often lack cellular diversity, spatial organisation, and maturity to replicate native tissues. They tend to replicate only certain aspects of tissues, failing to capture the full complexity of cell types, maturation levels, and functions. Better organoids could address these gaps by providing models that more accurately mimic the native tissue environment, enabling a deeper understanding of tissue complexity and functionality.

I aim to address these limitations by developing a data-driven strategy to guide organoid construction. By selecting toptimal cell type combinations based on their interactions in native environments, we could improve cellular diversity and maturity. The goal is to create a user-friendly computational tool for generating data-driven organoid construction hypotheses, using cardiac organoids as a proof of concept.

How do you envision better organoids contributing to drug discovery and medical research?

Pinheiro de Sousa: Breakthroughs in organoid technology could lead to more accurate and functional models, supporting safer and more effective clinical research. Regulatory shifts, such as the FDA allowing clinical trials without prior animal testing, highlight the urgency for such advancements. Improved cardiac organoids, for example, could be used in ischemic heart disease, which leads to the loss of billions of cardiomyocytes and has limited regenerative treatment options. Thus, organoids that are more like adult tissue could serve as physiologically relevant platforms for drug testing, disease modelling, and regenerative medicine – key for medical research and therapeutic development.

> “The synergy between computational and experimental biology is crucial for increasing impact in biological research”

How does your work on nanorobots tie into your research on organoids and precision medicine?

Pinheiro de Sousa: My work primarily focuses on finding ‘addresses’ in the vasculature rather than developing the nanorobots themselves. The vasculature forms a continuous pathway that reaches all parts of the body. Every living cell is located within a small radius (100 µm) of the nearest blood vessel to receive oxygen, with few exceptions. A proof of concept using the vasculature for delivery was demonstrated by Yuliang Zhao et al. (2018), where DNA origami nanorobots were designed to deliver thrombin, a blood coagulation protease, to tumour-associated endothelial cells via the surface protein nucleolin. Nucleolin functioned as both a targeting domain and a trigger for the nanorobot thrombin release.

This approach successfully induced intravascular thrombosis, causing tumour necrosis and inhibiting tumour growth in mice. Connecting this to my research on organoids, if precise drug delivery is to ever be tested in humans, will need more robust and physiologically relevant organoids, particularly vascularised ones, to serve as platforms for testing these delivery systems.

How does the collaboration between computational and wet lab scientists accelerate organoid research?

Pinheiro de Sousa: When I moved to EMBL-EBI, I used to think computational scientists were at a disadvantage because they were less involved in experimental design (although this has changed significantly in recent years), while wet lab scientists were the main drivers of experimental design and data generation. However, computational work provides valuable insights that can generate new hypotheses to guide data generation, making it essential for these two fields to collaborate more closely. Without these wet-dry lab collaborations, we miss opportunities and place science as a whole at a disadvantage. Greater collaboration, particularly on hypotheses that require expertise in both fields, would unlock significant benefits for research. In the context of organoids, this collaboration is especially critical, as it integrates computational models with experimental data. This partnership enables the rapid testing of hypotheses and improves the design of organoids by combining computational predictions with biological experiments.

How will bioinformatics and data science advancements impact research in the coming years?

Pinheiro de Sousa: The advancements in bioinformatics and data science are already profoundly influencing biological research, but their potential impact could be even greater if the communication gap between computational and experimental scientists is bridged. These two groups often ‘speak different languages’, making active and collaborative communication essential for progress.

Better dialogue is key to formulating relevant questions from the massive amounts of data generated daily; questions that are computationally insightful and experimentally testable in the wet lab. However, some biological problems are difficult or impractical to explore experimentally. With the right data, such challenges can be addressed through computational modelling, enabling in silico simulations of complex biological processes. This approach saves time and resources while opening avenues to explore

otherwise inaccessible scenarios. The synergy between computational and experimental biology is crucial for increasing impact in biological research. Computational models can guide wet lab experiments, while experimental results refine and validate computational predictions. This back-and-forth collaboration creates a feedback loop that can drive transformative discoveries and advance our understanding of complex biological systems.

Describe some of the collaborative projects you are involved in.

Pinheiro de Sousa: Some questions in science require a highly interdisciplinary approach, and it can be challenging for one person to understand all the areas needed to address such questions deeply. This is where collaborations become crucial. Collaborating with experts from different fields broadens your perspective and guides your project in new directions while still addressing the core question. I still collaborate with my former supervisor from Brazil, where the cardiac organoid experiments are being tested. My co-supervisor is based at EMBL-Barcelona, developing vascularised tissues in vitro.

Recently, we started a collaboration with a nanoparticle engineer from Manchester University, which will be relevant for downstream projects involving targeted delivery systems. One particularly enjoyable collaboration was with a postdoc I met at a Network Signaling conference. She is based at Yale University and was investigating interactions between neurons and oligodendrocytes in healthy and Alzheimer's brains. Using a combination of cell-cell communication analysis pipeline and subcellular proteomics, we identified distinct communication patterns in Alzheimer's patients' brains. This fruitful collaboration generated two works that have just been accepted, one in Nature Neuroscience and the other in Nature Ageing. This partnership was unique because I contributed to answering her questions rather than the other way around, which is how collaborations should ideally work – mutually beneficial in both directions.

What advice would you give to young scientists interested in interdisciplinary research like yours?

Pinheiro de Sousa: My advice would be to embrace curiosity and actively seek collaborations across different fields, as these experiences broaden perspective. Interdisciplinary research thrives on combining diverse perspectives, so don't hesitate to engage with experts outside your area of expertise. Attend talks and lectures beyond your field; they can inspire unexpected connections, as they did for me during my PhD. Building a solid foundation in your primary discipline is essential, but developing communication skills to bridge gaps between fields is equally important. Finally, stay open to continuous learning and adaptation, even though it can be challenging. It's difficult to fully grasp other fields' methods and limitations, which can be frustrating. While you can't master everything, you can learn enough to address your research questions meaningfully. This is why collaboration is crucial. Experts in other fields can guide you on what's possible and help focus your efforts, making interdisciplinary work productive and transformative. LIG

Accelerating biomedical research with data-driven modelling

The Center for Computational and Systems Biology at Vanderbilt University aims to revolutionise research into human diseases by integrating cutting-edge computational tools and biological data

The Center for Computational and Systems Biology (CCSB), launched at Vanderbilt University in early 2025, will focus on analysing vast amounts of data to look for new ways to tackle challenges. It brings computer science, engineering and biomedical researchers together with clinicians at Vanderbilt University Medical Center to accelerate discovery related to human diseases and conditions.

The centre will analyse extensive data generated through new technologies to find innovative solutions to complex questions about human biological systems. Ken Lau, professor of cell and developmental biology, is its director. Lau's work, focusing on cellular profiling technologies and mining data for new insights, has led to key discoveries in inflammatory bowel disease and colorectal cancer. He publicly shares his data, software and analysis protocols to benefit the biomedical research community, to contribute to a new era of open science.

Vanderbilt University

Professor Ken Lau, the director of the Center for Computational and Systems Biology (CCSB) at Vanderbilt University

Can you tell us about yourself and your role at CCSB?

Lau: I have a PhD in bioinformatics and proteomics from the University of Toronto. Then, I did my postdoctoral fellowship. It was a joint postdoctoral fellowship at Massachusetts Institute of Technology and Massachusetts General Hospital. Systems biology has been around for 50-plus years. When I finished my postdoc, systems biology was done using mechanistic modelling. It is an engineering concept where models are built by understanding individual components and assembling them using various modelling approaches, such as ODEs [ordinary differential equations] and Boolean logic modelling. Scientists have since transitioned from mechanistic modelling to a more data-driven approach known as data-driven modelling. In the mid-2000s, big data, AI, and machine learning were not yet established fields. During my postdoctoral fellowship, I applied data-driven modelling – now recognised as machine learning and AI – to what is now called multiplex or multimodal datasets. These types of data sets are generated all the time, and you can generate them at higher and higher resolution, measuring more and more things and increasing the resolution such that you can get to a single-cell level. There are millions of cells within a tissue organ, so you have millions of data points that can be measured in a multimodal fashion. So this is where the AI machine learning approaches come in.

Previously, mechanistic modelling required understanding how components interact before assembling a model. The approach is reversed now: the rules are unknown, but the available

data can constrain the possibilities, allowing models to be built. This process demands significant computational power, using data and computation to uncover the underlying rules of biology. You're essentially working backwards – starting with data points and using them to determine the underlying mechanistic model of a biological system.

As Director of CCSB, I have been conducting this research for quite some time. We lead major studies in the field, focusing on integrating this mindset into biomedical sciences at Vanderbilt. The university is making a push toward computing, investing in AI, machine learning, and computational biology. There is a strong collaboration between the Medical Center and the university in human disease. There is a focus on bringing this sort of mindset to the biomedical sciences, first, within Vanderbilt, but also to the wider scientific community. At Vanderbilt, there is a push towards building a connected computing college and, as part of one of the directives, there will be a lot of investment in the infrastructure of AI, machine learning, and computational biology.

How can this type of modelling help further research into human disease and other complex illnesses?

Lau: Infections cause many human diseases, and the approach to treating them is relatively straightforward – helping the body eliminate the infection. However, complex diseases such as diabetes and cancer arise from the dysregulation of networks involving cells, microbes, and cellular interactions. Using computational and systems biology to understand and intervene in these diseases is promising. Viewing them as single-agent problems can seem overwhelming, but taking a systems approach offers a more hopeful path.

