AZO NETWORK

INDUSTRY FOCUS

# The Digital Laboratory

An exclusive collection featuring top-tier articles, visionary experts, and essential industry insights

Sponsored by

LabVantage

December 2025 - Edition 2

# TABLE OF CONTENTS



# Foreword

Welcome to the latest edition of The Digital Laboratory Industry Focus eBook, sponsored by LabVantage Solutions. This special IFEB collection presents a timely exploration of how laboratories are evolving through the integration of artificial intelligence, automation, bioinformatics, and connected data platforms. As digital transformation reshapes the research and development landscape, these technologies are proving essential to accelerating discovery, enhancing reproducibility, and future-proofing laboratory operations.

In the realm of bioinformatics and data science, Bioinformatics Tools Every Lab Should Use outlines essential digital resources driving efficiency and insight in modern laboratories. Machine Learning Tool Identifies Metabolic Clues in Colorectal Cancer illustrates how AI-powered models are revealing new disease mechanisms and potential therapeutic targets.

Digital health and personalized medicine are also advancing through data-centric innovation. How Wearable Tech Is Reshaping Preventative Health explores the growing impact of wearable technologies in monitoring health trends and enabling early intervention. In parallel, Combination of Two Cancer Drugs Could Treat the Most Common Form of Dementia highlights how data-driven approaches are leading to unexpected treatment synergies.

Automation and artificial intelligence are at the core of modern drug discovery. Why Drug Discovery Needs Robots and Artificial Intelligence examines the growing role of intelligent automation in streamlining complex workflows. How to Future-Proof Your R&D Strategy with AI Labs provides strategic insight into building digital resilience and agility within research environments.

Finally, connected platforms and intelligent systems are transforming how laboratories operate. Why Data Platforms are Key to Scientific Progress emphasizes the importance of centralized data infrastructure, while Breaking Barriers in Life Science Innovation with AI and Connected Data showcases the power of integration across teams and tools. How Agentic AI and SaaS are Transforming the Future of Laboratory Operations looks ahead to a future defined by autonomy, scalability, and smart decision-making.

Together, these articles reflect the rapid digitization of scientific research and the technologies enabling its continued evolution.

# Why data platforms are key to scientific progress

**It's widely acknowledged that innovation drives a company's growth and product development, and for organizations with research and development labs, these environments are central to that innovation.**

Traditional laboratory software is built to manage workflows, but these systems often fail to address the modern challenge of enterprise data flows. Today, an organization's success increasingly depends on how effectively data moves across the enterprise to support informed decision-making.

Organizations that struggle to extract value from large volumes of data, or that aim to get more from their investments in data science and artificial intelligence (AI), can benefit from adopting a scientific data management platform as part of their digital infrastructure.

Integrating laboratory environments with the broader enterprise ecosystem enables organizations to better utilize the vast data lakes produced by labs.

Labs need to evolve from standalone units into strategic assets that are deeply connected to the organization's data architecture. A digitally native platform approach can help streamline this shift, making scientific data flow management more efficient and impactful.

This article looks at how adopting a platform-based approach to scientific data management, incorporating advanced analytics, semantic search, and lab automation, can enhance enterprise-level decision-making and lab efficiency, ultimately leading to more discoveries and stronger product pipelines.

*Image Credit: LabVantage Solutions*

## Maximizing scientific data in business decision-making

Organizations aiming to make the most of digital transformation and to harness scientific data for business decision-making stand to gain from implementing a comprehensive scientific data management platform. This type of platform connects R&D labs, QA/QC in manufacturing, and more, while also providing access points for supply chain partners.

Unlike siloed software systems, a digitally native scientific data management platform fully leverages organizational and external data, builds AI-enabled digital labs, and enables enterprise-wide data flows that support the entire product lifecycle—from early-stage concepts to full-scale commercialization.

Whether the focus is on industrial chemicals, pharmaceuticals, fuels, or food, an integrated platform ensures optimal lab performance and unlocks advanced analytics. The result is sharper insights, more informed decisions, and, ultimately, greater innovation and sustained growth.

## The disadvantages of siloed informatics

Key laboratory information has traditionally been housed in standalone systems, making it difficult for staff to locate, access, integrate, or reuse data effectively. These siloed solutions also restrict an organization's ability to enhance business processes across internal systems and supply chain partners.

At the same time, organizational data lakes hold immense potential for researchers aiming to drive new discoveries, extend product life cycles, or improve manufacturing efficiency.

However, when this data remains inaccessible, it can lead to missed opportunities. Researchers may be unaware of existing institutional knowledge, waste time and resources duplicating experiments, or find themselves manually piecing together data from multiple applications just to get a complete picture.

The impact of inaccessible data extends beyond R&D. QA scientists may lack access to crucial development data that could improve manufacturing outcomes and enhance product quality attributes. As a result, they often spend time on repetitive, low-value tasks instead of focusing on optimization and innovation.

Business leaders are also affected. Without visibility into lab activities and analytics, executives may struggle to gain clear insight into ongoing research, product pipelines, or the data needed to make informed investment decisions.

By reducing data fragmentation and implementing dashboards and other visualization tools, organizations can empower decision-makers at every level to better evaluate, validate, and analyze diverse data sources.

## Achieving a seamless data flow

Organizations of all sizes pursue digital transformation to boost productivity, improve efficiency, and reduce costs, while maintaining a strong focus on innovation.

Industry observers such as Frost & Sullivan[1] argue that a platform approach to lab informatics represents a solution to these challenges.

Frost & Sullivan's Frost Radar™ report on LIMS for the life sciences states that "users expect more from vendors, and vendors want to become end-to-end lab informatics solution providers rather than simply offering traditional laboratory information management systems [LIMS]."

Today's LIMS are far more advanced than earlier versions, often integrating features like electronic lab notebooks (ELN), scientific data management systems (SDMS), and lab execution systems (LES). Yet even with these expanded capabilities, they still fall short of fully supporting modern business processes.

Frost & Sullivan point out that organizations are demanding more—prompting a push for platforms that incorporate artificial intelligence, machine learning, and natural language processing.

These capabilities, they report, "would allow researchers and labs to better manage their data and extract insights at a faster pace to save time," while predicting that AI integrations with LIMS will increase "over the next few years."

Interest in these platforms is growing, as companies increasingly move away from fragmented solutions in favor of unified scientific data platforms that can seamlessly connect with broader enterprise systems.

By integrating lab data into the enterprise-wide digital ecosystem, organizations can streamline data flows, enabling leaders to bring products to market faster, reduce operational costs, and more effectively respond to customer needs.

## The business case for a platform approach

The business case for a platform approach encompasses several areas.

### Regulatory compliance

Regulated industries like pharmaceuticals can benefit from the implementation of automated compliance workflows, improving product quality, reducing failure rates, ensure data integrity, and facilitating robust audit trails.

### Security and privacy risk

All data traffic is secure, protecting both business and customer privacy from data integrity issues, cyberattacks, and other safety concerns.

### Efficiency and productivity

The elimination of data silos helps ensure smooth data exchange and collaboration across cross-functional teams throughout the enterprise. This streamlined approach can lead to stronger product pipelines, more discoveries, less repeat work, and improved adherence to quality parameters.

Moving away from time-consuming, low-value work to high-value science significantly boosts productivity, whether this is occurring in a single lab or across a global network of facilities.

### Insights with AI

The integration of innovative AI technology improves data analysis, modeling, and predictions, helping to facilitate robust comparisons of different experiments while enabling deeper scientific insight and more rapid discovery.

### Interoperability and standardization

Adhering to standardized protocols and data formats ensures data interoperability, simplifying data exchange and use across different platforms, software, and scientific disciplines.

*Image Credit: LabVantage Solutions*

### SAAS DELIVERY

LabVantage SaaS LIMS helps businesses:

- Reduce risk by improving data security, privacy, and regulatory compliance.
- Adapt to remote data management in response to the growth of work-from-home culture.
- Lower capital costs of cumbersome hardware and on-premises IT infrastructure.
- Stay up-to-date on the latest releases while avoiding disruptive product upgrades.

## The LabVantage scientific data management platform

LabVantage pioneered one of the industry's first laboratory informatics platforms, incorporating this into its LIMS alongside an ELN for flexible R&D, an SDMS for automated data capture, and an LES for compliant workflows.

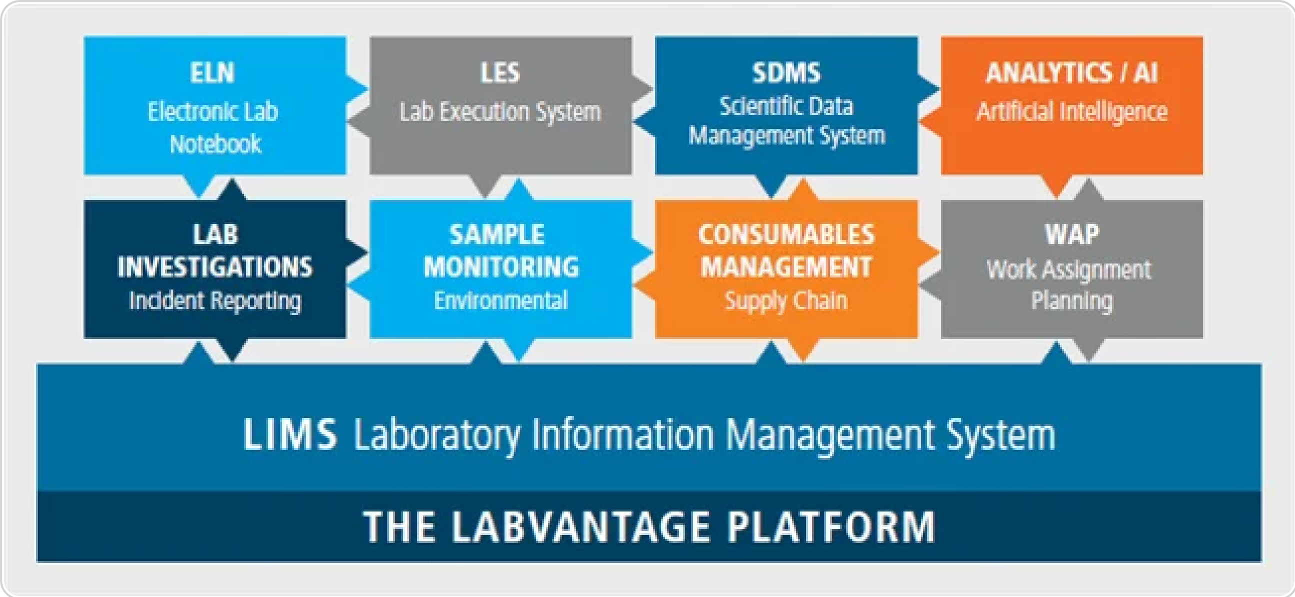
This platform acts as the hub of all labs across the organization and as a resource across the business. Thanks to its expanded capabilities, the platform can now be used to manage lab investigations, consumables management, sample monitoring, and work assignment planning.

The addition of AI-supported semantic search capabilities and advanced analytics has enabled a digitally native ecosystem that is able to serve the entire product lifecycle, from initial research and development to commercial manufacturing and QA/QC.

Its ability to manage both data flows and workflows allows this ecosystem to reduce operational costs while continuing to drive improvements in productivity, efficiency, decision-making, collaboration, and, eventually, time-to-market.

The entire scientific data platform is delivered with Software-as-a-Service (SaaS) technology, offering its users agility and scalability, and supporting innovation by meeting the FAIR data principles necessary for knowledge sharing and collaboration.

Scientists working in different types of laboratories and across multiple sites and geographies are empowered to do their jobs better, faster, and smarter, while business leaders are afforded the visibility to make more informed decisions on markets, products, and investments.




*LabVantage's scientific data management platform, which integrates solutions within a single architecture, licensing model, and services contract, provides customers with the flexibility to select and activate specific components, and scale use as needed. Image Credit: LabVantage Solutions*

## Case study 1: Streamlining R&D and QC to develop a tasty non-alcoholic beer

Expanding a successful product line to meet evolving customer preferences can give businesses a distinct competitive edge. A growing consumer interest in non-alcoholic beer is a timely example of this shift in demand.

For food and beverage manufacturers, adapting an existing recipe—or developing a new one—can be a costly and time-intensive process, often requiring multiple rounds of experimentation with various ingredient combinations.

*Image Credit: LabVantage Solutions*

One beer manufacturer addressed this challenge by using the LabVantage scientific data management platform, along with data from external sources, to identify the optimal formula for a new alcohol-free beer.

By tapping into its existing recipe database and applying AI-powered research, semantic search, advanced analytics, and automation, the company significantly reduced the number of experiments needed to achieve the desired flavor profile.

