THE CURRENT STATE OF DRUG DISCOVERY: IS THERE A BETTER WAY FORWARD?

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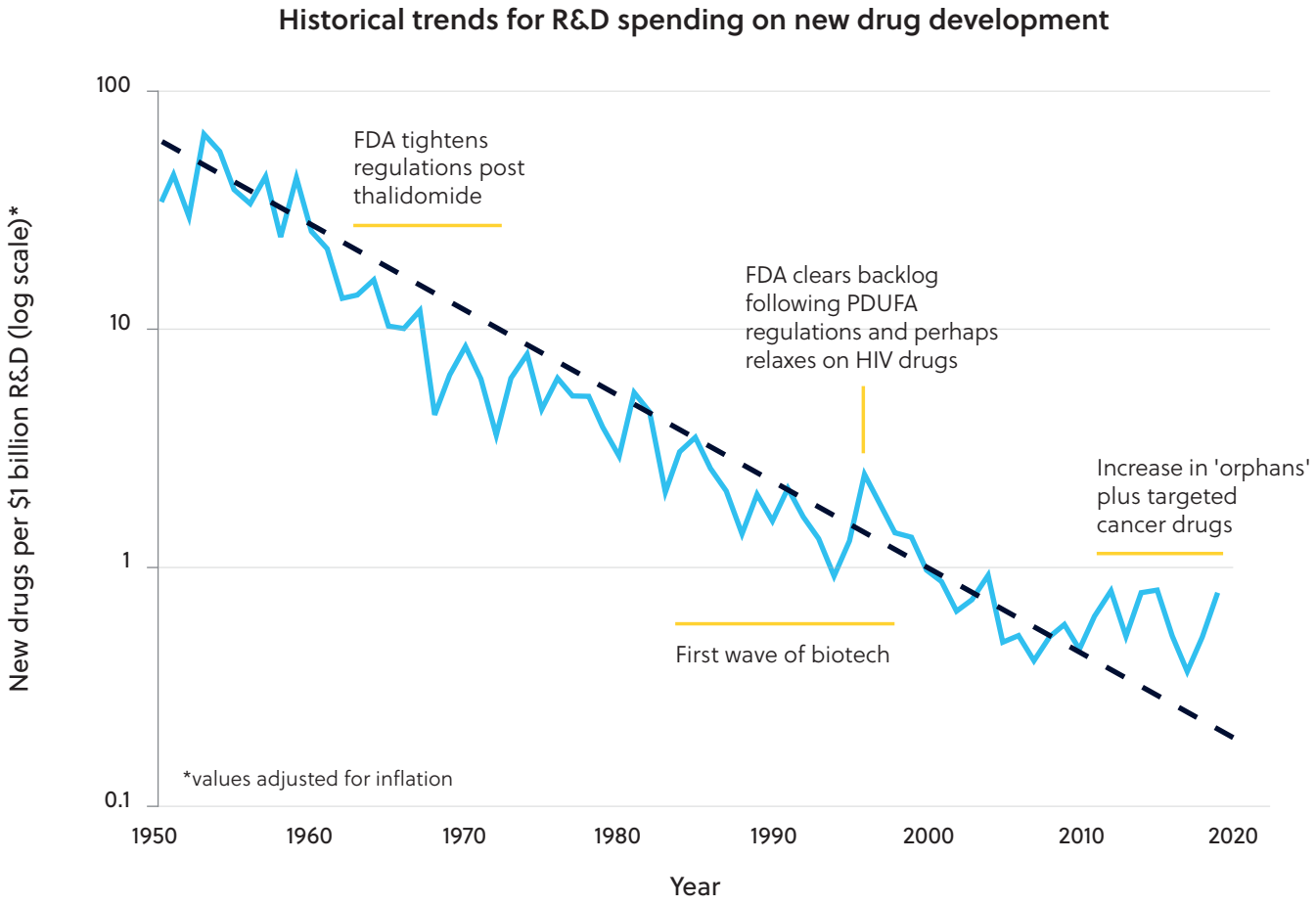
Introduction

In the complex world of pharmaceuticals, bringing a new drug to market is fraught with challenges, both old and new. Despite recent leaps in technology, including high-throughput screening (HTS), advancements in biotechnology, and sophisticated computational design, the path to true discovery is becoming increasingly arduous. This leaves us wondering why the process is not becoming more efficient with the advent of new, more powerful tools.