Addressing these complex diseases increasingly requires computational and systems-level approaches. Cancer, for example, exhibits extensive heterogeneity – patients have different genetics, and, even within an individual, primary tumours and metastases represent separate evolutionary processes. While personalised medicine was initially about tailoring drugs to populations; today, it involves analysing individual tumours and their genetic evolution. Historically, personalised cancer medicine was based on single-gene mutations and drug sensitivity, but this approach has had limited impact. Some cancers respond well to targeted treatments, but most involve robust networks of interactions requiring broader, systems-level understanding. The shift toward computational approaches has also changed the skill set required for biomedical research. Traditionally, students had biology backgrounds but, now, coding proficiency is essential. AI tools assist with coding, but the sheer volume of data makes it critical for researchers to leverage open-access datasets. Science is moving toward team-based research, with collaborations between data generators, analysts, and those developing machine-learning tools. Modern research also requires quantitative methods – simply presenting a microscopic image of a cell is no longer enough; researchers must provide statistical analyses and machine-readable formats for broader scientific use.

> "Using computational and systems biology to understand and intervene in diseases [such as diabetes and cancer] is promising"

Will you share CCSB data and tools?

Lau: We are committed to publicly sharing data and software tools. We aim to create an ecosystem where experts from different disciplines can collaborate. Computational research is often conducted in computer science departments, while biological research happens in biomedical departments, leading to communication barriers. We aim to lower those barriers, fostering collaboration between those who generate biological data and those who develop computational methods to analyse it. Vanderbilt is also centralising its computational resources. We currently use ACRE, a high-performance computing cluster, for routine tasks such as sequence alignment. However, AI research requires hundreds of GPUs, and Vanderbilt is working toward making these resources more accessible. Today, many departments maintain their own GPU clusters, but centralising these efforts will improve efficiency. We are also exploring quantum computing, which holds future potential.

How will CCSB help further research?

Lau: Regarding my own research, my lab focuses on the interface between inflammation, tissue damage, and tumour initiation. We prioritise early detection and intervention, even though it is not the most lucrative field. CCSB allows me to bring fresh perspectives and expertise. As director, my role is to recruit researchers with diverse expertise who can extract meaningful insights from complex datasets and to help experts from different disciplines to communicate effectively. AI and machine learning have been transformative, but they are not the sole focus of CCSB. The field is constantly evolving. For example, AlphaFold has revolutionised protein folding predictions, but we are always looking ahead – what comes after AlphaFold?

What are the next big challenges in computational biology?

Lau: One of the biggest challenges at CCSB is managing different expertise, personalities, and disciplines. Every field has its own culture and priorities, and even tenure and promotion criteria vary across departments. My role is to bridge these gaps and facilitate collaboration.

From a research perspective, a major challenge is working with publicly accessible data. While abundant, it is often disorganised, lacking standardised formats and annotations. Much of our work involves data wrangling – resolving inconsistencies, removing noise, and dealing with biases in human-annotated datasets. Ironically, despite being computational researchers, much of this process still requires manual intervention.

To improve data usability, researchers should avoid working in isolation and treat data accessibility as a priority rather than an afterthought. Large initiatives such as the Human Cell Atlas and the Human Tumor Atlas Network are working toward standardising data formats and metadata. We welcome collaborations with researchers generating similar data and can assist with proper annotation to enhance usability.

Ultimately, no single person can solve these challenges alone. Standardising data storage and accessibility is a collective effort within the global scientific community, requiring ongoing dialogue and collaboration. **LIG**

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Inside UCGD: how custom bioinformatics tools advance genomic research

UCGD's Carlson Holt discusses the role of UCGD Core in supporting researchers and providing services to support genetic discovery

In 2014, the State of Utah Science Technology and Research (USTAR) initiative and the University of Utah Health Sciences Center established the USTAR Center for Genetic Discovery (UCGD), intending to leverage Utah's unique resources to create a computational genomics hub in Utah. Today, the centre develops algorithms, software tools, analysis pipelines, and data management systems that enable researchers and clinicians to visualise and interpret genomic data.

Carlson Holt is the director of UCGD Core and helps to investigate the genetic basis for human disease by providing whole exome and whole genome sequence analyses for research and clinical projects, offering services to both academic and commercial users. The UCGD Core team specialises in variant calling and disease-gene discovery utilising tools developed by the Utah Center for Genetic Discovery, including VAAST, PHEVOR, VIQ, Smoove, Slivar, RUFUS and IOBIO.

Holt received his PhD from the University of Utah under Mark Yandell, before taking a postdoc position at the Ontario Institute of Cancer Research in Toronto, Canada. Yandell then recruited Holt back to UCGD and he has been there for the past 10 years. Holt has worked on a number of projects, including the development of the MAKER, a portable and easily configurable genome annotation pipeline that formed his PhD thesis project.

Carlson Holt is the Director of UCGD Core, part of the UCGD facility at the University of Utah

What enticed you to return to UCGD?

Holt: Mark Yandel, my boss. He's just a great person. And I love the work available here at the University of Utah – it has great computational resources; for example, the Center for High Performance Computing. I have access to thousands of CPUs and excellent storage resources for large data research. People don't realise how central the University of Utah has been in computation history.

You mention storage resources. How important are they for your work?

Holt: So much of what we do is data-limited. It's the biggest bottleneck. I have access to CPUs, but the I/O does not keep up with the CPUs. I just can't read and write the data fast enough, so having specialised fast storage is paramount. But storage is also a complex challenge; for example, one of the issues is you can't just buy a couple of 100GB. I have to buy four petabytes at a time. Finding the financial resources to make those large purchases every few years is difficult but also extremely important. My limiting factor is whether I can read and write the

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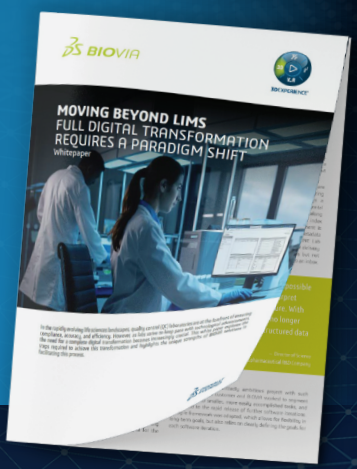

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data fast enough. And it doesn't matter how many CPUs I have. They're going to sit idle if my storage doesn't keep up.

You have to educate people on the importance of storage because it's not extremely exciting to hear about. CPUs are exciting, GPUs, AI, that's exciting. Storage is not, but it really is the bottleneck of everything here at UCGD. Every time we ask for money for a research project, medical genetics, etc, we always put in part of the budget for storage, and we make a very big point of explaining why it is important. Because otherwise these projects won't get done. It sounds like boring minutia, but it's the crux of everything.

How does the UCGD support genetics research?

Holt: The Utah Center for Genetic Discovery is this big academic initiative involving more than 50 researchers, scientists and developers. The three main PIs, Gabor Marth, Aaron Quinlan and Mark Yandel, are heavy hitters in bioinformatics. Mark developed MAKER, as well as other tools that are heavily used for genome annotation and human disease research. Gabor Marth created Freebayes, one of the first-ever variant callers. Aaron Quinlan developed BEDTools. Everybody uses BEDTools, and they also have several other tools they develop.

UCGD was created to share the software and software tools being developed by the centre with the wider academic community.

We take all of the research that is coming out of these labs and package it with our computational expertise because we're also part-time employees of the labs and have the computational resources. Collaborators have an easy location where they can go and say, "I want to use MAKER to annotate a genome" or "I want to use these other tools to explore human disease".

They can come to the centre, and we have the computational background, the tools we help develop and the computational resources that the university provides. We can get these collaborations going quickly based on a simple recharge model. If a collaborator only needs four hours of help, we can charge them four hours. If you need 25% of employees' effort for, say, three years, we can do that, too.

Who is a typical UCGD Core collaborator?

Holt: It's primarily academic, but we also work with commercial collaborators as well. One of the projects I can point to is something the University of Utah has that is called the Utah NeoSeq Project. What it does is this: sick children in the NICU [neonatal intensive care unit] are more likely to have a genetic basis for their condition. So the project team sequence the kids, and then we do the analysis through UCGD Core. We see if we can identify genetic reasons underlying their condition and we return that back to the clinicians. It goes directly back into the patients' treatment to see if we can identify something that's clinically actionable.

We have projects like that through the University of Utah, and we also have collaborations with Intermountain Health Network, where we're doing similar work with children in the NICU. We also work with the Undiagnosed Disease Network and Penelope Project, through Dr Lorenzo Botto at the University of Utah. These clinicians didn't have the bioinformatics expertise to do this part of their project, but they had the patients, the data sets, and the medical know-how. So we collaborate with them and provide this on a recharge basis. So those are a selection of three different projects. At the same time, we also do genome annotation. I annotated the Asian and African elephant genome in collaboration with labs at the University of Utah. If you have any kind of significant bioinformatics research, we will help you where we can.

Why does UCGD develop its own software tools?

Holt: We help develop a lot of these tools. I help develop MAKER; Barry Moore is one of the analysts in our group. He identified the first ever human disease identified by next-generation sequencing. It was the first time a new disease had been identified using VAAST, which was developed in the Yandel Lab. He commonly uses the successor to that tool, which is a Viqgem, to analyse human disease data sets to see if he can identify the potential cause, and that's a tool we developed at the University of Utah.

We have many of those types of tools. There's an active back-and-forth where we use the tools we've previously developed and the data sets we get to create new tools. Once those tools are developed, we can offer them as services through UCGD Core.

