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Simplifying drug discovery

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Taking the first step in drug development

Improving global healthcare outcomes relies on introducing innovative therapies that are either safer, more effective or address unmet medical needs. To achieve this, pharmaceutical companies go through drug development, a complex and expensive multistep process[1]. The average cost of developing a new drug is estimated to be around $1 billion, with some estimates reaching as high as $2.8 billion[2]. Combined with development timelines of 12–15 years[3], this makes drug development a significant investment for pharmaceutical companies.

The drug development pipeline follows a defined series of steps[3]:

Drug discovery

Research to understand the biological mechanisms of diseases and identify potential drug targets, biomarkers and novel drug candidates.

Preclinical development

In vitro and animal studies to determine the safety and efficacy of drug candidates and safe starting doses for first-in-human studies.

Clinical trials

Phase I–III clinical trials in humans to determine parameters such as maximum tolerated dose, therapeutic effectiveness, pharmacodynamics and pharmacokinetics.

Approval and commercialization

Demonstrating adherence to regulatory requirements to gain approval for therapeutic use and commercialization of developed drug products.

Drug discovery is the critical first step in drug development — the point at which pharmaceutical companies screen tens of thousands of targets, biomarkers and disease pathways to pursue new treatments. Experiments at this stage include genomics, transcriptomics, proteomics and other emerging molecular analyses.

Data analysis is therefore critical to determine which candidates should progress to the later stages and to the overall success of drug development. Bioinformatics enables drug developers to efficiently analyze large molecular datasets, facilitating drug discovery by identifying promising drug candidates more easily.

Bioinformatics-enabled drug discovery

Bioinformatics is a multi-disciplinary, data-driven science that spans genomics, transcriptomics, proteomics, population genetics and other high-throughput technologies[4]. Identifying new drug targets is driven by molecular data, meaning bioinformatics can improve all aspects of the process.

By comparing experimental disease conditions to controls and other groups, bioinformatics can[4]:

- Connect molecular information and changes to disease states.
- Identify drug candidates targeting molecular changes.
- Refine drug candidates to maximize therapeutic benefits and minimize side effects.

Bioinformatics enables pharmaceutical companies to make sense of discovery data, accelerating target identification and drug development. Big data technologies are also being used more often, highlighting the importance of bioinformatics in drug discovery.

The biopharma landscape in numbers:

Deloitte:

Measuring the return from pharmaceutical innovation

$2,284 million R&D costs to develop an asset from discovery to launch.

$362 million average forecast peak sales per pipeline asset.

4.1% internal rate of return of late-stage development pipeline.

Benchling:

State of tech in biopharma

70% of biopharma companies have adopted an R&D data platform.

53% of R&D scientists use 5+ unique scientific software applications day-to-day.

85% of companies expect at least 2x growth in R&D data.

Cloud-based platforms are the top priority for IT teams but not R&D teams.

BioRender:

State of science communication

96% of scientists agree that visual communication is critical to communicating science effectively.

Poor scientific communication can lead to canceled research and publication rejection.

Figures and illustrations are widely used by scientists but are time-consuming to create.

Pluto Bio:

The collaborative canvas for computational biology

Pluto is a dedicated bioinformatics platform designed to deliver a modern analysis experience built for biology. By enabling anyone to easily turn R&D data into publication-ready figures, **Pluto simplifies drug discovery** and allows biopharma companies to maximize their return on investment.

Big data, big discoveries

More data than ever before is being generated in drug discovery, fueled by emerging high-throughput technologies, including single-cell sequencing and multi-omics. Compared to bulk analysis and traditional -omics approaches, these techniques generate more data at a much more granular level, transforming disease understanding and revolutionizing drug discovery.

Single-cell sequencing technologies can answer key biological questions by uncovering disease-related mechanisms, actionable therapeutic targets and disease response heterogeneity. Therefore, incorporating single-cell analysis into discovery programs has the potential to improve both the quality of new drug targets and the clinical development of drug candidates[5].

Layering genomics, transcriptomics, proteomics and other levels of molecular data using multi-omics provides a holistic view of biology and disease. Multi-omics investigation of complex biological systems helps to understand cellular interactions better and identify new biomarkers and therapeutic targets[6]. Combining single-cell and multi-omics technologies in a single experiment can also explore the complex interplay between genotype and phenotype at high resolution[7].