Once the product was developed, the platform continued to support quality assurance during commercial production. For instance, if a product sample fails quality checks, the issue can be logged directly into the Lab Investigations module. This enables rapid root-cause analysis and timely corrective action, well before the product reaches the customer.

In this case, the use of the LabVantage platform helped the company cut research and development costs, shorten time to market, lower risk, and reduce quality concerns.

## The leading LIMS for growth and innovation

Frost & Sullivan named LabVantage the top growth and innovation leader in its LIMS report and Radar™, recognizing the company's strong position in a competitive landscape.[1]

Few vendors currently offer the level of integration LabVantage provides—combining LIMS with advanced scientific data management, analytics, and connections to enterprise systems beyond the lab.

LabVantage earned high marks for its "comprehensive portfolio" and "commitment to continued innovations." Frost & Sullivan also highlighted several of the company's key advancements.

Frost & Sullivan also highlighted a number of LabVantage's innovations.

One standout feature is LabVantage's application-specific solutions, which support particular industries and lab types with preconfigured workflows, enabling faster deployment and streamlined adoption.

The company's product portfolio continues to grow through a mix of internal development and external technology acquisitions, including investments in AI and natural language processing (NLP) that support scientific and unstructured data management.

A notable example is LabVantage's 2022 acquisition of Biomax Informatics, a knowledge management software provider.

Biomax Informatics' AILANI semantic search solution was recognized in the *Gartner® Hype Cycle™ for Life Science Discovery Research 2023*, where it was listed as a Sample Vendor in both the "Semantic Knowledge Graph Tools" and "Analytics Platforms for Research Informatics" categories.[3]

## Case study 2: Optimizing raw materials inventory for $2 million annual savings

Laboratory managers and scientists need real-time visibility into stock levels and warehouse inventory to operate efficiently. A digitally native scientific data platform can deliver significant savings across large enterprises by enhancing the ability to detect waste and automate inventory processes.

LabVantage's Consumables Management module offers a clear example of this impact. It helps identify expired chemicals before they're used in experiments and tracks ordering and consumption to promote optimal material usage.

Image Credit: LabVantage Solutions

One large paint manufacturer integrated this module into its LabVantage LIMS platform and saw a 90 % reduction in expired chemicals at a single site, translating into more than $2 million in annual savings from reduced chemical waste.

Increased inventory transparency also creates opportunities to share chemicals across labs, cutting down on redundant stockpiles of commonly used reagents. Additionally, the system can quickly pinpoint expired or compromised chemical lots and trace all affected experiments or tests, helping maintain quality and compliance.

## Improving data flows from the laboratory to the boardroom

Digital transformation is essential for leaders planning for their organizations' growth and innovation. Laboratories can no longer operate as their own islands, equipped with individual applications designed to support lab-specific workflows.

It is now a strategic imperative that organizations transition to integrated, digitally native solutions that are able to improve the flow of data across the entire ecosystem while effectively leveraging laboratory-centered data lakes. The choice of approach and partnerships in this endeavor are critical to its success.

LabVantage attributes its success in helping customers make this journey to its people, processes, and platform.

This article makes the case for a scientific data management platform approach to a digital enterprise, with case study examples bolstered by industry analysts like Frost & Sullivan.

It is important to work with only the best, most comprehensive, and integrative technologies as part of an organization's tech stack, with personnel trained and equipped to leverage these effectively.

It is also important to consider the people and processes within a potential scientific data advisor. For example, consider whether the advisor has global operations that can work in parallel with the organization's, and determine whether a potential advisor is skilled enough in the industry in question to offer appropriate solutions.

A potential scientific data advisor must be able to offer appropriate assistance as an organization evaluates, plans, and implements its transformation, supporting its client to understand and prepare for the change management required with novel and accessible solutions and processes.

LabVantage is uniquely positioned to deliver its modern scientific data platform to global organizations of all sizes and industries, thanks to its significant investments in its Customer Care and Professional Services Organization.

These advantages are key to supporting LabVantage's customers in making smarter, data-driven decisions that drive innovation and growth.

## References and further reading


1. Frost & Sullivan (2023). *Life Sciences Industry Trends | Life Sciences LIMS Market Analysis*. (online) Available at: https://store.frost.com/frost-radartm-laboratory-information-management-systems-for-the-life-sciences-industry-2023.html (Accessed 28 May 2025).
2. McKinsey & Company. "Digitization, Automation, and Online Testing: The Future of Pharma Quality Control." McKinsey & Company Life Sciences. Available at Digitization, automation, and online testing: The future of pharma quality control
3. Harwood, R. Gartner® Hype Cycle™ for Life Science Discovery Research, 2023. Available at Hype Cycle for Life Science Discovery Research, 2023

## Acknowledgments

Produced from materials originally authored by LabVantage Solutions, Inc.

## About LabVantage Solutions

LabVantage Solutions, Inc. is the leading global laboratory informatics provider. Our industry-leading LIMS and ELN solution and world-class services are the result of 35+ years of experience in laboratory informatics. LabVantage offers a comprehensive portfolio of products and services that enable companies to innovate faster in the R&D cycle, improve manufactured product quality, achieve accurate recordkeeping and comply with regulatory requirements.

LabVantage is a highly configurable, web-based LIMS/ELN that powers hundreds of laboratories globally, large and small. Built on a platform that is widely recognized as the best in the industry, LabVantage can support hundreds of concurrent users as well as interface with instruments and other enterprise systems. It is the best choice for industries ranging from pharmaceuticals and consumer goods to molecular diagnostics and bio banking. LabVantage domain experts advise customers on best practices and maximize their ROIs by optimizing LIMS implementation with a rapid and successful deployment.

---

**Sponsored Content Policy:** News-Medical.net publishes articles and related content that may be derived from sources where we have existing commercial relationships, provided such content adds value to the core editorial ethos of News-Medical.Net which is to educate and inform site visitors interested in medical research, science, medical devices and treatments.

# Bioinformatics Tools Every Lab Should Use

**Bioinformatics is the foundation of modern research, translating complex biological data into actionable insights by combining biology, computer science, and data analysis. Selecting the right computational tools is crucial for optimizing data management. This article explores key bioinformatics tools that every lab should integrate into their processes to stay at the forefront of innovative research.**

*Image Credit: Tartila/Shutterstock.com*

## Data Analysis: Sequence, Structure, and Visualization

Bioinformatics is essential for managing the rapidly growing life-science data that requires comprehensive databases and tools while ensuring efficient data access and analysis for scientific advancements.[1]

In biological research, transforming vast amounts of raw data into valuable information mainly requires three interconnected techniques: sequence analysis, structural modeling, and data visualization.

### Sequence Analysis

This process is a common starting point where raw biological data (DNA, RNA, or protein sequences) is analyzed for patterns, mutations, or functional elements.[2]

The results provide meaningful information relating to gene function, evolutionary relationships, biological processes, and disease mechanisms, forming the foundation for understanding molecular biology.[3]

### Structural Modeling

This builds upon sequence data to predict the 3D structures of molecules encoded by those sequences, offering insights into their functional properties and interactions.

The sequence data is used as input for creating models that represent how the molecules fold and interact. This technique is crucial for drug design, protein function analysis, and understanding the molecular dynamics of biological systems.[4]

### Data Visualization

As the final step, this process translates complex biological data into clear, interpretable visual representations, including heatmaps, plots, and pathway diagrams. It enables researchers to analyze large datasets, identify significant patterns, and effectively communicate findings.[2,5]

Together, these bioinformatics techniques enable the effective extraction, interpretation, and presentation of biological data, forming a powerful toolkit that drives discoveries in genomics, proteomics, drug discovery, and other areas of biomedical research.[6,7]


## Essential Tools for Modern Research

Scientific research relies on various bioinformatics tools for diverse applications. Below are a few essential examples commonly used in laboratories:[2,3,5-9]

## Sequence Analysis Tools

- BLAST (Basic Local Alignment Search Tool): Helps identify homologous sequences by comparing a query sequence to a database.
- Clustal Omega: Performs multiple sequence alignments, essential for evolutionary studies and functional annotation.
- Bowtie: Fast alignment of short-read sequencing data to reference genomes.
- T-Coffee (Tree-based Consistency Objective Function for Alignment Evaluation): is another multiple sequence alignment tool that combines progressive and consistency-based algorithms for accurate alignment,

These tools allow researchers to decode genetic variations, identify conserved sequences, and infer evolutionary relationships, making them crucial for molecular biology studies.

## Structural Modeling Tools

- AlphaFold: An AI-based tool used for the accurate prediction of protein structures.
- PyMOL: A molecular visualization tool used for viewing, analyzing, and manipulating 3D structures of biomolecules.
- Chimera: A molecular visualization tool used to view, analyze, and manipulate 3D structures of proteins, nucleic acids, and other macromolecules.
- MODELLER: A tool primarily used for predicting and constructing 3D protein structures based on known templates, when experimental structures are unavailable.

These tools facilitate the integration of genomic data with functional insights, supporting fields such as structural biology, pharmacology, and personalized medicine.

## Data Visualization Tools

- Cytoscape: For visualizing molecular interaction networks and biological pathways.
- IGV (Integrative Genomics Viewer): For visualizing large-scale genomic data such as alignments and mutations.
- UCSC Genome Browser: For exploring annotated genomes and visualizing genomic data.
- BioVinci: For generating a wide variety of biological and biomedical visualizations.
- CLANS (Cluster Analysis of Sequences): A tool used for sequence clustering and graphical representation of sequence relationships.

These tools help researchers detect patterns, highlight significant trends, and make data-driven conclusions that enhance biological research.

## Free & Accessible or Paid & Integrated: Which is Better?

In bioinformatics, choosing between free open-source and paid commercial software tools depends on multiple factors, including budget constraints, computational demands, user expertise, technical support availability, and research objectives. Each option has its advantages and limitations, making the decision case-specific.[10-13]

Free bioinformatics tools, such as BLAST, AlphaFold, MODELLER, and Cytoscape, are widely used because they are accessible and cost-effective and allow users to modify and improve them.

However, they require advanced bioinformatics expertise and strong computational infrastructure and often lack integration and usability, complicating data handling, especially in assembly and downstream analysis.[12,13]

Paid bioinformatics tools, such as Geneious, GLC Genomics Workbench, and Qlucore Omics Explorer, may address many issues of free alternatives, offering professional-grade software with seamless integration, dedicated support, robust infrastructure, and user-friendly interfaces.

They also tend to be optimized for performance by including built-in pipelines that simplify complex analyses without requiring extensive coding.[12,13]

However, the high cost of these commercial tools often makes them less accessible to many research labs, particularly independent researchers or smaller institutions with limited budgets. Additionally, the reliance on proprietary software also means users may have less flexibility in modifying algorithms or integrating third-party tools.[11,13]

## Making the Right Choice

While free tools offer flexibility and accessibility, paid solutions ensure seamless integration and support. Where feasible, a hybrid approach can provide the best of both worlds for research environments.

This approach combines open-source and commercial bioinformatics tools to enhance efficiency and cost-effectiveness, a common practice in modern research workflows.

Therefore, selecting the right tools requires balancing multiple factors to support diverse research needs while enabling researchers to extract meaningful biological insights.

## Key Takeaways on Bioinformatics Tools

The rapid expansion of biological data in modern research has made powerful computational tools indispensable in every lab. Bioinformatics has transformed medicine and science, driving breakthroughs and accelerating discoveries.

By leveraging the right tools, labs can optimize workflows, enhance data interpretation, and improve research efficiency.

As the field of bioinformatics continues to evolve and bridge the gap between biological data and medical insights, its advanced analytical capabilities will play an even greater role in shaping the future of biomedical research innovation.