The answers lie in a blend of scientific, technological, and operational hurdles the industry strives to overcome, including the increasing cost of drug development, data management optimization, software integration, and time constraints on drug discovery researchers.

Eroom's Law: Still relevant more than a decade later

Eroom's Law, coined by Jack W. Scannell in 2012,[1] refers to the observation that drug discovery is becoming more expensive and slower over time despite technological advancements, a seemingly counterintuitive trend in an era in which technology is supposed to streamline and accelerate our efforts. Even with the recent breakthroughs in treating orphan diseases and targeted cancer therapies showing promise in bucking this trend, the industry still has various obstacles to overcome.[2]



Data source:
Jones, Richard & Wilsdon, James. (2018). The biomedical bubble: Why UK research and innovation needs a greater diversity of priorities, politics, places and people. 10.13140/RG.2.2.15613.05609.

Scannell, J., Blanckley, A., Boldon, H. et al. Diagnosing the decline in pharmaceutical R&D efficiency. *Nat Rev Drug Discov* 11, 191–200 (2012).

Munos, B. Lessons from 60 years of pharmaceutical innovation. Nature Rev. Drug Discov. 8, 959–968 (2010).

While there is no definitive cause for this paradoxical observation, some potential reasons include:

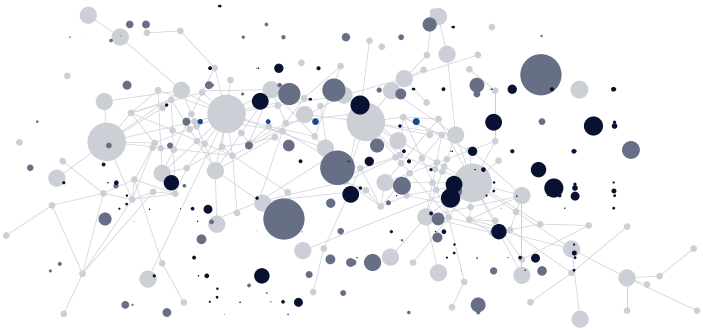
- Diminishing returns: As most of the 'low-hanging fruit' has been harvested, each new venture requires more resources with less certainty of success.
- Oversimplified discovery assays: Although HTS and target-based approaches speed up the initial stages of drug discovery, they often falter due to the complex, multifaceted nature of biological systems, leading to failures in clinical trials.
- Lengthy optimization cycles: Most drug development pipelines require numerous design-build-test cycles, often more than 20, highlighting the urgent need for methodologies to fast-track this progression.
- Data integration challenges: Integrating a vast amount of data into a cohesive, manageable system presents a significant bottleneck, slowing down the research process and complicating the path to discovery.

We must reimagine our data management approach

The era of big data has introduced new challenges for drug discovery teams working to manage the sheer amount of data available from internal and external sources. Intraorganizational data management can be challenging due to issues with versioning, file formats, connecting presentations back to source data, and the lack of a unified platform for storing and sharing information. These challenges are intensified when internal teams integrate data from unconnected and unorganized external sources, resulting in unstable data foundations.

Unconnected

Life sciences research and data are spread across hundreds of disconnected resources, such as databases, journals, and patents.



Unorganized

The same information is described differently across resources, making it difficult to compare data.

A single protein is known by many different names.