That's interesting. Can you give an example of how these tools evolve from your experience? It's an area that we are particularly interested in.

> "Storage really is the bottleneck of everything here. Every time we ask for money for a research project – medical genetics, etc – we always put in part of the budget for storage"

Holt: Okay, so an example would be VAAST. This software uses a burden test to identify the probable cause for genetic disease, but that might not give us enough statistical power in all situations, so we have a new version called VAAST 2, pVAAST (pedigree Variant Annotation, Analysis & Search Tool) that now uses pedigree-based information.

So we take the information based on the family to see how the disease separates, goes through the generations and in conjunction with the burden test, and now we have more statistical power. On top of that, we have developed prior probabilities based off of a connection network where we look at phenotypic and gene annotation. For example, if there's a GO term associated with a gene, but there are also other GO terms associated with it, we can look at the connections between multiple genes in the network and develop a probability network. That way, when we identify a gene with a specific phenotype, we're able to propagate probabilities across that network to identify new genes that may be associated, just based on that network connection. We found that that increased the power of identifying disease genes, and that was a tool called PHEVOR, which they came out with a while ago.

These tools build on top of each other. As part of a collaboration, we might identify that a tool works much better based on the work we're doing if we were to add something. So we develop a new tool, find out it works better, and then we can take on new collaborations to do similar work. **LIG**

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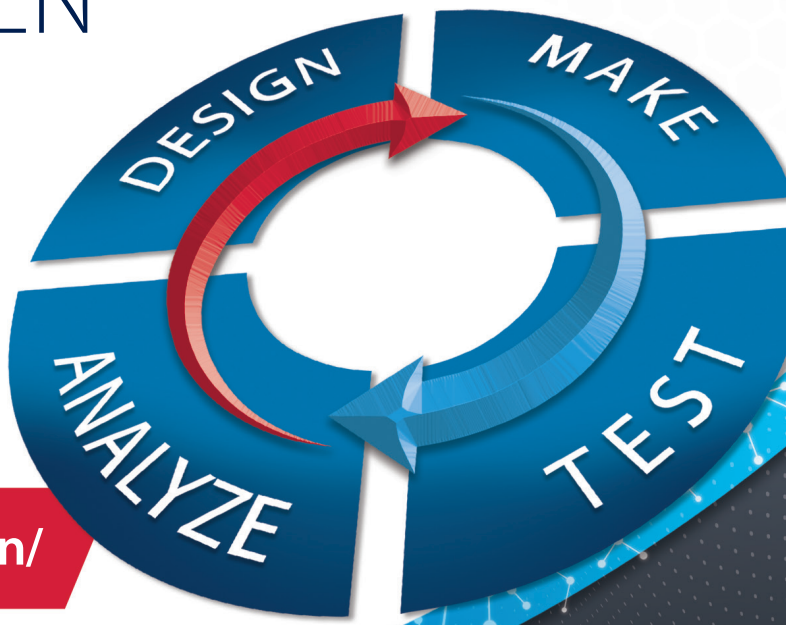

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From cancer data to treatment: Nancy Guo's precision medicine vision

Binghamton University's Nancy Guo discusses the use of AI to treat cancer patients earlier, leading to better patient outcomes and the development of new medicines and treatments based on data-driven research using precision medicine

Empire Innovation Professor Nancy Guo joined the Binghamton University faculty in autumn 2024. Guo is experienced in leading foundation AI-based multidisciplinary research as principal investigator (PI) of two National Institutes of Health (NIH) R01s and two National Science Foundation (NSF) grants. She obtained more than $45.5m in federal funding as PI/PD to develop technology and infrastructure to advance precision medicine. In addition to the software platform, Guo and her colleagues also developed a seven-gene lung cancer assay that accurately predicts the risk of tumour recurrence and metastasis while assessing the clinical benefits of chemotherapy. This invention has been validated in more than 1,600 patients to date, including a randomised phase 3 clinical trial. The FDA has now recognised its significance by classifying it as a 'Novel Technology' in its review process.

As the founding director of the Biomedical Informatics Resources Core of West Virginia Clinical and Translational Science Institute from 2009-17, she led statewide informatics initiatives and enhanced multi-state collaboration. She is fostering academic-industry partnerships for the clinical commercialisation of AI-based cancer treatment selection and drug development through her current NSF PFI-RP project.

Guo has not only been focused on software and assay development, but also identifying new drugs and new indications for existing drugs for the treatment of lung cancer and breast cancer. Through the patented AI software pipeline, Guo has made significant contributions to advancing cancer diagnostics and therapeutics.

Jonathan Cohen/Binghamton University

Nancy Guo, SUNY Empire Innovation Professor at the School of Computing at Binghamton University's Thomas J. Watson College of Engineering and Applied Science

Can you tell us about your role at Binghamton University?

Guo: I'm a newly hired SUNY Empire innovation professor. Specifically, this is a track for AI machine learning in healthcare. My expectation in this role is to establish a multidisciplinary, multi-institutional collaboration. Precision medicine is multidisciplinary. We need expertise from different fields. For example, we need people who

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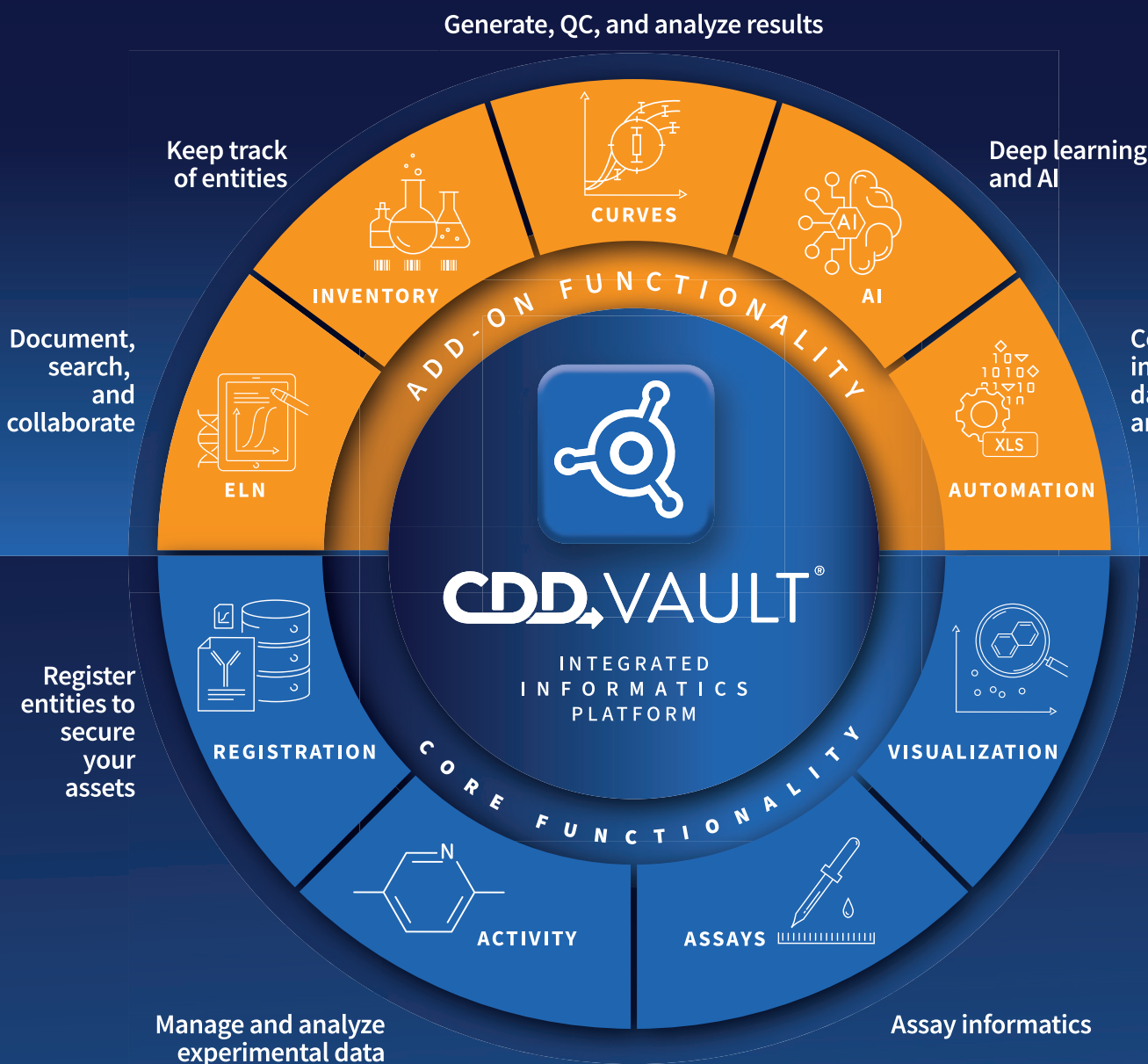

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understand AI, machine learning, and computer science, and we need people who understand hardware and biomedical engineering to make medical devices. We need clinical expertise involved from the beginning to understand their unmet needs. Inevitably, we also need expertise from biology and pharmacy if we are talking about medicine. We need experts to ensure the algorithms and the innovation we seek to develop make clinical and biological sense.

Why did you choose this path?

Guo: When I thought about my major in college at that time, I discussed it with my parents. My father was a university professor in engineering, specifically fluid dynamics, and my mom majored in chemistry. I was interested in understanding the human body and how it works systematically and precisely. Then, I took one class at university that taught us how to programme. Specifically, we learned how to use computer programming to compute a polling gene in DNA. I found that interesting. That's the only course where this was close to what I wanted to do. At that time, few universities had a bioinformatics degree programme. So, the best way to learn about these techniques is to learn computer science. I subsequently got into a project using computational methods to analyse EKG [electrocardiogram] results to analyse the heartbeat to detect heart attacks or abnormal heart events earlier.