## References


1. European Molecular Biology Laboratory - European Bioinformatics Institute (EMBL-EBI). (n.d.). Our story. [Online]. Available at: https://www.ebi.ac.uk/about/our-story/ (Accessed on 29 March 2025)
2. Gabler, F., Nam, S.Z., Till, S., Mirdita, M., Steinegger, M., Söding, J., Lupas, A. N., & Alva, V. (2020). Protein sequence analysis using the MPI bioinformatics toolkit. *Current Protocols in Bioinformatics*, 72(1), e108. doi: 10.1002/cpbi.108
3. Bono, K. (2022). Application of Sequence Analysis in Bioinformatics Study. *Journal of Proteomics & Bioinformatics*, 15(10):610. doi: 10.35248/ 0974-276X.22.15.610
4. Wenhao, G., Mahajan, S.P., Sulam, J., & Gray, J.J. (2020). Deep Learning in Protein Structural Modeling and Design. *Patterns*, 1(9). doi: 10.1016/j.patter.2020.100142
5. Shukla, V., Varghese, V.K., Kabekkodu, S.P., Mallya, S., & Satyamoorthy, K. (2017). A compilation of Web-based research tools for miRNA analysis. *Briefings in Functional Genomics*, 16(5):249–273, doi: 10.1093/bfgp/elw042
6. Clark, A.J., & Lillard, J.W. Jr. (2024). A Comprehensive Review of Bioinformatics Tools for Genomic Biomarker Discovery Driving Precision Oncology. *Genes (Basel)*, 15(8):1036. doi: 10.3390/genes15081036
7. Zhang, S., Liu, K., Liu, Y., Hu, X., & Gu, X. (2025). The role and application of bioinformatics techniques and tools in drug discovery. *Frontiers in Pharmacology*, 16, doi: 10.3389/fphar.2025.1547131
8. Stroe, O. (2023). Case study: AlphaFold uses open data and AI to discover the 3D protein universe. European Molecular Biology Laboratory - European Bioinformatics Institute (EMBL-EBI). [Online]. Available at: https://www.ebi.ac.uk/about/news/perspectives/alphafold-using-open-data-and-ai-to-discover-the-3d-protein-universe/

(Accessed on 30 March 2025)

9. Li, Q., Hu, Z., Wang, Y., Li, L., Fan, Y., King, I., Jia, G., Wang, S., Song, L., & Li, Y. (2024). Progress and opportunities of foundation models in bioinformatics. *Briefings in Bioinformatics*, 25(6):bbae548. doi: 10.1093/bib/bbae548
10. Huszar,T.I., Gettings, K.B., & Vallone, P.M. (2021). An Introductory Overview of Open-Source and Commercial Software Options for the Analysis of Forensic Sequencing Data. *Genes (Basel)*, 12(11):1739. doi: 10.3390/genes12111739
11. Kelliher, J.M., Xu, Y., Flynn, M.C., Babinski, M., Canon, S., Cavanna, E., Clum, A., Corilo, Y.E., Fujimoto, G., Giberson, C., Johnson, L.Y.D., Li, K.J., Li, P.E., Li, V., Lo, C.C., Lynch, W., Piehowski, P., Prime, K., Purvine, S., Rodriguez, F., Roux, S., Shakya, M., Smith, M., Sarrafan, S., Cholia, S., McCue, L.A., Mungall, C., Hu, B., Eloe-Fadrosh, E.A., & Chain, P.S.G. (2024). Standardized and accessible multi-omics bioinformatics workflows through the NMDC EDGE resource. *Computational and Structural Biotechnology Journal*, 23:3575-3583. doi: 10.1016/j.csbj.2024.09.018
12. Mangul, S., Martin, L.S., Eskin, E., & Blekhman, R. (2019). Improving the usability and archival stability of bioinformatics software. *Genome Biology*, 20(47). doi: 10.1186/s13059-019-1649-8
13. Smith, D.R. (2015). Buying in to bioinformatics: an introduction to commercial sequence analysis software. *Briefings in Bioinformatics*, 16(4):700–709. doi: 10.1093/bib/bbu030

## Further Reading

- All Bioinformatics Content
- Circular RNA profiles could serve as a biomarker of ovarian cancer
- Potential biomarker for lung cancer prognosis revealed
- Study reveals significant neighborhood preferences of tumor cells in Hodgkin lymphoma
- Bioinformatics in Research

**More...**

# How Wearable Tech Is Reshaping Preventative Health



The popularity of wearable health devices has surged, reflecting an increasing emphasis on preventive healthcare and proactive disease management. These devices, such as fitness trackers and smartwatches, enable continuous monitoring of vital physiological parameters, including heart rate, activity levels, sleep patterns, and even advanced metrics like electrocardiograms (ECGs) and blood pressure.

Their growth has been particularly notable during the coronavirus disease 2019 (COVID-19) pandemic, as they offered a practical means to remotely monitor patient health, minimize hospital visits, and reduce healthcare provider exposure to pathogens.

Beyond pandemic-related benefits, wearables hold significant potential for managing chronic conditions, notably cardiovascular diseases, by enabling early detection, personalized interventions, and enhanced patient engagement.

Despite their widespread adoption, challenges persist, especially concerning accessibility and consistent usage among older adults and socioeconomically disadvantaged groups. Addressing these barriers is crucial to ensuring that wearable technology effectively contributes to preventive health strategies and does not exacerbate existing healthcare disparities.[1,2]

This article showcases how wearables enable proactive health monitoring and transform personal and clinical healthcare approaches.

Image Credit: Maridav/Shutterstock.com

## How Wearables Work?

Wearable devices like wristbands and smartwatches contain miniature sensors that continuously track key physiological signals. Essential sensors include accelerometers, which measure movement; photoplethysmography (PPG) sensors, which use light to track heart rate and blood oxygen saturation ($SpO_2$); and temperature sensors that monitor skin temperature changes.

These sensors continuously collect and transmit data, enabling wearables to detect heart rate variability (HRV) and oxygen saturation levels, which are crucial for respiratory assessment.[3,4]

Wearables also analyze movement and physiological signals to track sleep patterns, identifying stages such as light sleep, deep sleep, and rapid eye movement (REM) sleep, which is associated with dreaming and cognitive recovery.

Integrated apps utilize proprietary algorithms to convert raw sensor data into meaningful insights, including detailed analysis of sleep cycles, summaries of daily activity, and real-time health alerts. Users interact with this processed information through user-friendly mobile applications.[3,4]

Overall, by combining advanced sensor technology, continuous health data tracking, and intuitive app integration, wearables offer personalized insights into heart health, respiratory status, and sleep quality, making everyday health management accessible, informative, and proactive.

## Preventative Health Benefits

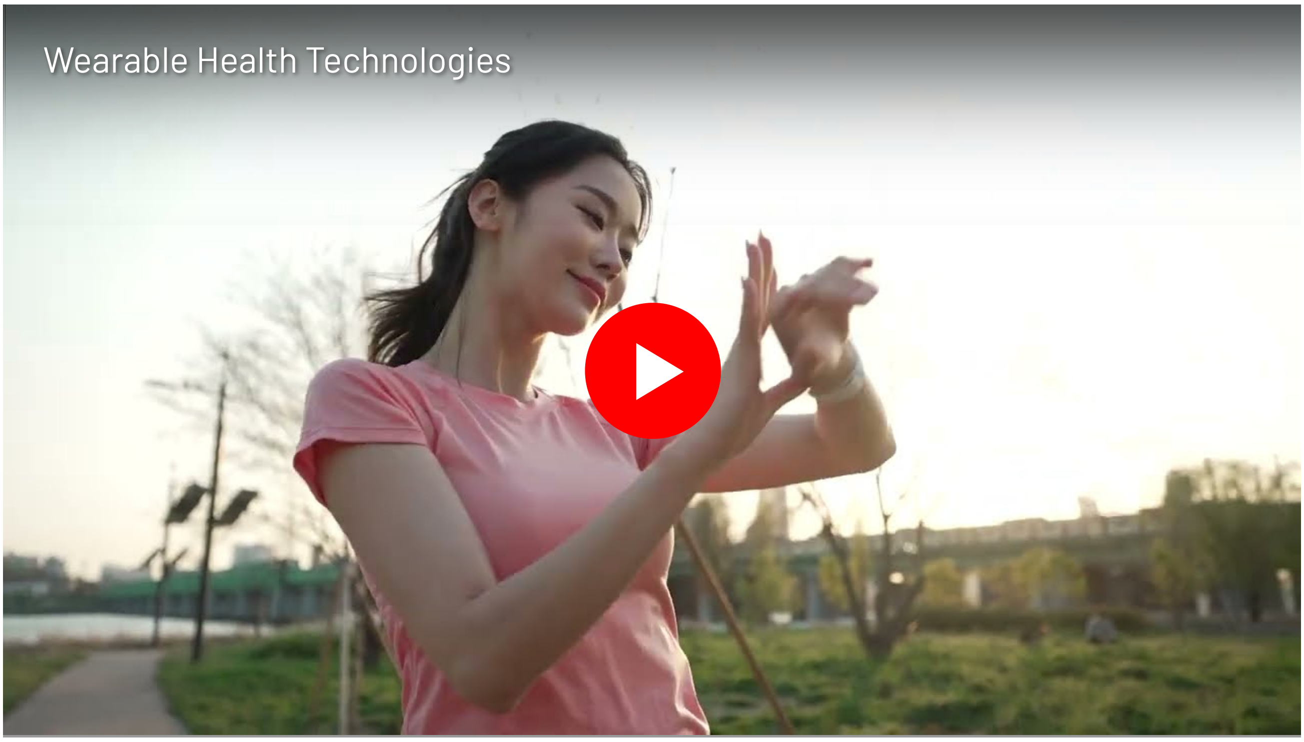
Preventative health strategies leverage early detection, chronic disease management, and behavior modification to enhance health outcomes. Early disease detection through wearable devices can significantly impact conditions like diabetes and atrial fibrillation (AFib).

Continuous glucose monitors (CGMs) offer real-time glucose readings, allowing timely insulin adjustments and substantially improving diabetes control. Similarly, smartwatch-based algorithms accurately detect AFib episodes, enabling early intervention and reducing stroke risk.

Chronic disease management also benefits from wearables by tracking vital signs, medication adherence, and symptom changes, leading to personalized care and reduced complications.[5]

Lastly, wearable devices facilitate behavior modification through biofeedback and activity tracking, promoting increased physical activity, improved sleep, and healthier lifestyle choices. These modifications are critical in managing chronic diseases and preventing their progression.

Despite challenges like data accuracy and patient adherence, ongoing advancements promise greater accuracy, user-friendliness, and integration into healthcare, transforming preventative health into an accessible and integral component of modern medicine.[5]




## Healthcare System Integration

Pilot programs integrating wearable devices with telehealth and electronic health records (EHRs) demonstrate significant promise for enhancing healthcare delivery.

Apple's advancements illustrate how integrating wearable technology into personal health journeys enables users to actively monitor diverse health metrics, including heart rate, mobility, and respiratory rates.

By consolidating data in the Health app and securely sharing it with clinicians, patients gain actionable insights and foster more meaningful patient-provider interactions.[4,6]

Similarly, successful implementation of wearables in clinical settings, as seen in Ochsner Health System and Kaiser Permanente programs, emphasizes clear problem identification, seamless integration into healthcare delivery, personalized experiences, and technology support.

Both systems adopted remote monitoring via wearable and digital health devices directly linked to EHRs, facilitating real-time clinical decisions, effective health coaching, and tailored patient education.[6]

Critical success factors identified include clinician engagement, alignment with reimbursement structures, and patient-focused technology support. For instance, personalized health coaching combined with wearable-generated data at Ochsner significantly improved hypertension management outcomes compared to standard care.[6]

These pilot initiatives underscore the transformative potential of integrating wearable technology with telehealth and EHRs, highlighting improved clinical outcomes, patient engagement, and healthcare delivery efficiency.

## Industry Landscape

The wearable technology sector is led by prominent consumer brands such as Apple, Fitbit, and Withings. These brands have popularized health monitoring by offering user-friendly devices that track physical activity, heart rate, sleep, and ECG.

Apple notably transformed the healthcare ecosystem with ResearchKit, an open-source platform enabling large-scale clinical research and health data collection. This platform significantly expanded wearable integration into clinical studies. Collaborations between these brands and healthcare institutions like the United Kingdom (UK)'s National Health Service (NHS) demonstrate growing trust and adoption.

NHS partnerships leverage wearables for remote patient monitoring, preventive healthcare, and chronic disease management, enhancing patient outcomes and reducing healthcare costs.[7,8]

Simultaneously, emerging companies like iRhythm and Whoop are entering the market, offering specialized medical-grade devices that provide precise data on metrics such as continuous cardiac rhythms, detailed sleep analysis, respiratory rates, and oxygen saturation levels.

These advanced functionalities facilitate clinical-level diagnostics and personalized healthcare interventions.[7]

The wearable landscape is rapidly diversifying, blending consumer-grade convenience with medical-grade accuracy. This evolution is driven by increasing healthcare demands, exemplified by pandemic-induced telehealth needs, marking a significant shift towards precision medicine, improved patient management, and expansive global health research.[7]

## Data Privacy and Limitations

Wearable health devices, such as smartwatches and fitness trackers, offer significant benefits by monitoring health data in real-time. However, their widespread use raises critical concerns regarding data privacy, regulatory frameworks, and device accuracy.

Personal health information (PHI) collected by these devices is inherently sensitive, necessitating privacy protections to prevent unauthorized access and misuse. Ensuring compliance with regulations like the General Data Protection Regulation (GDPR) or the United States (US) Health Insurance Portability and Accountability Act (HIPAA) is essential for maintaining public trust.[9]

Despite advancements, limitations persist, notably regarding data accuracy. Misleading or inaccurate health data can adversely impact medical decisions and user safety. Interoperability issues among diverse operating systems further complicate data management and integration into healthcare systems.