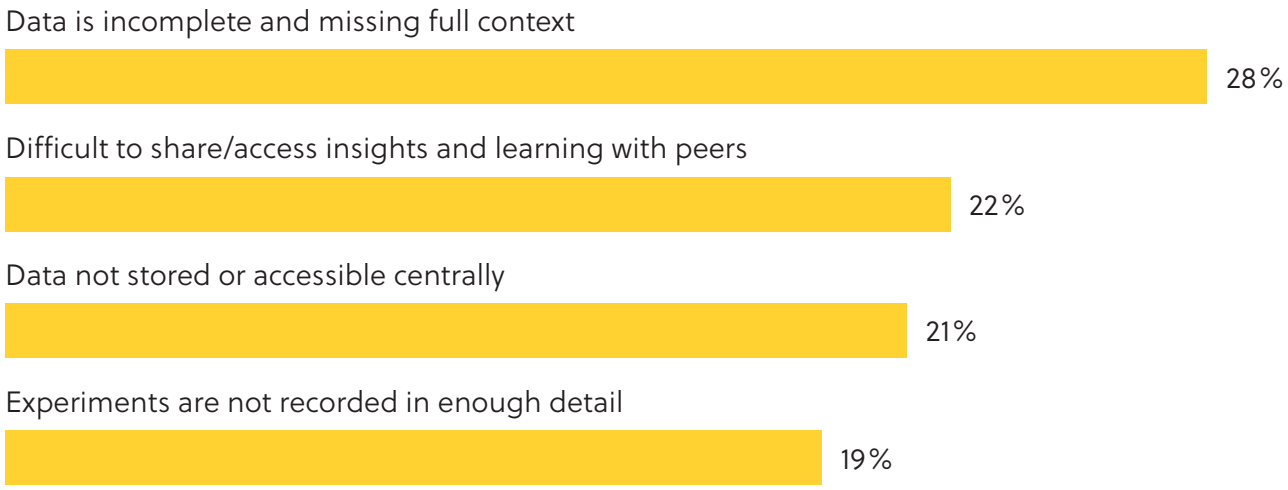
- Janus Kinase 3
- P52333
- HGNC:6193
- LJAK
- 'JAK 3'
- JAKL
- Tyrosine protein kinase JAK3

The drug discovery 'datasphere' is a behemoth, especially considering the various types and data sources available to researchers. These issues become increasingly problematic when Artificial Intelligence (AI) is deployed to process and analyze large data sets from various data streams. To derive true and actionable insights from your AI workflows, it is imperative to implement rigorous data management standards requiring access to clean, normalized, and harmonized data sets. Some of the information drug discovery researchers must manage for early discovery work is outlined in the table below.

Data category	Subcategory	Description
Chemical data	Compound data	Information about the molecular structures of compounds
	Synthesis data	Details on the synthesis and purification of chemical compounds
	Property data	Physical and chemical properties of compounds, such as solubility, stability, and molecular weight
Biological data	High-throughput screening (HTS) data	Results from screening large libraries of compounds for activity against biological targets
	Biomarker data	Information on biological molecules that indicate pharmacological responses, pathogenic processes, or pharmacokinetic processes
Pharmacological data	Pharmacodynamics	Data on the dose-dependent effects of a drug on its target
	Pharmacokinetics	Data related to drug absorption, distribution, metabolism, and excretion
	Toxicology data	Information on the potential adverse effects of drug candidates
Computational data	Molecular modeling and simulations	Data from computational models predicting how drug molecules interact with biological targets
	AI and machine learning (ML) models	Algorithms and predictive models used to analyze complex datasets and predict drug efficacy and safety

The seemingly infinite amount of data leaves researchers with the staggering task of discovering true insights among the noise. Beyond the sheer amount of data, researchers are further burdened by uncertainty about its reliability due to human errors in data handling and doubts about the accuracy of previous experiments.

Top reasons why earlier experiments are hard to improve



Data source: Synthace (2024). Lab automation & experimentation trends in life science R&D. Synthace.com, 2024, https://www.synthace.com/life-sciences-trends-automation-experimentation-report