Technologies are progressing fast, generating large volumes of complex data. Drug developers need bioinformatics that can keep up. Pharmaceutical companies that invest in bioinformatics can harness high-throughput technologies to unlock deep biological understanding and transform their drug discovery.

2
Driving drug discovery with data and bioinformatics

Drug discovery is becoming increasingly reliant on technologies that generate complex datasets, data analysis tools and bioinformatics platforms. However, one question that is often overlooked in the increasingly data-driven drug discovery landscape is:

Why is data important in drug discovery?

Simply put, data answers scientific questions.

Drug discovery raises many scientific questions, meaning that data is now indispensable for developers. The importance of data in drug discovery also highlights the importance of bioinformatics, which unlocks the potential of data by turning numbers into insights. Together, data and bioinformatics allow developers to address scientific questions and drive drug discovery forward.

How can bioinformatics unlock data in drug discovery?

- **Understanding disease mechanisms:** Revealing the molecular basis of disease including the biological pathways and networks that initiate disease and drive progression.
- **Biomarker discovery:** Identifying biomarkers, molecular signatures and changes in profiles characterizing disease diagnosis, prognosis and treatment response.
- **Target identification and validation:** Identifying new drug targets and validating them during discovery and development.
- **Personalized medicine:** Tailoring treatments using genetics, molecular profiles and patient subtyping.

Bioinformatics simplified

The Pluto platform is designed to address bioinformatics challenges. With Pluto, anyone can perform flexible data analysis and share beautiful, publication-ready figures and visualizations.

Pluto is a platform ready for big data, enabling the analysis of high-throughput experiments, including multi-omics. Data is backed up by security that ensures protection and adherence to compliance requirements.

Pluto's unparalleled efficiency simplifies bioinformatics, allowing scientists to break free from bottlenecks and focus on science.

Pluto's disease mechanism capabilities:

- Differential gene expression
- Pathway enrichment
- Protein-protein interaction network analysis
- Gene set enrichment
- Co-expression network analysis
- Gene regulatory network analysis
- Single-cell RNA sequencing

Data analysis that works therefore increases the chances of success in drug development. From target identification and candidate screening to characterizing side effects and drug resistance, an effective bioinformatics approach can simplify drug discovery and accelerate development[4].

However, there are several challenges that pharmaceutical companies must navigate to get the most out of bioinformatics in drug discovery:

- **Organizing big data**

High-throughput technologies are revolutionizing drug discovery. However, generating more data (and more complex data) makes data analysis more challenging. In the case of multi-omics, multiple different types of datasets from different sources need to be integrated and analyzed to produce meaningful results. Technologies are moving fast and bioinformatics needs to keep up to ensure that data is organized and analyzed effectively.

- **Accessible data analysis**

There isn't a standardized data analysis approach, making bioinformatics development challenging and affecting accessibility. Biologists spend a lot of time learning how to perform data analysis to help them make sense of data, with workflows often requiring coding expertise. Differences in data analysis approaches raise concerns regarding reliability and reproducibility and cause bottlenecks from both the time spent learning bioinformatics and the reduced time available to spend on experimental innovation.

- **Data sharing and collaboration**

Collaboration is essential in drug discovery but it can be challenging to share data and results. Pharmaceutical companies constantly collaborate to demonstrate the quality of their data to prospective partners, academia and government organizations. Pharmaceutical outsourcing now plays a major role in drug discovery, with collaboration and data sharing required to progress through development. Collaboration within organizations can stop companies from working in silos, a challenge that exists even for teams working in the same location.

- **Data security and storage**

Biological data in the pharmaceutical industry has unique challenges for data security and storage. Pharmaceutical companies must consider the sensitivity of the data they generate, either from patients or associated with intellectual property. Meeting regulatory requirements also requires developers to have the appropriate infrastructure in place for data storage.

Overcoming bioinformatics challenges can simplify drug discovery. Pharmaceutical companies that have confidence in their bioinformatics can focus their efforts on innovation, driving successful drug development and delivering life-changing treatments to the patients who need them.

3
Simplifying bioinformatics

A dedicated bioinformatics platform can help overcome data analysis challenges, improving efficiency in drug discovery and allowing efforts to be focused on innovation. A bioinformatics platform that works can provide pharmaceutical companies with a home for big data, simplified analysis, collaborative visualization and data security.

a. A platform for big data

Single-cell sequencing and multi-omics technologies generate high-dimensional datasets. Extracting insights from these data sources requires drug developers to run pipelines, preprocess data, perform downstream analysis and modify parameters. Due to the complexity of datasets, artificial intelligence (AI) may also be required for specific analysis methods, including cell-type annotation.