To address these challenges, healthcare organizations must implement strict data security measures, including encryption, regular risk assessments, and role-based data access controls. Furthermore, fostering transparency in data usage and encouraging industry self-regulation through guidelines and voluntary codes of conduct are vital.[9]

## Future Developments

Wearable biosensors represent a transformative advancement, merging healthcare with personalized wellness. Emerging technologies are enhancing their accuracy, comfort, and versatility.

Advances in microfabrication and flexible electronics facilitate unobtrusive, continuous monitoring of physiological metrics such as glucose, hydration, and vital signs through non-invasive methods like sweat analysis and minimally invasive microneedles.

Integration with artificial intelligence (AI) significantly expands their capabilities, allowing sophisticated data interpretation and predictive analytics. Machine learning algorithms analyze vast datasets collected in real time to predict health trends, diagnose conditions early, and deliver personalized health insights.[10]

Predictive analytics through AI-enabled biosensors empowers users and healthcare providers to proactively manage health, anticipate risks, and intervene before the onset of illness. This proactive approach is particularly valuable in chronic disease management, fitness tracking, and preventive medicine, where timely interventions can dramatically improve outcomes.

Future developments also anticipate hybrid wearable-implantable systems, combining external monitoring with internal precision to achieve comprehensive health surveillance. These integrated systems could revolutionize telemedicine and remote patient care, providing highly personalized, real-time health management.

Ultimately, advancements in wearable biosensors, AI integration, and predictive analytics promise a future of more efficient, preventive, and personalized healthcare.[10]

## References


1. US Food and Drug Administration (2023). *Remote or wearable patient monitoring devices EUAs*.
2. Dhingra, L. S., Aminorroaya, A., Oikonomou, E. K., Nargesi, A. A., Wilson, F. P., Krumholz, H. M., & Khera, R. (2023). Use of wearable devices in individuals with or at risk for cardiovascular disease in the US, 2019 to 2020. *JAMA Network Open*, *6*(6), e2316634-e2316634. 10.1001/jamanetworkopen.2023.16634
3. De Zambotti, M., Cellini, N., Goldstone, A., Colrain, I. M., & Baker, F. C. (2019). Wearable sleep technology in clinical and research settings. *Medicine and science in sports and exercise*, *51*(7), 1538.
4. Williams, J. (2023). Empowering people to live a healthier day: Innovation using Apple technology to support personal health, research, and care. *Apple Health Report*, 1-58.
5. Jafleh, E.A., Alnaqbi, F.A., Almaeeni, H.A., Faqeeh, S., Alzaabi, M.A., Al Zaman, K., Alnaqbi, F., Almaeeni, H. and Alzaabi, M.(2024). The role of wearable devices in chronic disease monitoring and patient care: a comprehensive review. *Cureus*, *16*(9).
6. Smuck, M., Odonkor, C. A., Wilt, J. K., Schmidt, N., & Swiernik, M. A. (2021). The emerging clinical role of wearables: factors for successful implementation in healthcare. *NPJ digital medicine*, *4*(1), 45.
7. Huhn, S., Axt, M., Gunga, H.C., Maggioni, M.A., Munga, S., Obor, D., Sié, A., Boudo, V., Bunker, A., Sauerborn, R. and Bärnighausen, T.(2022). The impact of wearable technologies in health research: scoping review. *JMIR mHealth and uHealth*, *10*(1), e34384.
8. Jardine, J., Fisher, J., & Carrick, B. (2015). Apple's ResearchKit: smart data collection for the smartphone era?. *Journal of the Royal Society of Medicine*, *108*(8), 294-296.
9. Bouderhem, R. (2023). Privacy and regulatory issues in wearable health technology. *Engineering Proceedings*, *58*(1), 87.
10. Vo, D. K., & Trinh, K. T. L. (2024). Advances in Wearable Biosensors for Healthcare: Current Trends, Applications, and Future Perspectives. *Biosensors*, *14*(11), 560.https://doi.org/10.3390/bios14110560


Empowering Faster, Smarter Decisions
Unlock Your Potential
labvantage.com/AZO11
LabVantage®
LIMS • ELN • LES • SDMS • AI

# Breaking barriers in life science innovation with AI and connected data

**Research and development teams rely on high-quality data to guide their decisions. They also stand to benefit from the use of generative AI to speed up discovery, along with more streamlined workflows that better connect research with manufacturing.**

This article explores practical ways to achieve these goals.

## When organizations move too slowly, the market moves on

Companies across every industry rely on the speed of their internal innovation cycles to stay competitive in markets driven by constant change and continuous improvement. But moving quickly from discovery to development to commercialization is no easy task.

Many organizations find themselves held back by unmanageable data silos, overly complex workflows, and fragmented infrastructures that prevent R&D and manufacturing teams from operating in sync.

To overcome these hurdles, innovators need closer collaboration between internal functions, such as manufacturing, labs, and quality teams, and external forces like customer demands and commercial partnerships.

At the heart of effective collaboration is one critical component: data. Whether collaboration is embedded in company culture or driven by strategic goals, access to real-time, high-quality scientific data and analytics is essential for building productive internal and external relationships.

These relationships are what enable faster decisions and better, more agile outcomes across the research and manufacturing value chain.

To make this possible, companies need an integrated data analysis environment, along with a dependable connection to accurate, contextualized internal and external data. The life sciences industry, in particular, has laid out a strong roadmap for achieving these goals.

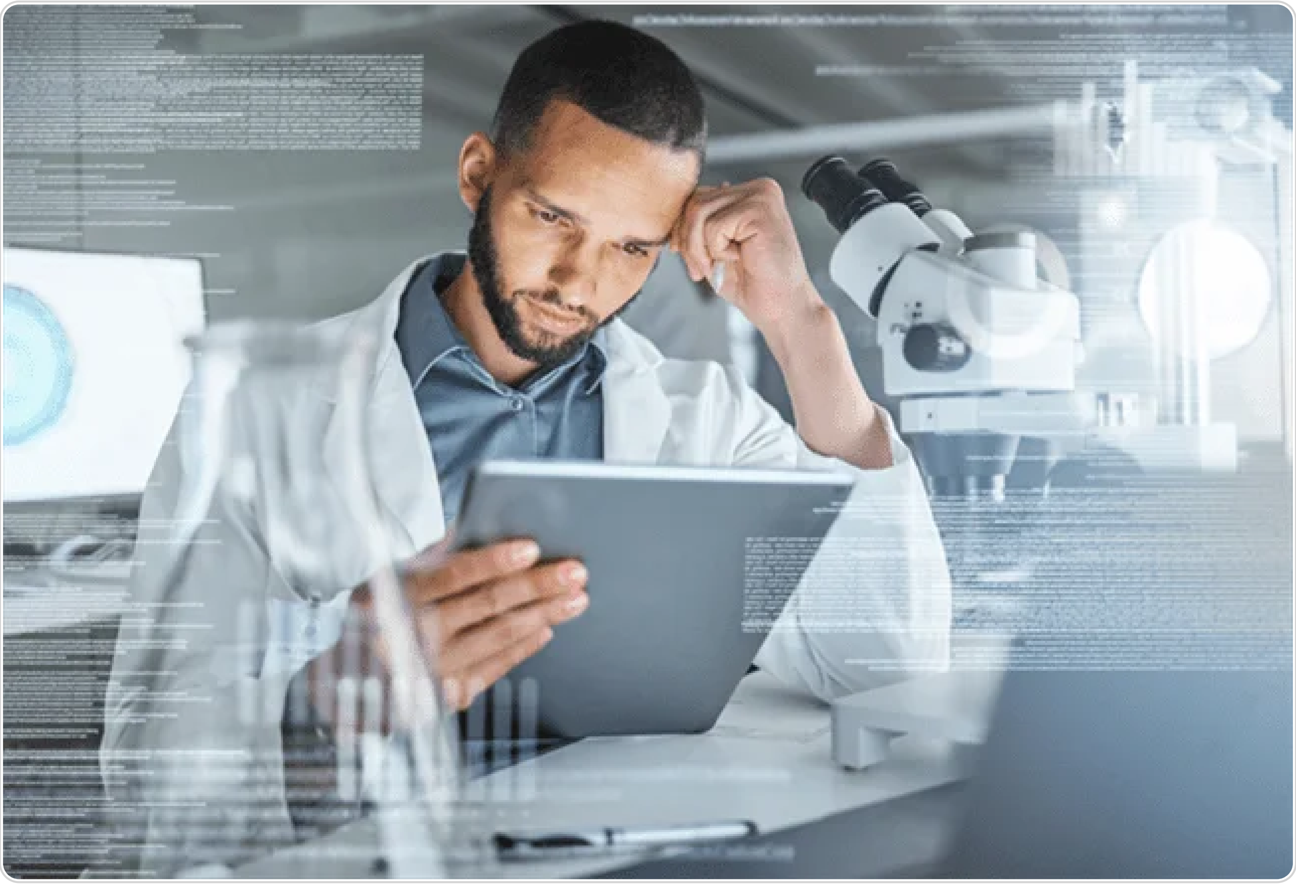


*Image Credit: LabVantage Solutions*

## Lessons from the life sciences: Putting R&D on the fast track

Patients rely on life science companies to bring new drugs to market quickly, but doing so remains a significant challenge in an industry long constrained by breakdowns between R&D and manufacturing, supply chain issues, scale-up difficulties, complex development pathways, and strict regulatory requirements.

Despite these longstanding obstacles, the industry successfully discovered, approved, and deployed COVID-related therapies in just two years. This remarkable acceleration was made possible through the use of high-quality, real-time scientific data that compressed innovation timelines from years into months.

Traditional, time-consuming methods of experiment design were replaced by digitally enabled workflows that provided immediate access to critical clinical data.

Beyond just accessing data, success hinged on the ability to analyze it effectively.

Predictive AI models were used to contextualize trial data and identify vaccine candidates with a high likelihood of success. AI-driven platforms also helped detect and resolve potential supply chain and manufacturing bottlenecks early, supporting faster, more confident downstream decisions and enabling rapid commercial scale-up once approvals were granted.

*Image Credit: LabVantage Solutions*

This collaborative, data-first model has reshaped the life sciences landscape—but its value extends beyond healthcare. Organizations across industries can apply these same principles to remove operational barriers, maximize returns on innovation investments, and accelerate the delivery of meaningful products to market.

## Rapid innovation starts with combining the right solutions in the right way

The LabVantage suite of AI-powered solutions was initially designed to accelerate drug discovery and clear the go-to-market pathway for precision medications. This advanced toolset now enables product innovators across a range of industries to work in a much more rapid and streamlined manner.

The LabVantage suite of technologies has enabled R&D labs in its customers' organizations to achieve:

- 50 % reduction in analysis effort.
- 60 % reduction in validation effort.
- $1 million reduction in cost per laboratory.

LabVantage supports its customers in removing potential R&D barriers, developing streamlined organization-wide workflows, and implementing an integrated data environment designed to drive rapid and forward-looking decisions via a range of fit-for-purpose solutions.

### The LabVantage LIMS platform

The LabVantage LIMS platform has been designed to fit seamlessly into customers' existing workflows.

It's a fully integrated, code-free laboratory informatics platform that affords users a single, scalable, user-friendly interface for accessing LabVantage's Laboratory Information

Management System (LIMS), Lab Execution System (LES), Scientific Data Management System (SDMS), Electronic Lab Notebook (ELN), and advanced analytics.

## LabVantage Analytics, powered by tcgmcube™

Discovery can be accelerated, lab throughput can be increased, and downtime can be reduced, thanks to LabVantage Analytics' AI-powered predictive analytics tools designed to connect users to actionable business insights.

LabVantage Analytics provides innovators a range of benefits, including:

- A single source of truth for all internally generated unstructured and structured data.
- Interactive dashboards and visualizations with powerful drill-down features.
- A comprehensive library of more than 1000 statistical and AI/ML models designed to support low-code AI workflows.