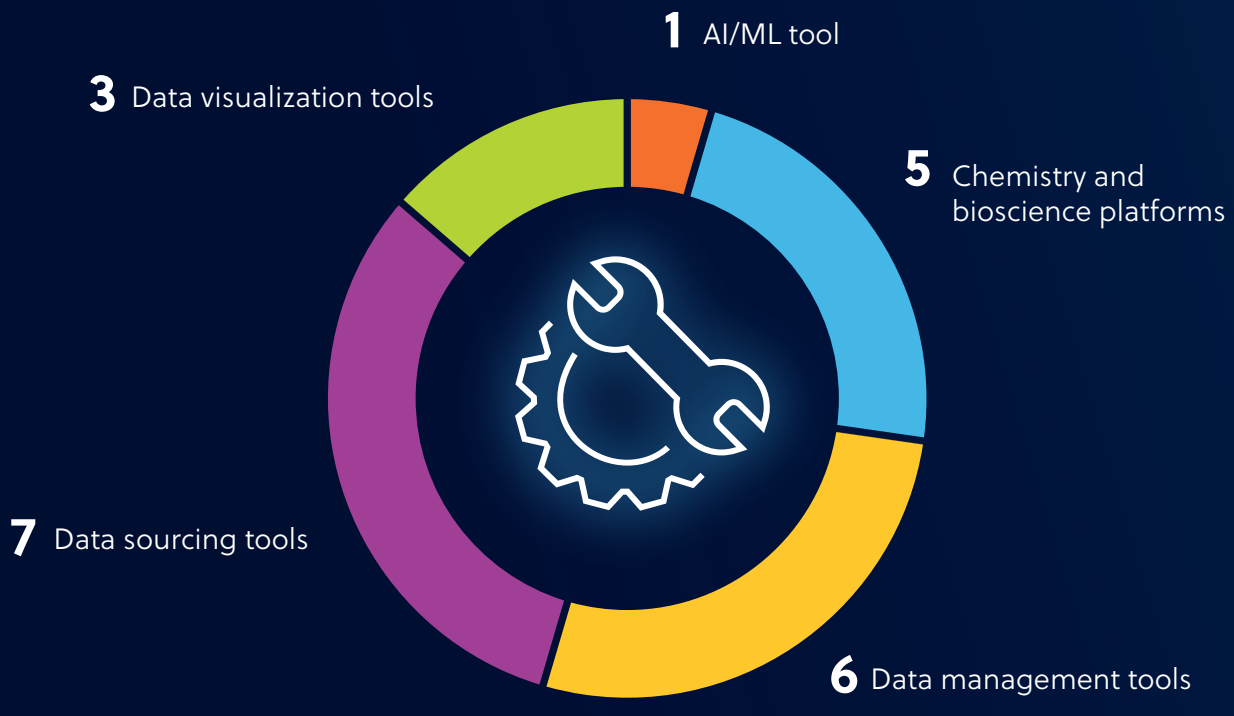
Unfortunately, this disordered state hampers productivity and obscures data clarity, making it difficult to build upon previous work.

Drug discovery software: Are we burdened by too many options?

Drug discovery researchers face a significant challenge in harmonizing many software tools and platforms essential for various workflow stages.[3] This includes data sourcing, management, and visualization—each integral to identifying and developing new drugs. The conundrum is whether the primary issue is an overabundance of software options or a scarcity of tools that adequately meet their specific needs.

The current software landscape is characterized by a wide array of specialized tools, each designed to perform distinct functions yet frequently lacking interoperability. This abundance might seem advantageous at first, offering bespoke solutions for different aspects of drug discovery. However, it can lead to researchers spending excessive time navigating between different systems, integrating disparate data formats, and learning multiple software interfaces.

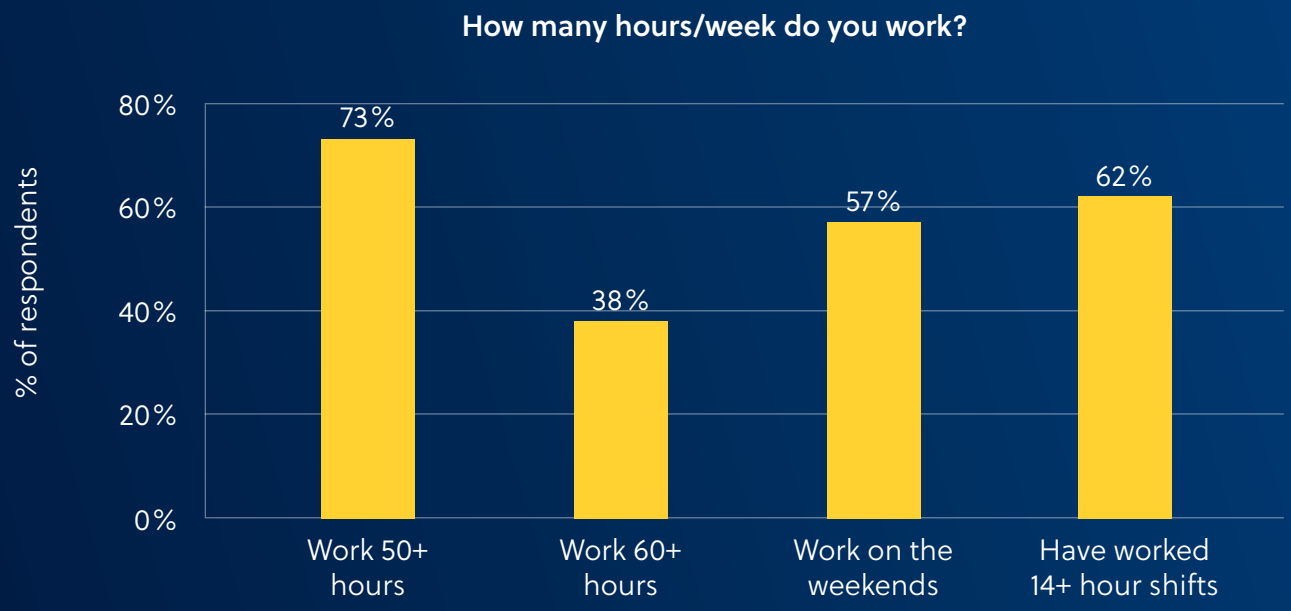
When surveyed, medicinal chemists identified 22 different tools and platforms they use for sourcing, managing, and visualizing biological data. This fragmented approach slows the research process, increases the likelihood of errors and data redundancy, and begs for a streamlined, integrated solution to simplify workflows and enhance efficiency.