How did you come to computational genomics?

When I switched to computer science for my master's. The technology to measure genes in the genome was becoming more established. About 6,000-7,000 genes had been catalogued and measured then. I decided that I needed to learn computer science to get involved in this research.

Can you talk about your breakthroughs in cancer research?

Guo: We first developed this AI technology, and then applied it to analyse cancer patient genomes. We decided to focus on lung cancer as this type of cancer has the second-highest incidence rates for both men and women, and the top cancer-related mortality rate for both men and women. The current trend is that more and more non-smokers have lung cancer. Through the research, we initially analysed the publicly available patient data. We could focus on 200 genes that we thought important. Then, we collected samples from multiple US hospitals. From that, we reduced the number of genes to seven and developed a microfluidic chip. This medical device can predict early-stage patients who may develop tumours that will metastasise and may benefit from chemotherapy. We found that these seven genes can be used to accurately predict the risk of tumour occurrence and metastasis in the earliest stage of cancer patients. These patients would receive surgery, but about 40% to 60% of them would develop tumour recurrence, followed by metastasis, and then die within five years after surgery. Before this research, there was just no way to tell whose tumour was more aggressive molecularly. After publishing this method, people such as oncologist colleagues would ask, "I have a patient. Can I use your funding to decide whether he needs chemotherapy?" But this was research funding; they couldn't use it. In 2023, Guo received a $565,994 grant from the NSF's Partnerships for Innovation Program to encourage the development of market-oriented prototypes and a multidisciplinary graduate training programme. This grant helped to accelerate the market-oriented development of prototype products and the AI tools used to diagnose cancer patients using the gene assays developed by Guo and her team.

> "Precision medicine is multidisciplinary. We need people who understand AI, machine learning, and computer science, and we need people who understand hardware and biomedical engineering"

Can you commercialise this technology?

Guo: From the research side, we felt that we had solved the problem, but the challenge was to turn that into something that could be used in hospitals. At that time, I got a grant from the NIH (National Institutes of Health) that focused on turning this idea into a product. Through that, I learned that you need to think about how to produce a commercial product so clinicians and doctors can use it in a clinical setting. One aspect of this was a one-on-one coaching programme and, through that, I learned that you need to register for a company, get a small business grant, find a licensing partner, and go through all that process before you can get a new product in a clinic. Once we had gone through that process, in 2020, we submitted the technology to the FDA, which gave us the status of novel technology. Through the process from research to commercialisation, I received tremendous help from the National Institutes of Health and National Science Foundation. They've been funding us and providing all kinds of programmes to train us in innovation and entrepreneurship, such as how to assess a current unmet clinical need.

What are the remaining challenges for your precision medicine research?

Guo: One ongoing area of research for us is how we translate research into products, and we're also looking at the next generation of technology. Everything we have done so far is based on 20 years of research, just from my group and all others, because we leverage many other public resources and data sets. So, before looking at the next generation of technology, especially AI, we must ensure that we stay at the forefront of biomedical research. So that really has something to do with how we structure the institute we're building. We know what is needed to continue, and then try to fill the current gap. Filling the gap means we are branching out. For example, my expertise is in genomic analysis and computational genomics. However, some people are experienced with medical image analysis, so how do we work with them? How can we integrate genomic research with medical imaging. There are many new emerging technologies, foundational AI models and large language models (LIMs). We need to think about how to leverage emerging technologies. But we will not just stop at research.

We can deliver products that can be implemented in the healthcare system. It is about improving existing technology, developing new technology and forming collaborations. **LIG**

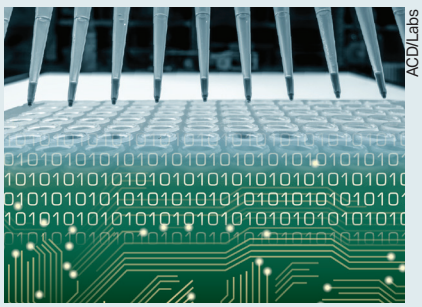
Case Study: Facilitating AI/ML in chemistry R&D – data science and high throughput experimentation

How leading pharma firms use Katalyst D2D to streamline AI/ML dataset creation, reduce workload, and gain data-driven insights

The past decade has seen a resurgence of interest in automating and parallelising chemistry. High throughput experimentation (HTE) accelerates reaction optimisation by enabling miniaturised reactions that consume less material and run in parallel. HTE provides data for reaction optimisation faster than traditional sequential experimentation and is ideal for producing comprehensive datasets for machine learning (ML). Pharmaceutical R&D organisations have invested in hardware to automate reaction execution and software to streamline these data-rich workflows.

Fragmented software across the workflow is particularly challenging in HTE given the large volumes of data generated. HTE teams at leading pharmaceutical organisations have adopted Katalyst D2D to integrate hardware and software into a single interface. The software has helped streamline parallel chemistry workflows, automate the collection and correlation of results, and ensure consistent data management. Users have been able to produce data for data-hungry AI/ML applications and investigate leveraging it.

We explore how teams at three top pharmaceutical organisations are preparing to leverage HTE data for AI/ML and achieving significant efficiency gains.



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HTE teams at leading pharmaceutical organisations have adopted Katalyst D2D to integrate hardware and software into a single interface

Satisfying AI/ML data requirements

ML models that predict reaction outcomes are an excellent way to accelerate drug discovery. Robust predictive AI/ML models for the prediction of successful synthetic experiments require:

- High quality data
- Consistent acquisition and processing of data
- Negative and positive results
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Generating consistent data

Company #1 took the first step of unifying its HTE data in a single solution with Katalyst D2D four years ago, looking to arrive at answers more quickly and leverage AI/ML to help design experiments. Having expanded HTE across discovery and process chemistry, it is now starting to pull data out of the software as JSON files and push it into data visualisation tools such as Spotfire to understand trends and investigate data science applications.

AI/ML dataset production

Company #2 began to mine data from Katalyst D2D for AI/ML applications within a year of deployment and has pipelined it into a data lake for AI/ML use. It almost doubled its HTE user base in 24 months (from 77 to >130 users) and averaged 560 HT experiments a year. The consistent, complete, and contextual data acquired and managed in Katalyst D2D has provided Company #2 with the ability to explore leveraging HTE data in AI/ML applications. "Katalyst D2D ensures that all the criteria for building robust predictive AI/ML models are met for our HTE screens. Katalyst D2D's ability to help scientists easily design large arrays of experiments and record data in a consistent fashion holds great promise for building efficient machine learning models" – Head of HTE, Company #2

ML model building

Company #3 generated and analysed 3,000 data points from an HTE amide coupling study to build a 'proof of concept' machine learning model for reaction yield prediction. "The robust database and data architecture [of Katalyst D2D] allows you to go from an experiment to a data science model very quickly, without the need to do very tedious data cleaning tasks. From a data science perspective, the data goes directly from running the experiment to being written to the Katalyst D2D database. The data can then be pulled from there into Python to do all your data science workflows [and that's] almost seamlessly" – Associate Scientific Director, Company #3

Leveraging AI in experiment design

More recently, Company #3 collaborated with the Doyle lab at UCLA to create a Bayesian Optimisation algorithm that could be applied to exploit known reaction information in the design of HT experiments. The resulting Experiment Design Bayesian Optimiser (EDBO+) algorithm was integrated into Katalyst.

The EDBO+ algorithm was tested using a common amide coupling reaction. The objective: to identify reaction parameters for maximum yield and minimal impurities.

20 reaction variables (different solvents, coupling reagents, bases, and a variety of reaction concentrations and reagent equivalents) represent a total design space of 1,296 reactions. Investigating these experimentally would require 14 rounds of experiments in 96-well plates, which is both time-consuming and also requires a significant amount of material.

Results from AI-enabled experiment design

Using the EDBO+ algorithm, the group identified optimal conditions for the amidation in 24 reactions (four rounds of six) – a fraction (2%) of the full factorial 1,296 design space. These savings of time, effort, and consumables represent the benefits researchers are hoping to realise from leveraging AI/ML technologies.

The future of data-driven R&D

HTE lends itself to consistent and efficient dataset production for AI/ML. In turn, integration of these technologies into HT workflows delivers measurable results. Teams are streamlining workflows and improving efficiency to accelerate time-to-market. As AI-driven approaches continue to evolve, the synergy between automation and data science will unlock new avenues of application, enabling scientists to push the boundaries of discovery to make smarter, data-informed decisions. **LIG**

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AI synthetic biology 'five to 10 years' from maturity

Reuben Harwood, Director of Research at Gartner's Healthcare and Life Sciences team, discusses the disruptive technologies reshaping life sciences – from AI and synthetic biology to quantum computing – and the timeline for their adoption

Reuben Harwood's research explores the rise of generative AI and accelerated use of AI more broadly to advance drug and scientific discovery. As Director of Research with Gartner's Healthcare and Life Sciences team, he leads the research and consulting company's coverage of genomics, multiomics, cell and gene therapies, synthetic biology and precision medicine.

Harwood has a doctorate in cancer research using precision medicine. He has supported Gartner clients for nine years across a variety of roles. Before working at Gartner, he was involved in the life sciences fields of bioinformatics, and molecular and cellular biology.

What are the most disruptive technologies in the markets that you cover?