## AILANI for semantic integration and search

The AILANI deep learning platform provides R&D teams with the analytical skills of a data scientist alongside the super-intelligence and efficiency of advanced AI-driven algorithms. The AILANI platform provides an intuitive interface able to answer users' R&D questions across proprietary and public sources. The system can:

- Recognize users' initial intentions and search for relevant insights across a range of disparate data sources.
- Facilitate groundbreaking research, discover hidden relationships, and promote interdisciplinary collaboration.
- Allow teams to access the data lake: a new data architecture able to meet today's need for the rapid analysis of diverse internal and external data types

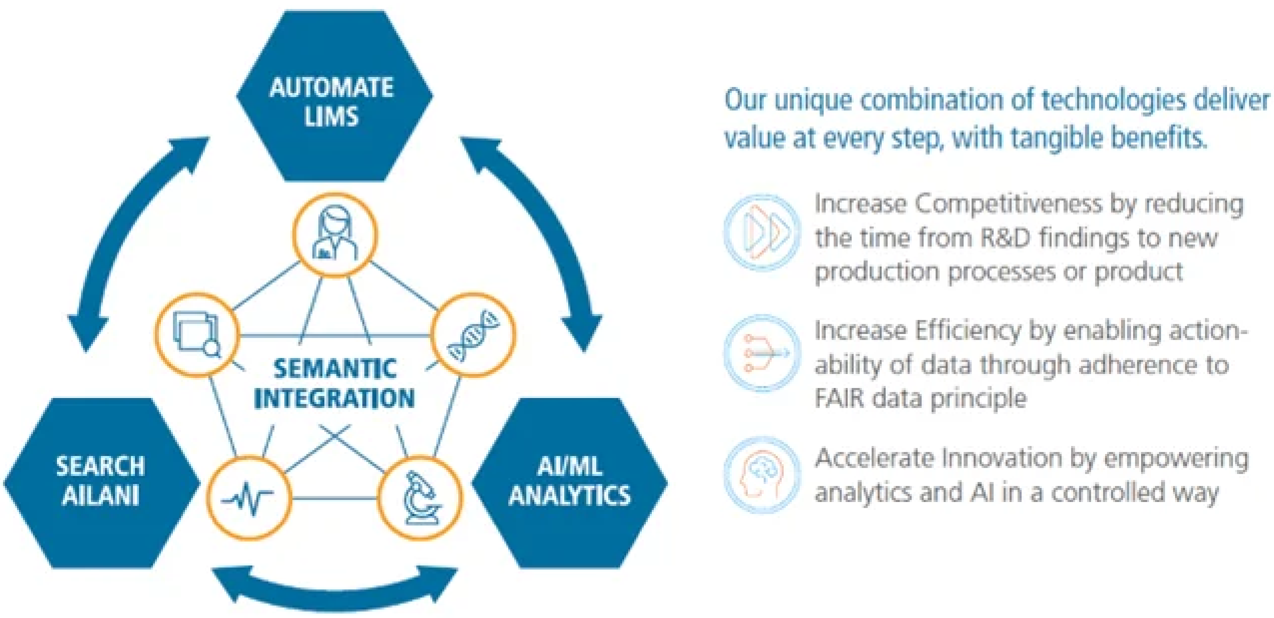


*Image Credit: LabVantage Solutions*

## Summary

LabVantage provides an ideal solution for organizations whose growth is limited by the absence of a focused, efficient research funnel that integrates seamlessly with manufacturing operations.

Designed with these challenges in mind, LabVantage technologies enable users to respond quickly and collaboratively to new discoveries, shifts in market demand, and the evolving needs of customers and partners.

## Acknowledgments

Produced from materials originally authored by LabVantage Solutions, Inc.

## About LabVantage Solutions

LabVantage Solutions, Inc. is the leading global laboratory informatics provider. Our industry-leading LIMS and ELN solution and world-class services are the result of 35+ years of experience in laboratory informatics. LabVantage offers a comprehensive portfolio of products and services that enable companies to innovate faster in the R&D cycle, improve manufactured product quality, achieve accurate recordkeeping and comply with regulatory requirements.

LabVantage is a highly configurable, web-based LIMS/ELN that powers hundreds of laboratories globally, large and small. Built on a platform that is widely recognized as the best in the industry, LabVantage can support hundreds of concurrent users as well as interface with instruments and other enterprise systems. It is the best choice for industries ranging from pharmaceuticals and consumer goods to molecular diagnostics and bio banking. LabVantage domain experts advise customers on best practices and maximize their ROIs by optimizing LIMS implementation with a rapid and successful deployment.

---

**Sponsored Content Policy:** News-Medical.net publishes articles and related content that may be derived from sources where we have existing commercial relationships, provided such content adds value to the core editorial ethos of News-Medical.Net which is to educate and inform site visitors interested in medical research, science, medical devices and treatments.

# Machine learning tool identifies metabolic clues in colorectal cancer

Scientists aiming to advance cancer diagnostics have developed a machine learning tool that is able to identify metabolism-related molecular profile differences between patients with colorectal cancer and healthy people.

The analysis of biological samples from more than 1,000 people also revealed metabolic shifts associated with changing disease severity and with genetic mutations known to increase the risk for colorectal cancer.

Though there is more analysis to come, the resulting "biomarker discovery pipeline" shows promise as a noninvasive method of diagnosing colorectal cancer and monitoring disease progression, said Jiangjiang Zhu, co-senior author of the study and an associate professor of human sciences at The Ohio State University.

"We believe this is a good tool for disease diagnostics and monitoring, especially because metabolic-based biomarker analysis could also be utilized to monitor treatment effectiveness," said Zhu, also an investigator in The Ohio State University Comprehensive Cancer Center Molecular Carcinogenesis and Chemoprevention Research Program.

"When a patient is taking drug A versus drug B, especially for cancer, time is essential. If they don't have a good response, we want to know that as soon as possible so we can change the treatment regimen. If metabolites can help indicate a treatment's effectiveness faster than traditional methods like pathology or protein markers, we hope they could be good indicators for doctors who are caring for patients."

The tool is not intended to replace colonoscopy as the gold standard for cancer screening, Zhu said, and further study with additional samples is planned before the pipeline would be ready for translation to a clinical setting.

The research was published recently in the journal *iMetaOmics*.

This work also represents an advance in machine learning techniques, combining two established methods to design the new platform: partial least squares-discriminant analysis (PLS-DA) for big-picture differentiation of molecular profiles, and an artificial neural network (ANN) that, in this case, pinpoints molecules that improve the platform's predictive value. The team called the resulting biomarker pipeline PANDA, short for PLS-ANN-DA.

> *We took the best of both worlds and put them together to leverage their strengths and complement each other to offset their potential weaknesses. We were looking at all kinds of possibilities to tease out the biomarkers that could be predictive or indicative of disease progression and the different stages of the disease. That gave us some strong confidence that this method has great potential for future diagnoses."*
>
> *Jiangjiang Zhu, co-senior author of the study and aassociate professor of human sciences, The Ohio State University*

Two sets of biological data extracted from blood samples were analyzed: metabolites, products of biochemical reactions that break down food to produce energy and perform other essential functions, and transcripts, RNA readouts of DNA instructions that predict related protein changes.

The biological samples are a significant part of the study's strength, Zhu said, because they were collected as part of large research projects: The Ohio Colorectal Cancer Prevention Initiative (OCCPI) and an Ohio State Wexner Medical Center clinical laboratory biobank. In all, 626 samples came from people with colorectal cancer – including patients with high-risk genetic mutations. Another 402 samples from age- and gender-matched healthy individuals were obtained by Jieli Li, co-senior study author and associate professor-clinical of pathology in Ohio State's College of Medicine.

"We, as humans, at different stages of our lives, actually have quite different biochemistry," Zhu said. "This valuable collection of samples enabled us to run high-throughput metabolomics analysis to understand the molecular changes from people who don't have cancer with people who have cancer, and also from early-stage to late-stage disease.

"We also have data from patients with genetic mutations that we can compare to the metabolite data to look at whether metabolic changes are an indication of predictive values for the genetic mutations. To our knowledge, this is the first time this has been done at this scope and scale because we are looking at literally hundreds of patients."

Biomarkers are tricky to rely on for diagnostics across different populations because of the many conditions that affect molecular profiles in living systems – so this study highlights several molecular changes with potential, but not certainty, in assessing colorectal cancer's presence and progression in a nationally representative group of patients.

The metabolism pathways linked to one family of compounds called purines, which are needed for DNA formation and degradation, stood out in the analysis because they were more active overall in cancer patients compared to healthy controls, and were less active with more advanced tumor stages.

"It's certainly an indication that this biomarker may be associated with the underlying mechanisms of cancer biology," Zhu said. "We are cautiously optimistic in saying that we're not only doing biomarker discovery, but we're also providing clues for mechanistic investigations."

The team plans to continue analyzing metabolites related to different types of biological signals to refine the PANDA biomarker pipeline.

"Some of the markers we identified are a little bit finicky, and there's a lot of noise within those signals, but we have pushed the field forward to develop potential next-generation biomarkers and the novel bioinformatics pipeline for colorectal cancer diagnosis and monitoring," Zhu said.

This work was supported by the National Institute of General Medical Sciences, an Ohio State fellowship and Pelotonia, which funded the statewide OCCPI. Zhu is also supported by the Provost's Scarlet and Gray Associate Professor Program at Ohio State.

Additional co-authors include first author Rui Xu, Hyein Jung, Fouad Choueiry, Shizi Zhang, Rachel Pearlman and Ning Jin, all of Ohio State, and Heather Hampel of the City of Hope National Cancer Center.

---

**Source:**

Ohio State University

**Journal reference:**

Xu, R., *et al.* (2025). Novel machine-learning bioinformatics reveal distinct metabolic alterations for enhanced colorectal cancer diagnosis and monitoring. *iMetaOmics*. doi.org/10.1002/imo2.70003.

# Why Drug Discovery Needs Robots and Artificial Intelligence



***Discover how AI and robotics are speeding up drug development, reducing failure rates, and ushering in a future where personalized medicines reach patients faster than ever before.***

*Image Credit: Shutterstock AI Generator / Shutterstock.com*

## Introduction

This article explores how artificial intelligence (AI) and robotics are revolutionizing drug discovery, cutting costs, accelerating timelines, and enabling rapid breakthroughs through automation and predictive modeling.

# An Introduction to AI in Drug Discovery

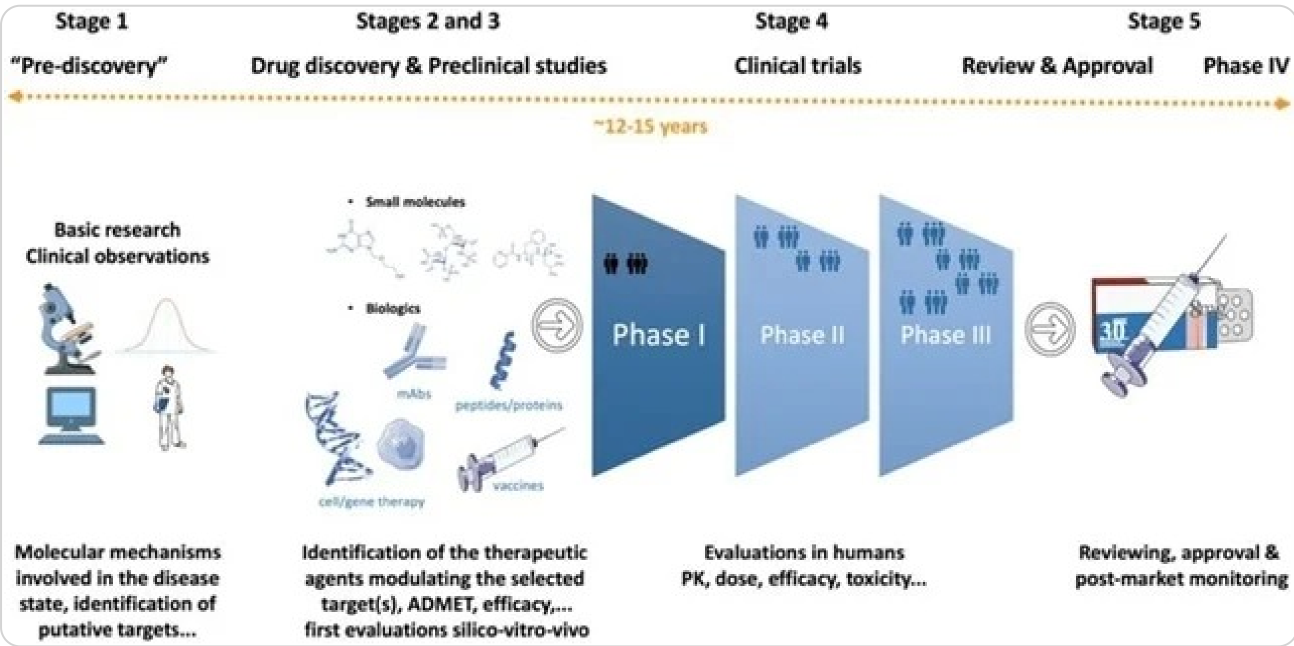
Traditionally, developing a new drug takes many years and requires a massive financial investment, often involving significant risk and a high likelihood of failure. AI models trained on extensive data sets, sophisticated mathematical models, and advanced computational algorithms have been developed in an effort to directly address these inefficiencies.