Data source: The Understanding Group. (2023). CAS Drug Discovery Research: Research Findings.

Researchers are on the brink of exhaustion

Drug discovery researchers are no strangers to long hours and the mounting pressure to innovate. Despite a widespread consensus on the importance of efficient time management for success, the reality is starkly different. Over 70% of drug discovery researchers reported working more than 50 hours per week, with 38% working more than 60 hours per week. Additionally, over half of the researchers surveyed work weekends and shifts exceeding 14 hours regularly.[4]



Data source:
Powell, Kendall (2016). Hard work, little reward: Nature readers reveal working hours and research challenges. Nature, https://doi.org/10.1038/nature.2016.20933

Stemcell Technologies (Accessed April 08, 2024), The demands of science. Stemcell.com. https://www.stemcell.com/efficient-research/demands-of-science-report

Unfortunately, these long hours don't always translate to rapid success. Researchers are often overwhelmed by administrative tasks, exhaustive literature reviews, and data management, with actual experimental work taking up less than a third of their time.

This realization highlights the urgent need for solutions that streamline literature review and data management, ensuring researchers can focus their time on performing the experiments that drive innovative breakthroughs.

Data source:
Effron, Jacob (2022). The changing world of life sciences R&D. Vitalsignshealth.substack.com. https://vitalsignshealth.substack.com/p/the-changing-world-oflife-sciences

Guzman, Dani (2020). Research administration: Relieving the pressure on researchers. Exlibrisgroup.com. https://exlibrisgroup.com/blog/researchadministration-relieving-the-pressure-on-researchers/