A bioinformatics platform ready for big data enables pharmaceutical companies to harness high-throughput technologies and gain detailed molecular insights at every level[7]:

Genomics: Sequencing complete DNA to identify mutations and better understand the underlying disease biology.

Transcriptomics: Total RNA or mRNA analysis to understand gene expression and explore what's happening in a disease at a specific time point.

Proteomics: Analysis of the complete set of proteins present at a given time to understand the functional mechanisms of biology and disease.

Metabolomics: Large-scale study of small molecules to understand metabolic activity, biochemical pathways and cellular interactions.

Single-cell analysis and multi-omics are rapidly developing, with best practices for experiments and data analysis constantly evolving. As this means data analysis is often exploratory, drug developers can benefit from a bioinformatics platform that facilitates experimentation. Bringing together datasets from different sources provides a foundation for discoveries fueled by single-cell analysis and multi-omics. Benchmarking and validating methods against publicly available datasets can also help with optimizing data analysis, which is particularly relevant in personalized medicine.

Unlocking the power of data

Pluto is designed to unlock the power of big data technologies such as single-cell sequencing and multi-omics.

By integrating multi-modal data sources and providing a platform for exploring big data, Pluto can solve bioinformatics challenges in drug discovery now and in the future.

Pluto's data handling simplifies high-throughput bioinformatics, empowering scientists to push experiments further and explore the limits of discovery.

Pluto's biomarker discovery capabilities:

- Receiver operating characteristic (ROC) curve analysis
- Principal component analysis (PCA)
- Hierarchical clustering
- Support vector machine (SVM) classification
- Random forest classification
- Cross-validation analysis
- Survival analysis (for prognostic biomarkers)
- Feature selection techniques
- Network-based biomarker identification

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b. Simplified and accessible analysis

The inaccessibility of bioinformatics workflows can have a substantial impact on drug discovery. Biologists learning bioinformatics when they need to analyze their data is an inefficient approach that can impact the reliability and reproducibility of results. Ultimately, this could lead to major setbacks, wasted resources and the progression of unsuitable drug candidates.

A standardized and traceable bioinformatics platform can help improve accessibility and drive innovation in drug discovery. Rather than learning how to analyze data, biologists can easily perform bioinformatics that they can rely on. By overcoming accessibility challenges, drug developers not only have more time to spend innovating but can also make more informed decisions because their results are reliable.

By performing analysis all in the same place, pharmaceutical developers can also minimize differences in bioinformatics workflows between experiments, improving the reliability and reproducibility of results. Accessible bioinformatics also feeds into collaboration as teams can align on data analysis and interpret results in a meaningful way.

The increase of AI-powered bioinformatics is also changing the meaning of standardization. It's becoming increasingly important to ensure that data is in the correct format before processing with AI. Preprocessing data in this way helps to avoid a "garbage in/garbage out" situation. Bioinformatics platforms compatible with raw data files can help address this issue, allowing controlled data analysis supported by AI.

Accessible data analysis

Pluto is designed with simplicity and user-friendliness in mind, enabling anyone to perform data analysis regardless of their bioinformatics expertise.

By providing standardized and traceable data analysis, Pluto can reduce bioinformatics bottlenecks and provide reliable and reproducible results.

Pluto's easy-to-use and interactive platform takes care of data analysis, allowing drug developers to innovate and deliver life-changing treatments.

Pluto's drug discovery capabilities:

- Drug repurposing analysis
- Connectivity mapping

c. Easy collaboration and sharing

Collaboration is an essential part of drug discovery but it can be challenging without a unified bioinformatics platform. Performing data analysis in one platform, exporting results and then sharing them via email is a slow and cumbersome process. Collaboration and sharing ideas about results make this process even slower, as not everyone may have access to the appropriate analysis software, and ideas can get lost in communication channels.

A bioinformatics platform designed to enable easy collaboration can help pharmaceutical companies share their innovative results and progress drug development. A connected and interactive platform promotes collaboration, allowing teams to share ideas and keep a record of communications all in one place.