Harwood: So much is talked about AI and machine learning these days. Machine learning-based workflows have been around for a long time in the life sciences. With the advent of foundation models and generative AI, we've all experienced huge growth in the adoption of AI technology through Chat GPT. A huge amount can be done through typical large language models and language models based on the language of life, DNA, RNA and proteins within biology. The topic of AI and machine learning is certainly a major focus.

On the technology front, you can also get into lab instrumentation. We all know the story of gene sequencing and the huge reduction in costs that has occurred through more and more enhanced techniques for gene sequencing. Similar kinds of transformations are happening in other areas, such as omics disciplines, transcriptomics and proteomics, which is looking at the RNA level and the protein level within cells and systems.

Other instrumentation can align with certain therapeutics. If you take the emerging classes of cell and gene therapies, you have things such as the CAR T-cell therapies for oncology. These are transformational therapeutics, but the ability to manufacture them is a major issue. A lot of instrumentation and technology are being developed to help automate and streamline these processes to support cell and gene therapies at scale.

Is synthetic biology mature enough to make an impact on life sciences?

Harwood: There are many researchers in the synthetic biology space, and it brings together biologists with your computational analytics part and the mathematics and engineering. It brings together a lot of different disciplines at Gartner. We have [predicted] the AI synthetic biology tools as five to 10 years to 'plateau', which is the part of the hype cycle where these technologies are mature within the market and well adopted.

Reuben Harwood is a Director Analyst with Gartner's Healthcare and Life Sciences team

There's a bit of time before synthetic biology tools are fully implemented. But you'll see synthetic biology tools used in many gene therapies. It was 2023 when the first CRISPR-based gene therapeutic received regulatory approval in Europe and the US. That was a significant milestone because CRISPR is a form of genetic engineering, a form of synthetic biology, designing the DNA sequence by correcting it at the genetic level.

Can quantum computing be included in this group of disruptive technologies?

Harwood: I track a lot of tech bio companies, these very technology-first drug discovery companies. [Many are]

advancing things in the quantum space, collaborating with partners like IBM and others, such as AWS and Google.

They've all got their quantum initiatives, and we're starting to see some progress in that space. However, the quantum technology itself is still a bit further away from the material technology. There is still longer to wait before content quantum-based computing is mainstream.

How does precision medicine impact lab markets?

Harwood: Precision medicine has been on the agenda for quite a while, which acknowledges that a one-size-fits-all approach doesn't work for the vast majority of disease indications. This field focuses on being able to tailor treatments to a specific patient – either to tailor dosing or to tailor an option of a few different therapeutics. However, it can also be used in designing and inventing a new drug, which can be the precision medicine component.

A large proportion of drugs that have received regulatory approval in recent years have come with biomarkers, which, in itself, are a way of targeting specific patients who will benefit from these drugs. Precision medicine is a reality from a drug development perspective.

Many of the therapies that we have just talked about, whether you're in the gene therapy space or cell therapy space, RNA therapeutics, are founded in the concept of precision medicine.

> "A huge amount can be done through typical large language models and language models based on the language of life, DNA, RNA and proteins within biology"

How is AI being implemented in drug discovery?

Harwood: The application of AI in clinical trials is fascinating. These include matching patients to trials, using generative AI to generate first drafts, and helping draft some of the content for regulatory submissions. Then you get into the manufacturing and supply chain spaces, where there are also different use cases for AI. One example could be electronic batch record mining. So investigating the electronic batch records and many other things.

AI is also being used on the commercialisation side. Selling off drugs and making sure that you sell drugs into the healthcare system and to hospitals and inform doctors and clinicians about your products. There really are a lot of use cases for AI in that area.

There are applications of AI across the life sciences, value chain, and generative AI has undoubtedly brought the potential for significant efficiencies and enhanced productivity. The reality is that life science companies are trying to work out how to build the data and infrastructure to support those different projects. One of the major pieces still being worked through is the data and analytics governance.

Is there a reliance on public data sets to train AI models in life sciences?

Harwood: There is a strong reliance on public data sets. Every life science company will be accessing public data sets in their R&D department, leveraging all of the information that is there to help them in multiple steps of the early drug discovery, the target identification and the candidate development stages of the life cycle of the drug development processes.

The use of these databases has been evident in things such as AlphaFold. So the development of AlphaFold by Google's Deep Mind leverages the data available in the PDB – the Protein Data Bank, which is an example of a very rich data set of protein sequences and their structures. Through access to this database, one can train a model to predict the 3D structures of proteins based on their sequence.

We need to do much more to develop such data sets for other areas or molecules on which we wish to build models. So, data sharing is important, and typically, life science companies have a lot of internal resources and a lot of internal data proprietary to their company.

You do see some partnerships between companies that have large data sets and some of the AI companies, and you'll see the partnerships established there where they leverage companies such as Nvidia to help them build models based on their data sets. So that's the flip side of this...

Even when they have proprietary data sets, there's a desire within these companies to build proprietary models. LIG

How AI is revolutionising cybersecurity in pharmaceutical companies

As cyber threats evolve and data breaches cost pharmaceutical companies millions, artificial intelligence emerges as an incredibly powerful tool for protecting sensitive medical data and valuable intellectual property, says Juan José López

The pharmaceutical industry faces increasingly sophisticated cyber attacks targeting valuable patient information and research data, particularly around blockbuster drug development. While the sector has made progress in cybersecurity, with data breach costs falling from $5.01m in 2022 to $4.82m in 2023, malicious attacks still account for 45% of breaches. However, AI is emerging as a possible solution, offering real-time threat detection, automated security monitoring and predictive capabilities that can identify vulnerabilities before they're exploited. For pharmaceutical companies navigating complex regulatory requirements such as GDPR and HIPAA, AI-driven security systems are becoming essential for protecting sensitive data and intellectual property.

Juan José López is Associate Director of Cybersecurity Architecture and Governance, Life Sciences Manufacturing, at Cognizant, which provides AI tools in several industries, including life sciences, healthcare, manufacturing, and engineering, to help organisations such as pharmaceutical and biotech companies to integrate digital transformation into their wider business strategies.

With more than 15 years of experience as a cybersecurity professional, López is a member of the ISA99 Industrial Automation and Control Systems Security committee and holds a Master's Degree in Implementing, Managing, and Auditing Information Security Management Systems.

Juan José López is the Associate Director of Cybersecurity Architecture and Governance, Life Sciences Manufacturing, at Cognizant

What is the scope of the cybersecurity challenge in life sciences?

López: In life sciences, sensitive data such as patient information and research findings are susceptible to advanced cyber attacks. This data is extremely valuable, especially when related to the development of blockbuster drugs, which can often be a company's most valuable asset. Traditional security measures are no longer sufficient, as cybercriminals have become increasingly sophisticated at exploiting gaps in organisations' defences.

AI offers the potential to enhance data management and strengthen cybersecurity by detecting and responding to threats in real time and identifying and mitigating vulnerabilities that are found in IT systems.

The pharmaceutical industry has progressed in data protection and cybersecurity over the past five years. The average cost of a data breach decreased from $5.01 million in 2022 to $4.82 million in 2023[1]. Detection (189 days) and containment (66 days) times for data breaches have also improved, falling below global averages[2].

Malicious attacks remain the

primary cause of data breaches in the pharmaceutical sector (at 45%), followed by human error (28%) and IT failures (27%). Phishing-compromised credentials and cloud misconfigurations are common attack vectors. Multi-cloud environments are the most vulnerable and incur the highest breach costs.

Data breaches are not just an inconvenience for the life sciences industry. They disrupt operations, manufacturing and supply chains. Intellectual property (IP) theft and patient data breaches also lead to financial losses and legal consequences. Companies may face fines for failure to comply with data protection regulations, such as Good Manufacturing Practices (GMP), Good Laboratory Practices (GLP), Global Data Protection Regulation (GDPR), and the US Health Insurance Portability and Accountability Act (HIPAA). For example, HIPAA fines average $1.5m per violation. Non-compliance with the EU's new NIS2 Directive may also result in fines of up to €10m or 2% of revenue (essential entities) or €7m or 1.4% of revenue.

In what areas can AI be used for cybersecurity?

López: There are several key areas. Generative AI can offer real-time analysis of vast data to identify patterns and anomalies indicative of potential security breaches, enabling immediate response and prevention of attacks. AI-driven systems continuously monitor network traffic, user behaviour and system activities to detect potential cyber threats. AI can also predict future cyberattacks by analysing historical data and trends. This foresight allows pharmaceutical companies to really bolster defences and allocate their resources strategically.

AI algorithms can control access to sensitive data, ensuring only authorised personnel can handle it. This helps organisations comply with data protection regulations such as GDPR and HIPAA, keeping their data safe and compliant. AI automates routine security tasks such as monitoring traffic, updating protocols and managing access controls. This reduces workload, minimises errors and ensures consistent security enforcement throughout the whole organisation.

AI enables pharma companies to analyse data from various external sources, providing a comprehensive view of potential threats. This collaborative intelligence helps organisations stay vigilant and adopt effective strategies from their industry peers. AI also standardises threat intelligence formats for seamless sharing and utilisation.

Complementing human insight, AI can bridge the cybersecurity skills gap in the pharmaceutical industry by augmenting existing teams and providing insights for humans to consider. Generative AI can even help with training staff through simulated attacks.

How can AI tackle these threats?