Pharmaceutical companies worldwide are increasingly using AI to predict clinical trial outcomes, identify therapeutic targets, and optimize molecular designs. Technologies such as AlphaFold from DeepMind, which accurately predicts three-dimensional (3D) protein structures, and generative AI platforms that design medicinal molecules exemplify the transformative role of AI in drug discovery.

Although the United States Food and Drug Administration (FDA) has not yet approved an AI-generated drug for human use, several compounds developed through AI, such as treatments for fragile X syndrome and idiopathic pulmonary fibrosis, are currently being investigated in clinical trials.[1]

## The Drug Discovery Problem

Drug discovery remains a challenging, costly, and time-intensive process. In fact, current estimates indicate that the approval of a single new drug typically costs about $2.8 billion USD and takes approximately 12 to 15 years.



*Drug discovery and development. The main stages are represented in a highly simplified manner. The process varies depending on the molecular mechanisms expected to be linked to the disease and the type of therapeutic agents that needs to be developed. The approximate cost is around US $2.8 billion and the time needed to complete the entire process is around 12–15 years.*[2]

The drug discovery process comprises multiple stages, beginning with basic research to identify therapeutic targets linked to specific diseases. Scientists then screen large numbers of potential compounds through computational methods, laboratory assays, and animal models. Despite rigorous preclinical testing, high failure rates persist, particularly during human clinical trials, where many drug candidates fail due to unforeseen toxicity or inefficacy.[2]

The coronavirus disease 2019 (COVID-19) pandemic highlighted the critical need for accelerated drug development, which required revolutionary technologies like AI to expedite target validation and compound screening. Nevertheless, advancements in this area have been limited due to the lack of complete data, combined with biological complexity and stringent regulatory requirements, all of which emphasize the urgent need for more efficient and innovative solutions to enhance the speed, affordability, and success rate of drug discovery processes.[2]

## Robotics in the Lab

Robotics has transformed laboratory practices, particularly in drug discovery, by utilizing automated platforms for tasks such as liquid handling and high-throughput screening (HTS). Advanced robotic systems enable precise and rapid screening of vast compound libraries, significantly enhancing efficiency, consistency, and scalability.

At the U.S. National Institutes of Health (NIH) Chemical Genomics Center, robotic automation facilitates quantitative HTS (qHTS), where multiple compound concentrations are simultaneously tested to generate comprehensive concentration-response data. This robotic system incorporates precise liquid dispensers, multifunctional robotic arms, and sophisticated software capable of handling complex assay workflows, thereby reducing manual intervention, reagent consumption, and human error.[3,4]

Several companies and institutions exemplify this automation trend. Insilico Medicine, for example, combines robotics with AI to expedite compound identification and drug development, whereas Evotec employs robotic platforms for efficient large-scale biochemical screening. Emerging lab automation startups are further advancing robotic technologies by integrating microfabrication and adaptive handling mechanisms to enhance system speed and reliability.[3,4]

Robotic systems are associated with numerous advantages, including increased throughput, reproducibility, and operational consistency. For example, robotic systems at the NIH have generated millions of concentration-response curves from various assays, which improves the reliability of screening data for chemical probe identification. These platforms are also designed to accommodate diverse assay formats, including cell-based, biochemical, and complex multi-step procedures.[3,4]

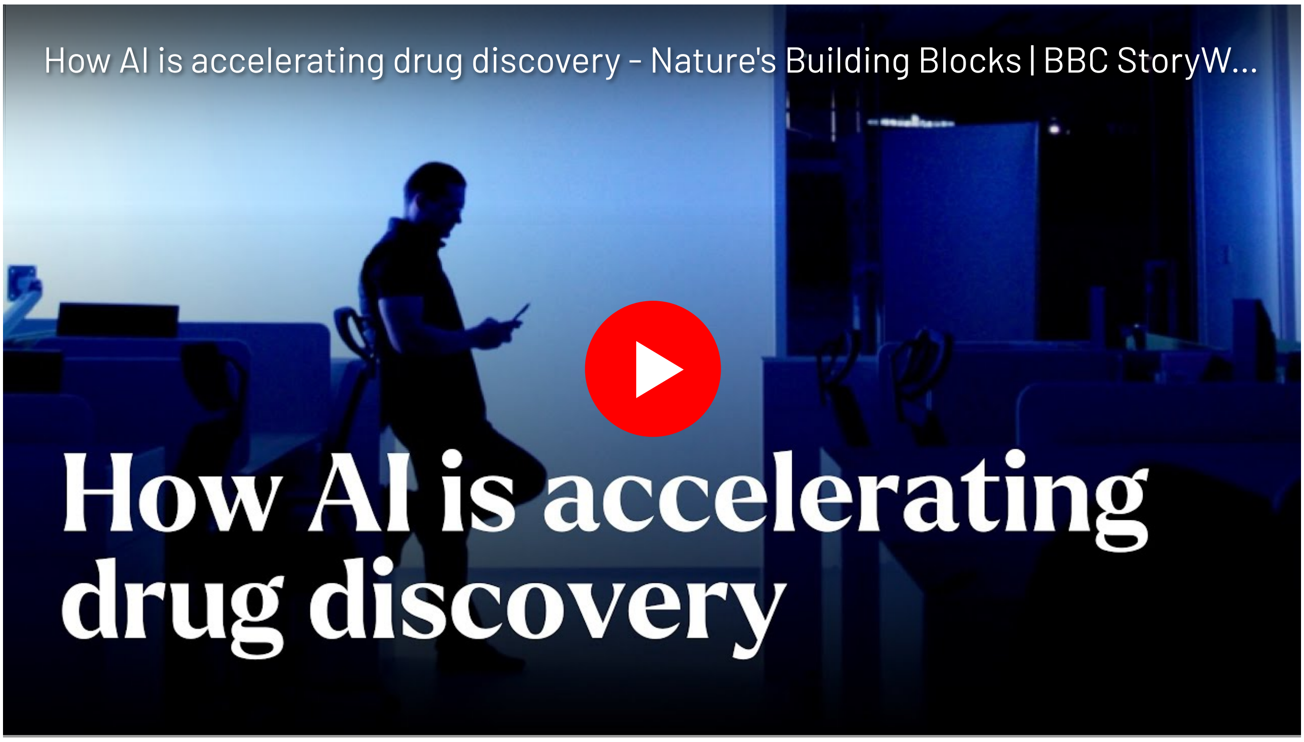
## The Role of AI

AlphaFold accelerates target identification by accurately predicting protein structure from amino acid sequences. Likewise, BenevolentAI integrates machine learning (ML) algorithms to discover new drug targets and rapidly progress them into clinical trials. Atomwise employs neural networks to perform virtual screening to identify molecules with high binding affinity to targets.[5,6]


*A flow chart of the role of AI in drug development[3]*

Combining AI with robotics creates closed-loop discovery systems that automate and optimize drug discovery cycles. These platforms perform iterative tasks, including hypothesis generation, automated experimentation, analysis, and refinement, which collectively increase research speed, scale, and consistency.[5,6]

Techniques like graph neural networks and reinforcement learning further enhance molecule generation and optimization. Ultimately, AI-driven drug discovery promises improved efficiency and personalized treatments tailored to individual patient needs, accelerating the translation of novel therapies from laboratories into clinical practice.[5,6]




## Challenges

Complex neural networks, which are often described as "black boxes," are difficult to validate, which creates uncertainty around their predictions. Addressing these concerns requires the simplification of AI architectures by removing redundant neural network layers without losing accuracy, thereby increasing the transparency and trustworthiness of AI models.[5,6]

Another ethical concern regarding AI and machine learning (ML) is data bias, which can lead to inaccurate outcomes, especially when algorithms are trained on non-representative or incomplete datasets. This bias has the potential to reinforce health disparities, rather than reduce them.

Regulatory agencies like the United States FDA and European Medicines Agency (EMA) are adapting their frameworks to remain aligned with these rapidly advancing technologies. Nevertheless, recently proposed legislation struggles to address AI's dynamic and self-learning nature, especially in generative models that continuously produce new data.

Ethical questions are also becoming increasingly prominent, including who is responsible when an AI-driven medical error occurs. There is also growing concern over data privacy, algorithmic fairness, and long-term societal impact.[7]

Flexible yet rigorous regulations, global cooperation, and clear ethical guidelines are essential to ensure the safe, effective, and equitable deployment of AI-ML in healthcare.

## The Future

The pharmaceutical landscape is witnessing a surge in collaborations between technology firms and pharmaceutical companies. These partnerships are fostering innovation through advanced data analytics, automation, and computational modeling. The startup ecosystem is also increasingly contributing fresh perspectives and agile development models.

To thrive in this evolving field, expertise in data science, automation operations, and AI-based modeling is becoming essential. As AI tools are embedded in research workflows, the future promises more efficient, precise, and patient-specific drug development.[8]

## Conclusions

AI and robotics are not replacing scientists; rather, these technologies are empowering researchers to work faster and more efficiently. Together, humans and machines form a hybrid model that is redefining drug discovery.

Whereas scientists bring creativity, clinical insight, and ethical oversight, AI accelerates data analysis, and robotics automates repetitive lab work. This collaboration shortens timelines, reduces costs, and increases precision.

As these technologies continue to evolve, the future of pharmaceutical research will be shaped by a synergy between human intelligence and ML. Ultimately, this hybrid approach promises faster, more personalized, and accessible therapies for patients worldwide.

## References

1. Niazi, S. K., & Mariam, Z. (2025). Artificial intelligence in drug development: reshaping the therapeutic landscape. *Therapeutic Advances in Drug Safety*, *16*, 20420986251321704. **DOI:** 10.1177/20420986251321704, https://journals.sagepub.com/doi/10.1177/20420986251321704
2. Singh, N., Vayer, P., Tanwar, S., Poyet, J. L., Tsaioun, K., & Villoutreix, B. O. (2023). Drug discovery and development: introduction to the general public and patient groups. *Frontiers in Drug Discovery*, *3*, 1201419. **DOI:** 10.3389/fddsv.2023.1201419, https://www.frontiersin.org/journals/drug-discovery/articles/10.3389/fddsv.2023.1201419/full
3. Oyejide, A. J., Adekunle, Y. A., Abodunrin, O. D., & Atoyebi, E. O. (2025). Artificial intelligence, computational tools and robotics for drug discovery, development, and delivery. *Intelligent Pharmacy*. **DOI:** 10.1016/j.ipha.2025.01.001, https://www.scienced

irect.com/science/article/pii/S2949866X25000097

4. Michael, S., Auld, D., Klumpp, C., Jadhav, A., Zheng, W., Thorne, N., Austin, C.P., Inglese, J. and Simeonov, A. (2008). A robotic platform for quantitative high-throughput screening. *Assay and drug development technologies*, *6*(5), 637-657. **DOI:** 10.1089/adt.2008.150, https://www.liebertpub.com/doi/10.1089/adt.2008.150
5. Qureshi, R., Irfan, M., Gondal, T.M., Khan, S., Wu, J., Hadi, M.U., Heymach, J., Le, X., Yan, H. and Alam, T. (2023). AI in drug discovery and its clinical relevance. *Heliyon*, *9*(7). **DOI:** 10.1016/j.heliyon.2023.e17575, https://www.sciencedirect.com/science/article/pii/S2405844023047837
6. Schöning, J., & Pfisterer, H. J. (2023). Safe and trustful AI for closed-loop control systems. *Electronics*, *12*(16), 3489. **DOI:** 10.3390/electronics12163489, https://www.mdpi.com/2079-9292/12/16/3489
7. Pantanowitz, L., Hanna, M., Pantanowitz, J., Lennerz, J., Henricks, W.H., Shen, P., Quinn, B., Bennet, S. and Rashidi, H.H.(2024). Regulatory aspects of AI-ML. *Modern Pathology*, 100609. **DOI:** 10.1016/j.modpat.2024.100609, https://www.sciencedirect.com/science/article/pii/S0893395224001893
8. Singh, S., Gupta, H., Sharma, P., & Sahi, S. (2024). Advances in Artificial Intelligence (AI)-assisted approaches in drug screening. *Artificial Intelligence Chemistry*, *2*(1), 100039. **DOI:** 10.1016/j.aichem.2023.100039, https://www.sciencedirect.com/science/article/pii/S2949747723000398

# How agentic AI and SaaS are transforming the future of laboratory operations

***"In labs around the world, scientific teams are applying the software-as-a-service model to generate more data than ever before. And while that data has enormous potential to drive innovation, it's highly fragmented, created by different instruments, stored in different systems, and interpreted through different points of view.***

*For years, labs have responded to this challenge by centralizing their data. Add another system. Build another data lake. But whether your lab data is spread across ten systems or gathered in a big central location, it's not usable if it's not contextualized.*

*That's where Lab 4.0 comes in, bringing with it the promise of digital transformation as a gateway to better, faster decisions. Centralizing data is no longer enough—today, labs seek to transform that data into smart, contextualized, and actionable insights. At the heart of this evolution are two key innovations.*

*First, there's the extension of software-as-a-service into its next generation: service-as-a-software, or what we call SaaS 2.0. Then there's the emergence of agentic AI, which harnesses contextual awareness and scientific domain expertise to understand what users need, even when users themselves aren't sure.*

*These innovations add up to more than a product update. They're enabling a whole new philosophy for how work gets done in the lab. It's about putting lab workers directly in conversation with their data, ensuring they get a meaningful, contextualized response—not after days of hands-on analysis, but in the moment, right when it's needed.*

*This evolution won't start with a big bang. It's a journey made up of small, high-impact changes: one repetitive task eliminated, one key insight surfaced, one workflow simplified. At LabVantage, we're committed to making that journey with our customers, helping every lab become a lab of the future one step at a time."*

— **Mikael Hagstroem**: CEO, LabVantage Solutions Inc.