Even with these challenges, the future is bright

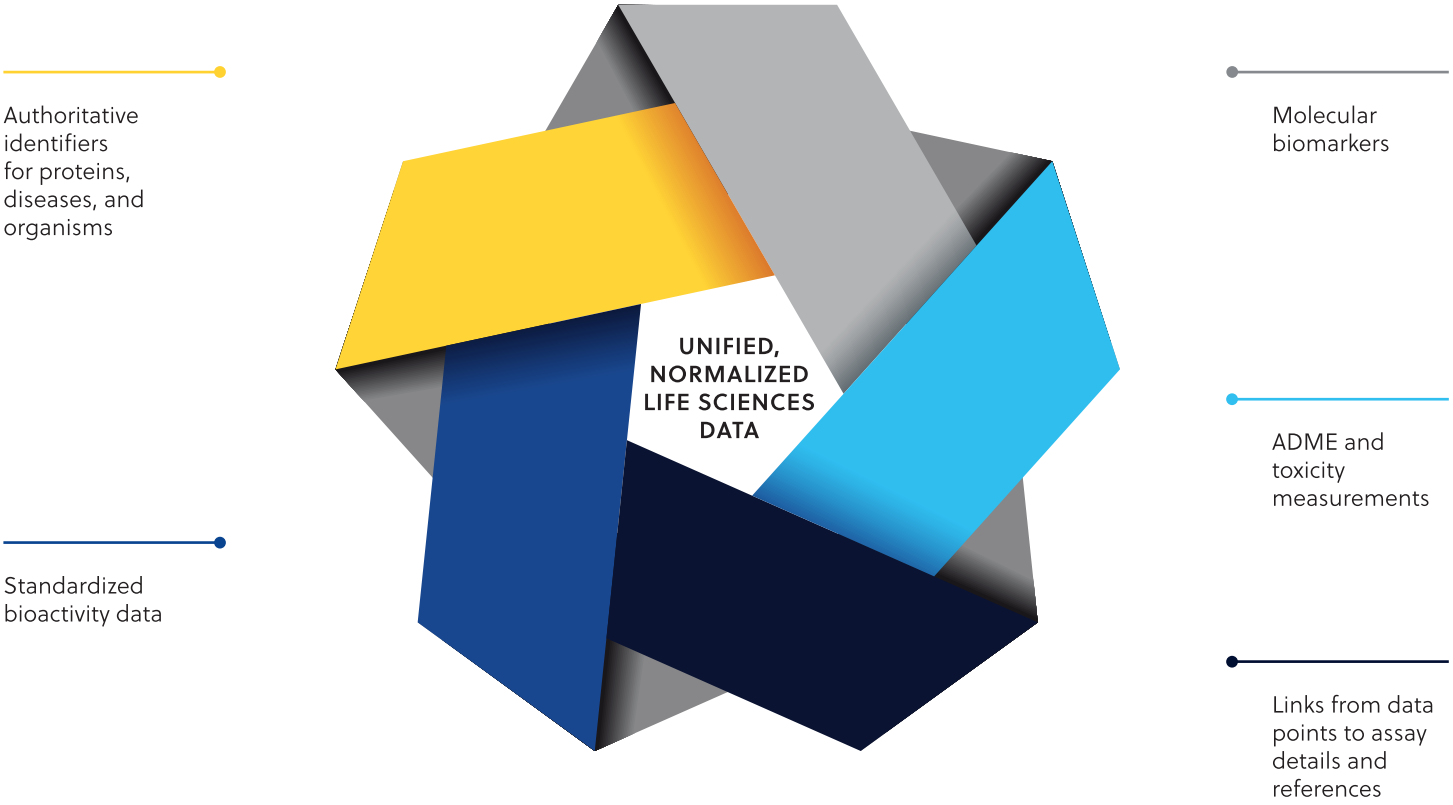
The increasing stakes in drug discovery demand a bold reevaluation of how scientists use their time, the methodologies they employ, and the tools they use. Only then can scientists hope to accelerate a drug's journey from the lab to the patients who need these breakthroughs most. By rethinking their approaches and harnessing the full potential of technological advancements, scientists can chart a course toward a more efficient, effective, and profitable future in drug discovery.

Say goodbye to missed insights and wasted time

Overcome your data sourcing challenges to unlock the full potential of your drug discovery workflows with the CAS BioFinder Discovery Platform™. CAS scientists use unmatched human expertise to deliver the insights you need to accelerate your discovery process, ensuring your time is spent on tasks that move your program forward.

Establish a robust data foundation and streamline your early discovery work with access to the world's largest collection of harmonized and curated scientific data—all linked to the references, methods, and assays used for its generation.

CAS experts analyze and curate all data in the CAS Content Collection™ to normalize measurements, assign authoritative identifiers, correct inconsistencies, and derive insights to build novel connections from once disparate information. The result is an unparalleled breadth of high-quality data that life science researchers can rely on, making CAS BioFinder™ the authoritative source for biological data you can trust.



Learn how the CAS BioFinder Discovery Platform can increase the efficiency of your drug discovery research at cas.org/solutions/biofinder-discovery-platform

1. Scannell, J., Blanckley, A., Boldon, H. et al. Diagnosing the decline in pharmaceutical R&D efficiency. Nat Rev Drug Discov 11, 191–200 (2012).
2. Jones, Richard & Wilsdon, James. (2018). The biomedical bubble: Why UK research and innovation needs a greater diversity of priorities, politics, places and people. 10.13140/RG.2.2.15613.05609.
3. Synthace (2024). Lab automation & experimentation trends in life science R&D. Synthace.com, 2024, https://www.synthace.com/life-sciences-trends-automation-experimentation-report.
4. Stemcell Technologies (Accessed April 08, 2024), The demands of science. Stemcell.com. https://www.stemcell.com/efficient-research/demands-of-science-report

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