López: Incorporating AI into the digital transformation of pharmaceutical companies can revolutionise threat detection and risk mitigation strategies. AI can enhance security measures, reducing the likelihood of data breaches and ensuring compliance with regulatory requirements. In particular, new generative AI tools – a type of AI that uses machine learning and automation to mirror human problem-solving skills – can analyse vast amounts of security data across various systems in real time, providing accurate recommendations without requiring manual intervention.

AI-driven cybersecurity solutions offer many benefits but can pose challenges when it comes to implementation. Following a few steps can help ensure any AI-driven cybersecurity digital transformation project runs smoothly.

AI systems rely on high-quality data to function effectively, but challenges can arise in accessing this information due to silos in legacy systems and different departments. Collaboration with experts at the project's outset is crucial to ensure accurate and up-to-date data. These experts can support auditing an organisation's data, identifying relevant databases and systems, and assessing data quality. Following an audit, planning an AI-enabled cybersecurity solution tailored to the company's specific needs is possible.

Integrating AI-driven cybersecurity solutions with a range of complex IT infrastructures, including legacy systems, can be challenging. Legacy systems may require customisation and upgrades for seamless integration. Early consideration of this issue is crucial to avoid unforeseen costs and ensure an effective solution.

Expert support reviewing the capacity of both existing and new AI-enabled digital systems can ensure the finished system is cost-effective and compliant to avoid the financial and reputational repercussions of failing to meet

> "Intellectual property theft and patient data breaches also lead to financial losses and legal consequences"

the requirements of GDPR, HIPAA and related legislation. A workforce skilled in generative AI technologies is essential to the success of any new AI cybersecurity system. The sooner upskilling begins, the better, as it helps ensure that companies have the in-house expertise to harness new AI-enabled systems effectively.

An engaged team is vital for the new AI security system to succeed, but some business employees may be sceptical about the tool's capabilities and trustworthiness. Involving team members in the planning and implementation process early can help them understand the new system and appreciate its full potential for supporting their day-to-day work.

AI systems must adapt swiftly to evolving cyber threats. Regular training and updates are essential but can be resource-intensive. Early planning for reviews and updates can help streamline the resources needed.

Deploying cutting-edge technologies like AI can be daunting for life sciences companies with complex legacy infrastructure. Collaborating with a specialised digital transformation partner with expertise in harnessing AI's potential can help organisations overcome integration barriers.

Such a partnership ensures the development of an effective AI-driven cybersecurity system seamlessly integrated with critical systems, minimising disruption and delivering optimal performance. **LIG**

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[1] https://securityintelligence.com/articles/cost-of-a-data-breach-2023-pharmaceutical-industry/

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In drug discovery: why partnerships could hold the key to better biological data analysis

Dr Rob Grundy MBE explains how collaborative approaches to AI implementation could help both large and small organisations overcome traditional drug discovery bottlenecks while avoiding costly technology investments

The pharmaceutical industry faces persistent challenges with high failure rates in clinical trials, creating significant burdens for companies, investors, and patients. Dr Rob Grundy MBE, Director of Innovation Partnerships at Catalyst, suggests that a collaborative approach to AI adoption could be the key to overcoming these obstacles.

Rather than making substantial internal AI investments, he advocates for partnership models that enable shared access to advanced machine learning tools and collective learning opportunities. This approach, he argues, could help unlock the 'dark biology' that traditional peer-reviewed research has missed, while avoiding the trap of being locked into outdated technology investments.

With more than 25 years of experience in pharma and biotech, Grundy brings considerable expertise to this perspective. His career spans leadership roles at major pharmaceutical companies including Schering-Plough, GSK, and Almac Discovery. As the founder of Anglezarke Life Sciences and former CEO of Intelligent OMICS, an AI-driven drug discovery company where he now serves as a senior adviser, he has championed innovative approaches to drug development. His influence extends to policy-making, having chaired Matrix, Northern Ireland's Science and Technology policy panel, and served on the UK's chief scientific advisors network.

> "You can't just throw away years and years of iterative experience in any process by replacing it with AI; that's just not going to work"

Tell us about your role at Intelligent Omics

Grundy: My role within Intelligent Omics has been to use a powerful machine learning-driven approach to analyse large data sets gathered from disease patients. This computational approach allows us to understand biology better. If we understand biology and how disease biology differs from healthy biology, then that will help us identify better targets for drug discovery. The alternative is iterative peer-reviewed research into disease biology, which we've always done. But it is fundamentally flawed because it's open to bias and the non-publication of negative results.

The proof that it's inefficient is the significant failure rate of experimental medicines in the clinic, which is to the detriment of patients, pharmaceutical companies, and investors in those pharmaceutical companies. The whole thing is grossly inefficient and needs to be improved. If we can use data and the cost of computation in months or weeks, rather than years, we can present an alternative view of biology. This can reveal dark biology that was previously unappreciated and provides a meaningful alternative approach to developing new drugs.

How does AI integrate into this field of research?

Grundy: Analysing the biology and the processes involved in drug discovery has produced a huge amount of data. The execution of healthcare also

Dr Rob Grundy MBE, Director of Innovation Partnerships at Catalyst

produces a massive amount of data. The question is, how do we employ that data to develop better drugs?

An increasing number of tools will allow us to do that. As AI becomes more sophisticated and pursued by a larger number of organisations, there will be an overwhelming number of tools. Undoubtedly, this will allow us to better use the data that we generate. My hypothesis for this presentation is that the tools are out there, but how can large and small organisations access them efficiently?

I suggest that partnerships allow us to do that in a cost-efficient way that doesn't expose us to investment in technologies that we may only need from time to time. The learnings achieved by using these tools against the big data we're producing across disease biology can be shared and learned within collaborative environments. In that way, you increase the menu of tools that are available to you.

> "Suppose you have biology that isn't represented in sufficient numbers in a clinical population. In that case, you'll never be able to get the effects you need in a clinical trial"

My observation as a service provider in this area is that once an organisation invests in internal AI or machine learning capability, it prevents them from engaging with additional solutions outside of the area in which that investment has been made. In a time when technology is moving so fast, that doesn't make sense. You should always be able to take advantage of new technology as it emerges, for the purposes that you understand it will add value.

If you're prevented from doing that

because of the investments made, you're unable to invest in leading-edge technology, and that won't benefit the organisation. There has to be a more efficient way to access evolving technology that reduces risk exposure and induces reduced expenditure.

How can organisations best employ AI for biological data?

Grundy: We must understand where the value can be utilised and where more traditional methods might be better employed. It will always be a hybrid approach. AI will be transformational. We just don't know how yet. It's bound to be an iterative process of using AI and comparing it with traditional methods to ensure you've augmented what you do traditionally rather than replacing it.

It's all about augmentation. You can't just throw away years and years of iterative experience in any process by replacing it with AI; that's just not going to work. I don't believe anybody's doing that, but you must take a sensible and diligent approach.

If you want to do something new by employing an AI tool, make sure that you expose it to a level of diligence by comparing it to your traditional methods, understanding how it's improved, and understanding where the complementarity is. But that requires effort, and so it's counterintuitive. If you're going to do it properly, you probably won't reduce the effort level, but you will increase the quality of what you do.

What are the challenges? Is data quality a challenge for AI?

Grundy: Data quality is certainly a consideration, a factor. I'm not going to say it's a challenge or an issue because I don't think it is. It's a part of the process. The process begins with identifying data sets. The second stage is quality control of those data sets. The third stage is either abandoning the data set because its quality isn't there or subjecting it to treatments that allow it to be used.

We use principal components analysis and t-SNE plots, which allow us to understand how data is distributed. Then, we make a decision on whether this is a reliable data set. Data quality will always be a consideration, and that's where you start, right? If you know your technique well, you will know what you require of the data and how to treat it to make it appropriate for use.

Duplication of effort is a significant issue in drug discovery. Part of that is the necessity to be competitive. You don't want to share that you've got data with another organisation trying to achieve the same aim. But there's a certain tragedy if you're trying to cure a disease with an unmet medical need. That is something we wrestle with in the drug discovery and development industry as a whole, which is the duplication of effort that can be avoided to make medicine development more efficient.

> "You don't want to share that you've got data with another organisation trying to achieve the same aim. But there's a certain tragedy if you're trying to cure a disease with an unmet medical need"

How does bias impact AI research using biological data?

Grundy: Initiatives such as AllTrials, initially driven by Ben Goldacre, compel clinical research practitioners to publish all their negative or positive results. So, that's getting better. Bias is inherent in published medical research, but it's also inherent in the AI tools that are developed. For example, take AlphaFold from DeepMind. Everybody celebrates that as a great way to understand complex protein structures and how we might target them, but it's built on a biased data set. It's built on the available data, which is largely positive, and that means that there are gaps in that data that prevent you from seeing the whole picture. A tool such as AlphaFold will never be perfect until you get a significant quorum of negative data to complement the positive data from the groups that are adding to the data sets from which things like AlphaFold are built.

If you go back to bias in drug development, the best example, to my mind, is Alzheimer's disease. So, in Alzheimer's disease, for probably two or three generations of medical research, we've pursued two very narrow hypotheses, the amyloid and the tau hypotheses, which have consumed billions of research dollars. We still don't really have a meaningful cure for Alzheimer's disease or understand how it works.

Increasingly, data is telling us that this is a disease of cellular metabolism, of inflammation, and characteristics like amyloid and tau are probably only manifestations of the disease, not causes of the disease. But because so much has been invested in those narrow hypotheses, it's prevented more investigation of the other elements of disease.

I think that's a real problem that is a product of peer review. The problem with peer review as a process to discover drugs is that research gets funded based on what's published. Data gets published based on what everyone agrees is good quality data. If the majority of the people asked to agree on what makes good quality data have a certain interest in an area of biology, then everything moves in that direction. This can result in a mischaracterisation of the real situation in disease.