*Image Credit: LALAKA /Shutterstock.com*

# The evolution of laboratory informatics

## SaaS 1.0: A necessary first step

For laboratories, the initial wave of SaaS was revolutionary. New, cloud-based LIMS platforms replaced on-premise systems, providing greater flexibility, lower maintenance costs, and improved scalability. No more making do with outdated legacy systems, labs could now access the most recent features without incurring a significant cost.

No more tedious data entry—labs could now rely on quick, dependable results without bottlenecks or time-consuming manual tasks. And no more disconnected teams—with a cloud-based platform, labs could collaborate with other areas, such as manufacturing, in real time. However, this shift to SaaS 1.0 brought new challenges.

The amount and variety of data generated in the lab increased exponentially, resulting in a deluge of analytical outputs, instrument data, sample logs, QC records, and more, much of which was trapped in organizational silos, making it difficult to access, analyze, and use.

Data lakes emerged as a potential solution, but aggregating siloed data in a single location only addressed half of the issue. Managing and contextualizing large amounts of data is not usually a core competency for scientists.

They are trained to generate insights rather than wrangling spreadsheets, navigating siloed systems, or piecing together incomplete datasets. However, without those steps, lab workers are repeating completed tasks, overlooking critical test steps, and wasting hours looking for information that should have been readily available.

These inefficiencies are caused not only by data overload, but also by the inability to use the data. They not only slow down innovation, but also introduce risk, reduce reproducibility, and drain resources. To address these challenges, labs required an evolution of SaaS 1.0 rather than a replacement.

Enter SaaS 2.0, which is designed not only to centralize data but also to understand, connect, and use it for scientific purposes.

## From data access to data fluency

The core SaaS 1.0 concept of software-as-a-service provided labs with a flexible, cloud-based platform. SaaS 2.0 transforms that dynamic into service-as-a-software by adding agentic AI to the platform.

Agentic AI enables laboratory workers to communicate with intelligent agents in natural language. The "service" in service-as-a-software is what follows: These AI agents respond to conversational prompts, understand lab workflows, initiate tasks, and provide contextualized data when it is needed.

These embedded AI agents are not simply chatbots or analytical tools. They are digital coworkers who have received extensive domain-specific training based on company and laboratory data. These technologies are transforming lab workflows and accelerating scientific progress.

Traditional SaaS and SaaS 2.0: A Comparison. Source: LabVantage Solutions

| | **Software-as-a-Service (Traditional SaaS)** | **Service-as-a-Software (SaaS 2.0)** |
|---|---|---|
| **Core philosophy** | Cloud-delivered software | AI-driven services that enable lab workers to talk to their data |
| **What users can expect** | Manual software operation | AI agents that respond to natural language prompts |
| **Workflow design** | Standardized | Personalized and adaptive |

| | | |
|---|---|---|
| **Intelligence** | Limited automation | Context-aware AI that understands scientific workflows and user intent |
| **Interoperability** | Prone to siloed operations | Built for interoperability and API integration |
| **Data handling** | Basic reports | Predictive and domain-specific analytics |

### Glossary of terms

**SaaS 2.0:** SaaS 2.0 uses a "service-as-a-software" philosophy, allowing lab workers to "talk to their data" through AI agents who provide contextualized, actionable insights.

**Semantic framework:** A semantic framework is a structured, ontology-based system that contextualizes lab data, allowing AI agents to interpret and adapt to scientific environments while also providing insightful, accurate information to laboratory workers.

**Agentic AI:** Agentic AI refers to intelligent, domain-trained agents that understand lab workflows, respond to natural language, and act as digital coworkers to support scientific tasks in real time.

**Digital workforce:** The term "Digital Workforce" refers to AI agents embedded in SaaS 2.0 platforms. These digital collaborators are trained to handle repetitive tasks, uncover valuable insights, and accelerate research by collaborating with scientists.

## The SaaS 2.0 philosophy in practice

### Human-centered by design

What does it mean, practically, to transition from data access to data fluency? It involves implementing a digital interface designed for how people actually work in a lab.

People may have different workflows, preferences, and levels of technical proficiency, but they all have one thing in common: they want context-rich answers to their most pressing scientific questions, based on lab data and ready for rapid, effective application at the bench. In other words, lab workers need a way to communicate with their data.

Not as data scientists writing SQL queries or deciphering complex visualizations, but as individuals conversing naturally, as you would with a coworker who understands your language, context, and goals. That is exactly how the intelligent agents that drive SaaS 2.0 are designed: as coworkers and collaborators.

They can interpret intent, apply lab-specific logic, and provide immediate answers alongside lab personnel. They allow teams to focus on science rather than software. The interactions between lab workers and their digital coworkers do not end with the initial question.

Because these AI agents operate within a semantic framework, they can handle follow-up inquiries, observe and adapt to changing workflows, and fine-tune their responses in real time as user needs or goals change.

### Built for the unique challenges of lab work

This transition to SaaS 2.0 and a digital workforce is only effective if the workforce is grounded in reality. There is no room for AI-generated hallucinations or traceability issues. That is why the data fabric that supports SaaS 2.0 is critical, particularly in the highly regulated lab environment.

The key is to govern AI agents with rigorous data ontologies. This means creating structured, domain-specific guidelines to define how data relates to lab workflows. Using these ontologies, AI agents can improve their contextual understanding and apply lab-specific logic to provide accurate and traceable insights. This means:

- **Reliable results without hallucinations:** By grounding SaaS 2.0 agents in verified internal data, the risk of receiving a fabricated or misleading response is reduced.
- **Built-in traceability:** Lab-specific AI agents provide proven data to support critical insights, eliminating the need for guesswork.
- **Deep domain expertise:** AI agents based on lab ontologies can provide contextual fluency for technical and highly regulated environments.

## Real-world results: Three ways that SaaS 2.0 will transform lab work

### 1. Smarter searches and deeper insights

Until now, navigating petabytes of data from large-molecule studies or reviewing results across multiple sites was a monumental task, driven by keyword searches and requiring hours of hands-on technical work. The concept of "talking to your data," a key innovation of SaaS 2.0, changes everything.

AI agents can quickly extract relevant knowledge from a lab worker's conversational query by using domain-specific large language models (LLMs) that have been refined for lab environments.

This will significantly speed up the process of identifying promising compounds, predicting test results, analyzing supply chain dynamics, and completing other high-value lab tasks.

### 2. AI-powered automation, personalized for labs

Reducing operational overhead is one of the most immediate benefits of investing in the SaaS 2.0 evolution. AI agents can proactively evaluate lab activities to detect redundancies, identify gaps, and incorporate them into personalized workflows.

This is not about replacing lab workers; it is about allowing them to focus on higher-value scientific work while a trusted digital coworker handles the repetitive, time-consuming tasks that previously slowed progress.

### 3. Compliance that labs can trust

Regulatory expectations are constantly changing, often in favor of more stringent oversight—especially in the age of AI. This increases the pressure on labs to demonstrate the pedigree of compliance-related data. Where did it come from? What method was used to create it? What is the full lineage?

Probabilistic methods that rely on pattern recognition to answer these questions will not withstand regulatory scrutiny, which is why SaaS 2.0 is based on semantic ontologies that allow for data centricity.

This means that each result can be traced back to its source. Because the AI powering SaaS 2.0 is based on verifiable internal data and lab-specific logic, it can evolve in lockstep with changing compliance standards.

## Welcome to the lab of the future

SaaS 2.0 is a watershed moment in lab informatics because it allows for contextual conversations with data. Lab workers will be able to work directly with context-aware AI agents to speed up critical decisions, shorten the path to breakthrough innovations, and ensure regulatory compliance in a rapidly changing environment.

This may be a big promise, but getting there does not always require a big leap. It starts small: a missed test detected just in time, a duplicate step avoided, and a smarter insight delivered when it is most effective.

These everyday victories serve as the foundation for connecting lab teams to their digital platform, resulting in a more intelligent, efficient, and future-ready Lab 4.0.

## About LabVantage Solutions

LabVantage Solutions, Inc. is the leading global laboratory informatics provider. Our industry-leading LIMS and ELN solution and world-class services are the result of 35+ years of experience in laboratory informatics. LabVantage offers a comprehensive portfolio of products and services that enable companies to innovate faster in the R&D cycle, improve manufactured product quality, achieve accurate recordkeeping and comply with regulatory requirements.

LabVantage is a highly configurable, web-based LIMS/ELN that powers hundreds of laboratories globally, large and small. Built on a platform that is widely recognized as the best in the industry, LabVantage can support hundreds of concurrent users as well as interface with instruments and other enterprise systems. It is the best choice for industries ranging from pharmaceuticals and consumer goods to molecular diagnostics and bio banking. LabVantage domain experts advise customers on best practices and maximize their ROIs by optimizing LIMS implementation with a rapid and successful deployment.

**Sponsored Content Policy:** News-Medical.net publishes articles and related content that may be derived from sources where we have existing commercial relationships, provided such content adds value to the core editorial ethos of News-Medical.Net which is to educate and inform site visitors interested in medical research, science, medical devices and treatments.

# How to Future-Proof Your R&D Strategy with AI Labs

**As industries contend with exploding data volumes, rising costs, and pressure to speed up innovation, traditional R&D lab models are struggling to keep pace. Enter AI labs, integrated environments that bring together artificial intelligence (AI), machine learning (ML), robotics, and smart data systems.**

*Image Credit: Gorodenkoff/Shutterstock.com*

**These AI labs help organizations move from reactive research centers to agile innovation engines. By enabling faster insights and more informed decision-making, AI labs are not just enhancing efficiency, they're helping businesses stay competitive in a rapidly evolving landscape.**

**Here, we will look at how AI labs can help organizations future-proof their R&D strategies.**

## What is an AI Lab?

An AI lab is far more than an automated workspace. It's aintegrated framework that embeds intelligence into every stage of the R&D process. At the foundation are three core capabilities.

First, machine learning enables researchers to process and interpret vast datasets. These models can uncover patterns, predict experimental outcomes, and even suggest optimized parameters before a single test is run. In pharmaceuticals, for example, generative AI is now being used to design molecular structures that would be difficult—or impossible—to discover through conventional methods. This not only reduces the trial-and-error phase but also significantly accelerates early-stage drug development.[1,2]

Next, robotics brings consistency and scale to the lab. Automated systems can perform complex tasks like high-throughput screening or material synthesis with remarkable precision. At Argonne National Laboratory, the Polybot system exemplifies this approach by autonomously exploring millions of material combinations to develop high-performance electronic polymers. What once took months of manual testing can now be done in days.[3]

Equally important are smart data systems that unify information from various sources, lab instruments, clinical trials, supply chains, into a single, interoperable platform. These systems make it possible to analyze data in real time, uncovering trends and anomalies quickly while enabling seamless collaboration. Initiatives like the National AI Research Resource (NAIRR) pilot are working to make such tools more accessible, leveling the playing field for researchers and institutions of all sizes.[4]

Together, these components create a closed-loop system where models guide experimentation, data informs decisions, and feedback accelerates progress.

## Why R&D Needs a Smarter Backbone

Keeping pace with innovation is all about staying viable in a landscape that's constantly shifting. The traditional model, with its long timelines and high failure rates, is increasingly unsustainable.

Take pharmaceuticals, for example. Developing a single drug typically takes over a decade and costs upwards of $2.6 billion. And what's worse is that around 90 % of candidates fail during clinical trials. AI labs are making a measurable difference here by enabling predictive modeling and virtual screening, methods that can reduce discovery timelines by nearly half and shave costs by up to 30 %.[1,2,5,6]

But the challenge isn't just time and money. Data is also a big problem. Today's labs generate terabytes of information on a daily basis, far more than any team of humans can process manually. AI tools like DeepMind's AlphaFold are already helping scientists decode protein structures that were once elusive, unlocking new insights in fields like neurodegenerative disease.[1]

There's also a growing regulatory dimension. Agencies such as the US Food and Drug Administration (FDA) are introducing evolving guidelines for AI and ML use in clinical settings. To stay compliant and responsive, organizations need agile, data-driven systems. AI labs support this with capabilities like real-time pharmacovigilance, where adverse drug reactions can be detected and reported through automated analysis of real-world data.[2,7]

The broader economic stakes are substantial. By 2030, AI is projected to contribute $250 billion annually to the pharma sector alone. Those who move early stand to gain the most.

## What AI Labs Can Deliver—Today

AI labs are changing research by making it faster and more efficient. They help scientists run experiments quickly and work well with existing systems, ultimately accelerating innovation across various scientific fields.

### Increased Throughput and Reproducibility

AI labs can easily automate repetitive tasks, allowing researchers to concentrate on high-value projects. For instance, Cerebras' AI supercomputing contributions to the NAIRR pilot allow scientists to run exascale simulations, accelerating materials discovery by orders of magnitude. Meanwhile, Polybot's automated workflows at Argonne ensure consistency in production, successfully minimizing coating defects in electronic polymers while simultaneously achieving important conductivity benchmarks, advancing both efficiency and innovation in the field.[3,4]

### Predictive Experimentation and Real-Time Decision-Making

AI also enables new types of experimentation. Generative models like Insilico Medicine's GENTRL can simulate molecule interactions and generate viable drug candidates in weeks. Digital twins—virtual replicas of lab environments—allow teams to test hypotheses without physical constraints. Janssen's Trials360.ai platform uses this concept to optimize clinical trial design, leading to fewer protocol deviations and more efficient study execution.[5,8]

### Seamless Integration with Existing Infrastructure

Importantly, AI labs don't require organizations to start from scratch. They can be integrated with existing infrastructure. Many labs, for instance, are retrofitting traditional Lab Information Management Systems (LIMS) with AI capabilities that automate routine data analysis, detect equipment maintenance needs, and even forecast supply chain demands. At Merck, AI-powered forecasting tools have improved inventory accuracy, aligning production more closely with real-time market trends.[2]

## Building Your Own AI Lab: Where to Start

Creating an AI lab doesn't happen overnight, but it doesn't need to be overwhelming either.

### Step 1

The first step is to understand your current capabilities. A solid gap analysis can identify whether your instruments are IoT-ready, whether your data streams can be standardized, and whether your teams are culturally prepared to adopt iterative, data-driven processes. Upskilling programs—like those at Roche's AI Hub—are one effective way to close skill gaps and prepare teams for the shift.[8]

### Step 2

Next, focus on data infrastructure. Interoperability is crucial, particularly in industries where privacy and security matter. Projects like the NAIRR Secure initiative are exploring how federated learning can analyze sensitive data (like patient records) without compromising privacy. Cloud services from AWS and Google offer scalable, secure environments for managing this kind of data, while open-source communities like Hugging Face encourage collaborative development.[2,4]

### Step 4

Build Strategic partnerships, as these can also accelerate the process. No single organization has to do it all alone. Pfizer's work with IBM is a prime example—by combining internal expertise with AI modeling capabilities, they cut drug design time by up to 90 %. Similar collaborations are emerging across the sector, with startups like Exscientia partnering with Bayer and Bristol Myers Squibb to fast-track drug discovery.[8]

### Step 5

Finally, it's wise to start small. Pilot projects are a manageable way to prove ROI and build internal buy-in. AstraZeneca's collaboration with BenevolentAI led to five new drug targets for chronic kidney disease in just a few months—a milestone that typically takes years.[8]

## Case Studies: AI Labs in Action

Several organizations are already seeing the results:

- **Argonne National Laboratory's Autonomous Materials Lab:** At Argonne National

Laboratory, the autonomous Polybot system has dramatically accelerated materials discovery by exploring a million different parameter combinations. The resulting data has been shared publicly to drive collective progress in polymer research.[3]

- **Pfizer's AI-Driven Drug Development:** Pfizer, working with IBM, was able to compress four months of drug design work into just weeks during the development of Paxlovid. The AI system rapidly screened 20,000 compounds, identifying those with the strongest therapeutic potential.[8]
- **Insilico Medicine's Generative Chemistry:** Insilico Medicine developed a promising fibrosis treatment in just 18 months, about 75 % faster than the standard timeline, by combining reinforcement learning with quantum chemistry simulations to prioritize synthesizable drug candidates.[2,5]

## R&D's Next Chapter: Smarter, Not Just Faster

Modernizing R&D isn't about replacing scientists with machines; it's about enabling them to do more. AI labs give researchers the tools to scale their ideas, test them quickly, and refine them with precision. But technology alone isn't enough. Culture matters too.

Organizations that treat AI as a strategic capability, not just a cost-saving tool, are the ones most likely to lead. This includes investing in cross-functional teams, encouraging risk-tolerant experimentation, and ensuring that AI systems are transparent and ethically grounded. The US National AI R&D Strategic Plan emphasizes the importance of these principles, calling for fairness, accountability, and alignment with public values.[3,6]

In the long run, AI labs are not just improving research—they're reshaping how discovery happens.

## Want to Learn More?

**Curious about where AI is heading next in science and industry? Here are a few directions worth exploring:**

- **AI Liability and Accountability: Who is Responsible When AI Makes a Harmful Decision?**
- **Advancing Healthcare Security Using AI**
- **The Real Limitations of AI in Life Sciences**

## References and Further Reading

1. Viswa, C. A. *et al.* (2024). Generative AI in the pharmaceutical industry: Moving from hype to reality. *McKinsey & Company.* https://www.mckinsey.com/industries/life-sciences/our-insights/generative-ai-in-the-pharmaceutical-industry-moving-from-hype-to-reality
2. Gencer, G. (2025). AI in Pharma: Use Cases, Success Stories, and Challenges in 2025. *SCW.AI.* https://scw.ai/blog/ai-in-pharma/
3. AI-driven, autonomous lab at Argonne transforms materials discovery. (2025). *University of Chicago News.* https://news.uchicago.edu/story/ai-driven-autonomous-lab-argonne-transforms-materials-discovery
4. Democratizing the future of AI R&D: NSF to launch National AI Research Resource pilot. (2024). *NSF - National Science Foundation.* https://www.nsf.gov/news/democratizing-future-ai-rd-nsf-launch-national-ai
5. AI in Pharma and Biotech: Market Trends 2025 and Beyond. (2025). *Custom Software Development & Engineering Company | Coherent Solutions.* https://www.coherentsolutions.com/insights/artificial-intelligence-in-pharmaceuticals-and-biotechnology-current-trends-and-innovations
6. Gursoy, F., & Kakadiaris, I. A. (2023). Artificial intelligence research strategy of the United States: Critical assessment and policy recommendations. *Frontiers in Big Data*, *6*, 1206139. DOI:10.3389/fdata.2023.1206139. https://www.frontiersin.org/journals/big-data/articles/10.3389/fdata.2023.1206139/full
7. Gupta, D. (2025). How AI Is Reshaping Pharma: Use Cases, Challenges. *The Whatfix Blog | Drive Digital Adoption.* https://whatfix.com/blog/ai-in-pharma/
8. Buntz, B. (2025). How 11 Big Pharma companies are using AI. *Pharmaceutical Processing World.* https://www.pharmaceuticalprocessingworld.com/ai-pharma-drug-development-billion-opportunity/

Disclaimer: The views expressed here are those of the author expressed in their private capacity and do not necessarily represent the views of AZoM.com Limited T/A AZoNetwork the owner and operator of this website. This disclaimer forms part of the Terms and conditions of use of this website.

# Combination of two cancer drugs could treat the most common form of dementia

A study comparing the gene expression signature of Alzheimer's disease with those elicited by 1,300 approved drugs found a combination of two cancer medications that could treat the most common form of dementia.

Scientists at UC San Francisco and Gladstone Institutes have identified cancer drugs that promise to reverse the changes that occur in the brain during Alzheimer's, potentially slowing or even reversing its symptoms.

The study first analyzed how Alzheimer's disease altered gene expression in single cells in the human brain. Then, researchers looked for existing drugs that were already approved by the Food and Drug Administration (FDA) and cause the opposite changes to gene expression.

They were looking specifically for drugs that would reverse the gene expression changes in neurons and in other types of brain cells called glia, all of which are damaged or altered in Alzheimer's disease.

Next, the researchers analyzed millions of electronic medical records to show that patients who took some of these drugs as part of their treatment for other conditions were less likely to get Alzheimer's disease.

When they tested a combination of the two top drugs - both of which are cancer medications - in a mouse model of Alzheimer's, it reduced brain degeneration in the mice, and even restored their ability to remember.

> *Alzheimer's disease comes with complex changes to the brain, which has made it tough to study and treat, but our computational tools opened up the possibility of tackling the complexity directly. We're excited that our computational approach led us to a potential combination therapy for Alzheimer's based on existing FDA-approved medications."*
>
> *Marina Sirota, PhD, the interim director of the UCSF Bakar Computational Health Sciences Institute, professor of pediatrics, and co-senior author of the paper*

The findings appeared in *Cell* on July 21. The research was funded in part by the National

Institutes of Health and the National Science Foundation.

## Big data from patients and cells points to a new Alzheimer's therapy

Alzheimer's disease affects 7 million people in the U.S. and causes a relentless decline in cognition, learning, and memory. Yet decades of research have only produced two FDA-approved drugs, neither of which can meaningfully slow this decline.

"Alzheimer's is likely the result of numerous alterations in many genes and proteins that, together, disrupt brain health," said Yadong Huang, MD, PhD, senior investigator and director of the Center for Translational Advancement at Gladstone, professor of neurology and pathology at UCSF, and co-senior author of the paper. "This makes it very challenging for drug development - which traditionally produces one drug for a single gene or protein that drives disease."

The team took publicly available data from three studies of the Alzheimer's brain that measured single-cell gene expression in brain cells from deceased donors with or without Alzheimer's disease. They used this data to produce gene expression signatures for Alzheimer's disease in neurons and glia.

The researchers compared these signatures with those found in the Connectivity Map, a database of results from testing the effects of thousands of drugs on gene expression in human cells.

Out of 1,300 drugs, 86 reversed the Alzheimer's disease gene expression signature in one cell type, and 25 reversed the signature in several cell types in the brain. But just 10 had already been approved by the FDA for use in humans.

Poring through records housed in the UC Health Data Warehouse, which includes anonymized health information on 1.4 million people over the age of 65, the group found that several of these drugs seemed to have reduced the risk of developing Alzheimer's disease over time.

"Thanks to all these existing data sources, we went from 1,300 drugs, to 86, to 10, to just 5," said Yaqiao Li, PhD, a former UCSF graduate student in Sirota's lab who is now a postdoctoral scholar in Huang's lab at Gladstone and the lead author of the paper. "In particular, the rich data collected by all the UC health centers pointed us straight to the most promising drugs. It's kind of like a mock clinical trial."

## A combination therapy poised for primetime

Li, Huang, and Sirota chose 2 cancer drugs out of the top 5 drug candidates for laboratory testing. They predicted one drug, letrozole, would remedy Alzheimer's in neurons; and another, irinotecan, would help glia. Letrozole is usually used to treat breast cancer; irinotecan is usually used to treat colon and lung cancer.

The team used a mouse model of aggressive Alzheimer's disease with multiple disease-related mutations. As the mice aged, symptoms resembling Alzheimer's emerged, and they were treated with one or both drugs.

The combination of the two cancer drugs reversed multiple aspects of Alzheimer's in the animal model. It undid the gene expression signatures in neurons and glia that had emerged as the disease progressed. It reduced both the formation of toxic clumps of proteins and brain degeneration. And, importantly, it restored memory.

"It's so exciting to see the validation of the computational data in a widely used Alzheimer's mouse model," Huang said. He expects the research to advance soon to a clinical trial so the team can directly test the combination therapy in Alzheimer's patients.

"If completely independent data sources, such as single-cell expression data and clinical records, guide us to the same pathways and the same drugs, and then resolve Alzheimer's in a genetic model, then maybe we're onto something," Sirota said. "We're hopeful this can be swiftly translated into a real solution for millions of patients with Alzheimer's."

---

**Source:**

University of California - San Francisco

**Journal reference:**

Li, Y., *et al.* (2025). Cell-type-directed network-correcting combination therapy for Alzheimer's disease. *Cell*. doi.org/10.1016/j.cell.2025.06.035.