Are there other issues?

Grundy: Reproducibility is another problem. Many projects seek to develop novel medicines based on experiments that haven't been appropriately reproduced. It's a bit like setting the course for a rocket travelling towards the moon. If you're off by a single degree, you'll miss.

It's the same [when] developing drugs. Suppose you have biology that isn't represented in sufficient numbers in a clinical population. In that case, you'll never be able to get the effects you need in a clinical trial. Getting it right early and having the information you've analysed properly is really important. **LIG**

The innovation imperative: Pioneering new modalities for therapeutic leadership

A look at how multimodal strategies are reshaping pharma and biotech, and what it takes to succeed in this new era

Advancements in molecular and genetic research are driving personalised, targeted therapies, and expanding treatment possibilities. In order to stay competitive, companies must find ways to adopt multimodal strategies, requiring cross-functional collaboration and robust data management. Outsourcing is increasingly important, which makes secure data exchange and analysis critical.

Multimodal drug discovery incorporates diverse approaches, from small molecule to monoclonal antibodies, gene edition and CAR-T therapies, enabling treatment of previously 'undruggable' targets. Combining therapies, such as targeted treatments with immunotherapies, enhances efficacy, especially in complex diseases such as cancer. Personalised medicine further tailors treatments based on genetic and disease-specific factors.

These strategies can present both risks and opportunities. Scientific, financial, and regulatory uncertainties are challenges, but, on the flipside, success can establish companies as leaders in new and exciting areas. Strategic partnerships across biotech, pharma, academia and tech firms are key to accelerating innovation and mitigating risks. The approach also extends beyond combining different drug types to include the integration of diagnostics, delivery systems, and AI-driven digital tools, which are important for managing multimodal research data. Pharmaceutical companies are recognising the need for digital transformation across their value chains, investing in automation and digital solutions to improve efficiency, quality, and resilience.

Strategic considerations for pharma and biotech companies

Larger pharmaceutical companies, with their greater resources, are able to pursue multiple research modalities concurrently. Their particular challenges are in the optimisation of internal workflows, and managing outsourcing effectively. Smaller biotech companies need to try to maximise the resources at hand, making tricky decisions about funding and prioritising specific drug development paths. They need to analyse the potential return on investment for each modality, focusing on areas where they can excel and differentiate themselves. Organisations of all sizes, however, face the same challenge of generating, organising, and analysing data efficiently and at scale.

Collaboration is an important part of developing new drug modalities. Partnerships between biotech startups, large pharmaceutical companies, academic institutions, and technology firms can bring together diverse skills, knowledge, and resources. For example, startups often have ideas but lack the resources to bring a product to market, while large companies have resources and market access but may need the fresh perspectives of smaller firms. Collaborations also enable risk-sharing – important when exploring new modalities. However, establishing and managing these partnerships, particularly when it comes to outsourcing, can present challenges around legal agreements, intellectual property, and data sharing. Efficient data exchange and management are key for successful collaborations, with FAIR (findable accessible, interoperable and reusable) data, and robust systems and expertise to manage and analyse the data generated in modern drug discovery.

> “Modern, accessible software technology plays an important role in managing the complex data and processes involved in drug development”

The future of drug discovery

The future of drug discovery will be shaped by technological advancements, scientific breakthroughs, and evolving industry dynamics. AI and machine learning have the potential to accelerate the drug discovery process from target identification to clinical trial design. Collaboration is essential for accessing specialised skills and technologies, and companies that prioritise data strategy, and streamline communication and data exchange, will have a competitive edge. Modern, accessible software technology plays an important role in managing the complex data and processes involved in drug development. Platforms that enable seamless integration, collaboration, and FAIR data management will be essential.

The Revvity Signals perspective

Many drug development technology initiatives fail because traditional IT systems, designed for structured commercial data, cannot handle the variability of experimental research data. Success in digital transformation requires first understanding the research workflow, then implementing a systematic approach: capturing raw data from scientific instruments, converting it to structured, human/machine-readable formats, and automatically assembling it into analysable datasets suitable for AI-driven insights. This ensures experimental data can be used for decision-making, while aiding collaboration across global research teams.

Revvity Signals aims to support multimodal drug discovery with a connected software solution that minimises the amount of software that scientists need to use, freeing them to focus on high-quality science. The Signals Research Suite is designed to work across modalities, recognising the balance between chemical and biological approaches. It provides tools and workflows tailored to individual and team needs, facilitating collaboration within and between organisations. For example, in antibody-drug conjugates (ADCs), which involve multiple modalities, the suite helps manage complex data and workflows associated with components, ultimately providing a holistic view of the final product. The future of drug discovery is promising, but challenges remain. Regulatory hurdles, ethical considerations, and the need for sustainable practices must be addressed. However, with rapid scientific and technological advancements, and the support of software solutions, the industry is well-positioned to overcome these challenges and deliver groundbreaking healthcare innovations. LIG

Contact Revvity Signals to ind out more.

Designing laboratory robots: Verifying automation technologies

Professor Ana Cavalcanti discusses her pioneering work in developing and verifying robots for laboratory research

Professor Ana Cavalcanti is a professor at the University of York, working in the Department of Computer Science. Professor Cavalcanti holds a chair in emerging technologies from the Royal Academy of Engineering. She oversights modelling, simulation, code generation, and testing concerns in this critical role.

Cavalcanti is also the director of RoboStar, a centre of excellence dedicated to research and technology transfer in software engineering for robotics. The research and development work there covers various aspects of model-based software engineering, including modelling, simulation, testing, and verification. The group also reviews control software, physical models of the platform and scenarios, environment assumptions, and human behaviour.

RoboStar is one of the largest research groups in the world, bringing a diverse membership of researchers working in robotics under a single umbrella. Its membership comprises UK researchers from the universities of York, Sheffield, Surrey, King's College, and Thales, as well as researchers from around the world, including Brazil, China, France, Germany, and Norway.

The University of York

Professor Ana Cavalcanti is a professor at the University of York, working in the Department of Computer Science. Professor Cavalcanti holds a chair in emerging technologies from the Royal Academy of Engineering

Can you tell us about yourself and your role at the University of York?

Cavalcanti: The mandate of the Chair in Emerging Technologies was to create a centre of excellence, so I created – and am now the Director of – RoboStar, a centre of excellence in software engineering for robotics.

We all have a shared vision: to develop an end-to-end approach to designing and verifying mobile and autonomous robots. In terms of your interest in lab automation, RoboStar York is part of the community here at the University of York that is centred around our Institute for Safe Autonomy, and we have a CDT, a Centre for Doctoral Training in the area of Autonomous Robotic Systems called ALBERT - Autonomous Robotic Systems for Laboratory Experiments.

I am leading the panel, and Professor Ian Fairlamb, the co-director of ALBERT from our chemistry department, is also on the panel, which is focused on many things such as safety and lab automation.

What does end-to-end mean in the context of robot design?

Cavalcanti: It's an end-to-end process that develops, designs, and verifies robots. What I mean by end-to-end is current practice. This is a generalisation; I'm always cautious about that. The state of practice is that colleagues want to develop a new robot, and they start by writing code. Programming should be the last stage of the software engineering process. The RoboStar vision focuses

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on being model-centric. We will start developing a system by writing models. By end-to-end, RoboStar provides support to describe and validate these models, just like a civil engineer would write a CAD model and then do some checks. We would do the same thing. We write the models and then check: is this system going to deadlock? Is this system going to have any undesirable properties? We can do that even before the system is built, just as civil engineers do, but we don't stop there. That's the start of the design.

From those models, we want to derive value. Our vision is that we want a world where writing code is something of the past. You write the models. You get the code for simulation, and you get the same code for deployment. That's important because, from an engineering point of view, when you use one code or model for simulation, and then you come to put it on your robot deploy, it is a different piece of code. You then have the possibility of introducing errors and you want to eliminate that. We also want to generate tests automatically. End-to-end means that we cover from the modelling stage to the deployment stage.

What are the main challenges to developing autonomous lab robots?

Cavalcanti: We are tackling this challenge on a very broad spectrum. It's a multidisciplinary problem with challenges in all areas. So the first one is to understand what is adequate for the humans currently in the lab. What do they need, want, and what would be useful for them? All these three things are different.

We start by thinking about the human aspect and how humans can effectively interact with robots. Regarding the development of the robots, there are challenges associated with the software and the hardware. For the hardware, some exciting pieces of work are taking place in ALBERT related to providing the robots with the ability to manipulate very fragile equipment and sensitive materials. This must be done so that we can ensure that they will not cause a problem by spilling materials or potentially interfering with an experiment that may have consequences when dealing with dangerous chemicals.

Software engineering is key to the design of trustworthy mobile and autonomous robots. RoboStar is developing technology to put software engineering on the same standing as traditional engineering disciplines, where models, supported by tools and mathematical foundations, drive the whole production process: simulation, testing, deployment, and provision of evidence of quality.

How do you control all this? This comes in software. How do you develop the applications? The challenge is not only to write the code, but also to provide the evidence so that we can rely on that code. There will be sociological issues, business issues, and ethical issues. Robotics is a multidisciplinary field, and introducing autonomous robots into our society is a multidisciplinary issue.

What are the techniques for verifying robots, particularly in the laboratory?

Cavalcanti: We use three techniques to verify the software used in robots. The techniques have different purposes. In general terms, testing can be done in two ways: testing in simulation, where you have complete control over the control and observability of the system, because everything is in software and you can interfere here and there to capture the information you need – that's verification by simulation; the next is verification by testing the deployed robot. In that case, you want the tests in simulation to be converted to tests run in deployment.

There is another very exciting way of doing the verification. With these models, we can automatically generate mathematical descriptions of them. With those mathematical descriptions, you can generate the tests, you can generate the code, and that can also carry out mathematical proof. It's abstract, but I always go back to the CAD models so people can understand what's going on.

An engineer can prove that the water output in a tap is good enough for the dimensions of the pipes to support the pressure and flow of water. We have the same opportunity. In our models, we can describe how the software will be organised and orchestrated, and how it will communicate, for example. We can prove, mathematically, there is no deadlock. No deadlock means the robot will not freeze as our laptops sometimes do. A freeze may not be a problem. However, safety is a domain-specific challenge. If a robot goes down steps in a hospital and freezes, it may fall and hurt someone. We use these proofs to guarantee expected behaviour. That's the exciting part of RoboStar.

Is it possible to move to a process that only uses these mathematical proofs as verification?

Cavalcanti: No, I don't believe that. Especially in the domain of robotics and physical systems in general, but certainly in the domain of robotics. The objective is not to remove the need for tests, but to carry out proof you can detect the problem earlier and give you stronger guarantees. Everything needs to be consistent.

> "Having AI components introduces new challenges. They are a black box..."

Robot control software runs in a robot, a machine that will be subject to faults and wear and tear. A robot will be moving in a lab, for example. That's our vision: to have labs designed for humans and to have robots working alongside humans.

That is a highly complex environment. The robot cannot know when a human will pass in front of them. They cannot know when the humans will move around the reagents or instruments for the experiment that the robot needs. It is very complex, and we must use our entire arsenal to solve those problems. And so it's not about removing the need for tests. It's about using the best techniques to deal with each of the problems at hand.

Does AI impact the work you're doing on the development of robotic systems?

Cavalcanti: Having AI components introduces new challenges. They are a black box and, in terms of the work we want to do, the main challenge is determining the specifications. For safety, we take the view that it is not about the AI component. Safety is not a property of any single component of a system. It's a system-level property.

So, our techniques cater for the fact that you may have AI techniques implement some of your components. We can model those components. We can capture the mathematics characterising the behaviour of that component and use that at the system level to ensure properties. I'm not saying it's a solved problem, because you need to work at the component level to make those system-level claims, and the technology for those components is very much in development. It is getting better, but it is a challenge. The challenge is at the level of the systems, and we are tackling that in a European project called RoboSapiens. LIG

Designing laboratory robots: derisking the discovery of novel compounds

Professor Ian Fairlamb from York University discusses how the development of laboratory robots can accelerate discovery and reduce the risk for chemists

Researchers at the University of York are developing the science, engineering, and socio-technology that underpins building a robot for laboratory automation for chemistry and related sciences. Autonomous Robotic Systems for Laboratory Experiments (ALBERT) is an autonomous robot that conducts laboratory experiments that are cleaner, greener, safer and cheaper than anything achievable with today's conventional techniques and technologies. York's Institute for Safe Autonomy provides international leadership for this research area.

The University of York

Professor Ian Fairlamb is a professor in the Department of Chemistry at York University and the co-director of Autonomous Robotic Systems for Laboratory Experiments (ALBERT)

Can you tell us about your role at York and as co-director of ALBERT?

Fairlamb: I started at the university as an academic in 2001, joining as an organic chemist. I made organic molecules for the drug, pharmaceutical, agrochemical, and materials industries, developing organic reactions from a traditional perspective. The methods we used for reactions were similar to how they would have been conducted 100 years ago. The innovation was in the chemistry tools – focusing on the molecules the catalysts used and making processes more efficient and cleaner.

Around the mid-2000s, I became aware of commercial robotic systems capable of conducting chemical reaction screenings. In my lab, we typically screened reactions one at a time. We used a classic round-bottom flask, mixing everything with all the variables involved, following a slow and laborious process. However, using a tool from Chemspeed systems, we found we could screen reactions in a more high-throughput manner.

By 2011/12, we had built a relationship with ChemSpeed Technologies, which is based in Switzerland. The company agreed to establish its UK arm within our university environment, which really was a game changer for me, as it allowed insight into the technology at a deeper level. A workflow engineer from ChemSpeed was then based with us, and we developed a strong relationship, working to integrate all of this technology into our research moving forward.

High-throughput chemical reaction screening existed long before the 2000s, but this was the first commercial product I encountered. One disadvantage of the system, which is true for all high-throughput commercial systems, was that it was highly integrated and complex, relying on advanced software. While the value of the equipment was clear, the software accompanying it was equally important and became even more critical over time. Both elements were necessary.

What drove the creation of ALBERT?

Fairlamb: We created the York Robotics

for Chemistry Lab. It is a relatively small initiative, but our system works well for us. It serves approximately 30 to 40 researchers, but we aim to expand it in the coming years. ALBERT represents the next level of advancement.

We started considering whether we were designing the right robots for chemistry experiments. My interaction with Professor Ana Cavalcanti, from computer science, and Professor Jim Woodcock, arose from an open conversation about how technology might assist us. This discussion evolved to include colleagues from across the university, spanning various disciplines – not only the core sciences but also psychology, law, mathematics, and other fields. This led to an organic, bottom-up approach to exploring this topic.

A striking moment for me was when a social scientist observed how humans conducted experiments and interacted with technology in our lab, providing insights into potential improvements. ALBERT is focused on developing new robotics for chemistry labs, incorporating advanced robotics technology, while also questioning whether we are designing the most effective robots for the tasks and how humans will interact with them. One key question is whether robotics can be integrated into a standard chemistry lab while minimising accidents and potential issues. These labs were designed for human use and follow a traditional layout replicated worldwide.

Another question is whether robots should be placed in standard laboratories at all, or if fully automated labs should be created where human access is limited or unnecessary, depending on the chemistry involved. This is where we currently stand. Collaborating with colleagues from different disciplines has been an exciting endeavour. Our fields use distinct terminologies, making communication a challenge at times. My ambition is to develop automated robotic labs through commercial equipment or custom-built solutions. That is my vision for chemistry at this point.

Where can robotics and automation make a significant impact in chemistry research?

Fairlamb: For me, high-throughput screening is one of the most impactful areas. Standard liquid handling units already provide significant capabilities, but robotics' advantage is their ability to interact with these systems.

For example, we use a Schlenk line, a glass apparatus allowing reactions in an inert nitrogen or argon atmosphere. Many of our reactions are oxygen- or moisture-sensitive. This equipment has existed for a long time, but integrating robotic systems with motorised taps and programmable controls would really enable fully automated operation, reducing human intervention.

All chemistry experiments undergo rigorous risk assessment and are conducted in the safest environment. However, to mitigate risk further, removing human hands from certain processes would be beneficial. Accidents still occur occasionally, and robotics could be crucial in risk reduction.

Another significant concern is the development of novel materials and compounds with unknown biological effects. Many of the molecules we design are intended to have biological properties, but their effects remain uncertain until tested. As a result, all new molecules must be treated as potentially toxic. Although researchers use protective equipment, employing robotic systems for synthesis would be a safer alternative.

> “Robotics has the potential to handle more complex sample preparation tasks”

What is being automated today, and where can scientists further expand the toolkit?

Fairlamb: Many instruments, such as nuclear magnetic resonance (NMR) spectroscopy, are now automated, which is a common method for characterising compounds. For instance, proton NMR experiments provide insights into molecular connectivity in organic compounds. These experiments are typically queued in an automated system, often using a carousel for sample loading. Students and postdocs place their samples in the system, which typically runs overnight and provides results by the next day. This process has been effective for a long time.

The same applies to liquid chromatography-mass spectrometry (LCMS), which analyses reaction samples. Each sample can be queued for LCMS analysis if a 96-well plate is screened for different reaction conditions. The samples are then processed overnight, and the results are available for data analysis by morning.

Beyond physical automation, data processing is also becoming more automated. Instead of manually analysing reaction outcome data, we now have tools that input results directly into an app, generating trends and correlation maps within days. This process would have taken six to eight weeks just a few years ago.

Advancements in automated data processing have significantly improved efficiency. In the future, robotics has the potential to handle more complex sample preparation tasks. More advanced robotic systems could eventually take over responsibilities currently managed by students and postdocs, further streamlining laboratory workflows.

Can more advanced robotics be developed for sample preparation in the future, or is that still a long way off?

Fairlamb: No, that is not far off. If you look at the setup at Liverpool University, the team there likely already has examples. The main challenge is the cost of robotics, as commercial systems can be expensive. Additionally, the lab must be configured to allow a robot to move around efficiently.

This is where ALBERT plays a role. My colleagues at the Institute for Safe Autonomy emphasise the importance of setting up the environment correctly. I am still learning in this area, but it is a complex challenge for a robot to recognise what it needs to interact with and what it should ignore – including people. I believe this is an area where we will see significant development in the coming years.

There is also a piece of software called Organa – it is interesting. Its developers have set up an electrochemistry experiment with a robotic arm. It performs relatively straightforward tasks but learns as it progresses. Initially, it is given experimental details, and then it conducts a series of experiments based on what it can identify and what it is instructed to do.

This approach has significant potential. Currently, it may be somewhat idealised in its implementation, but every development has to start somewhere. Most chemists looking at it now would likely find it impressive but not practical for everyday lab use. However, it offers insight into what may be possible in the future. **LIG**

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