Pharmaceutical companies that invest in collaborative bioinformatics platforms can more effectively demonstrate the quality of their data and transform drug discovery. A bioinformatics platform built around collaboration can help drug developers share results with:

- Other pharmaceutical companies, biotechs or prospective partners
- Academic and research institutions
- Government organizations

Outsourcing is also a vital part of the pharmaceutical industry, allowing companies to access specialist facilities or services and streamline drug development. Contract research organizations (CROs) and contract development and manufacturing organizations (CDMOs) can cover the entire drug development pipeline, from early discovery to commercial manufacturing. A bioinformatics platform that enables collaboration is a great tool for managing data from partners and simplifying the outsourcing process.

A space for collaboration

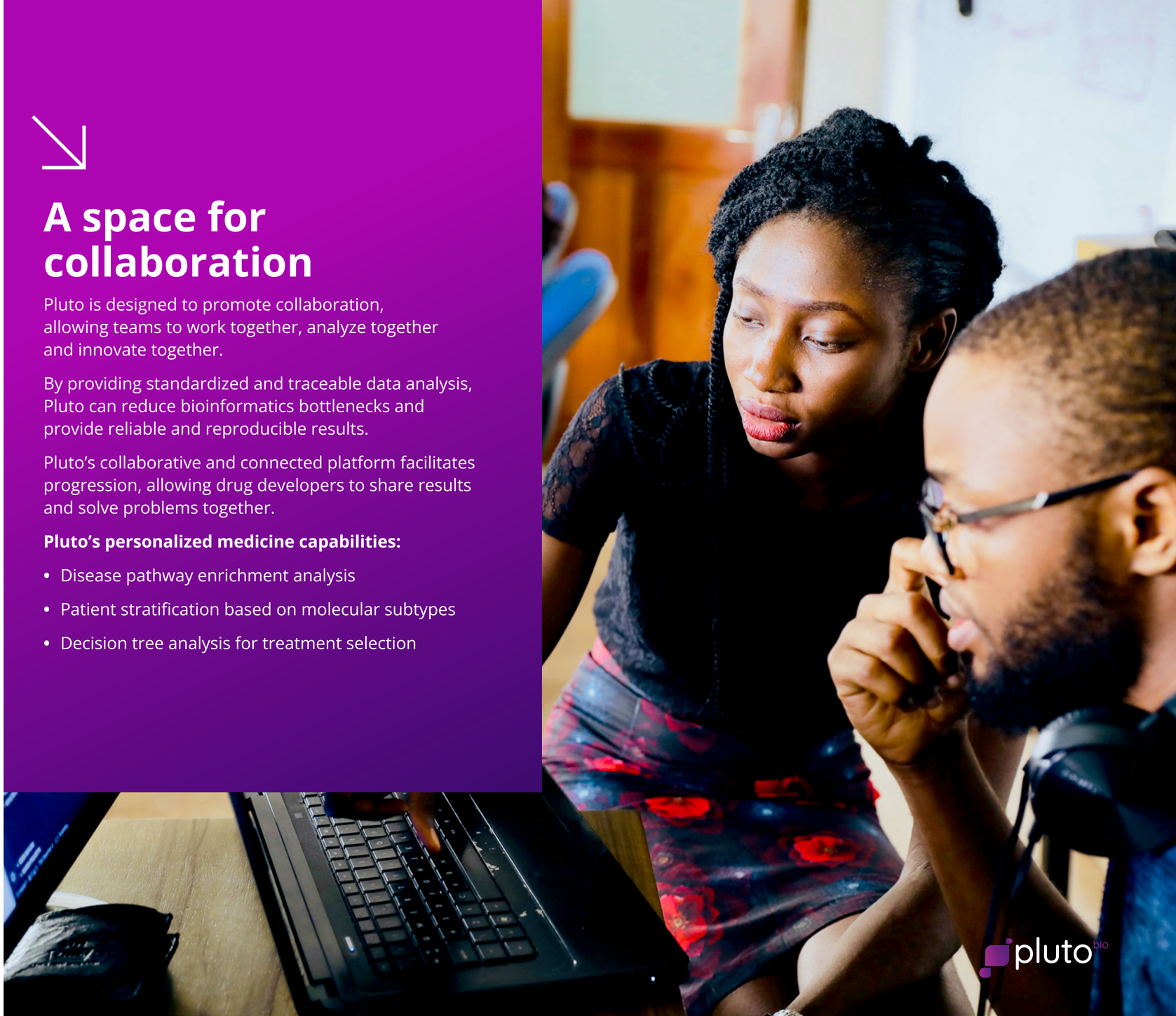
Pluto is designed to promote collaboration, allowing teams to work together, analyze together and innovate together.

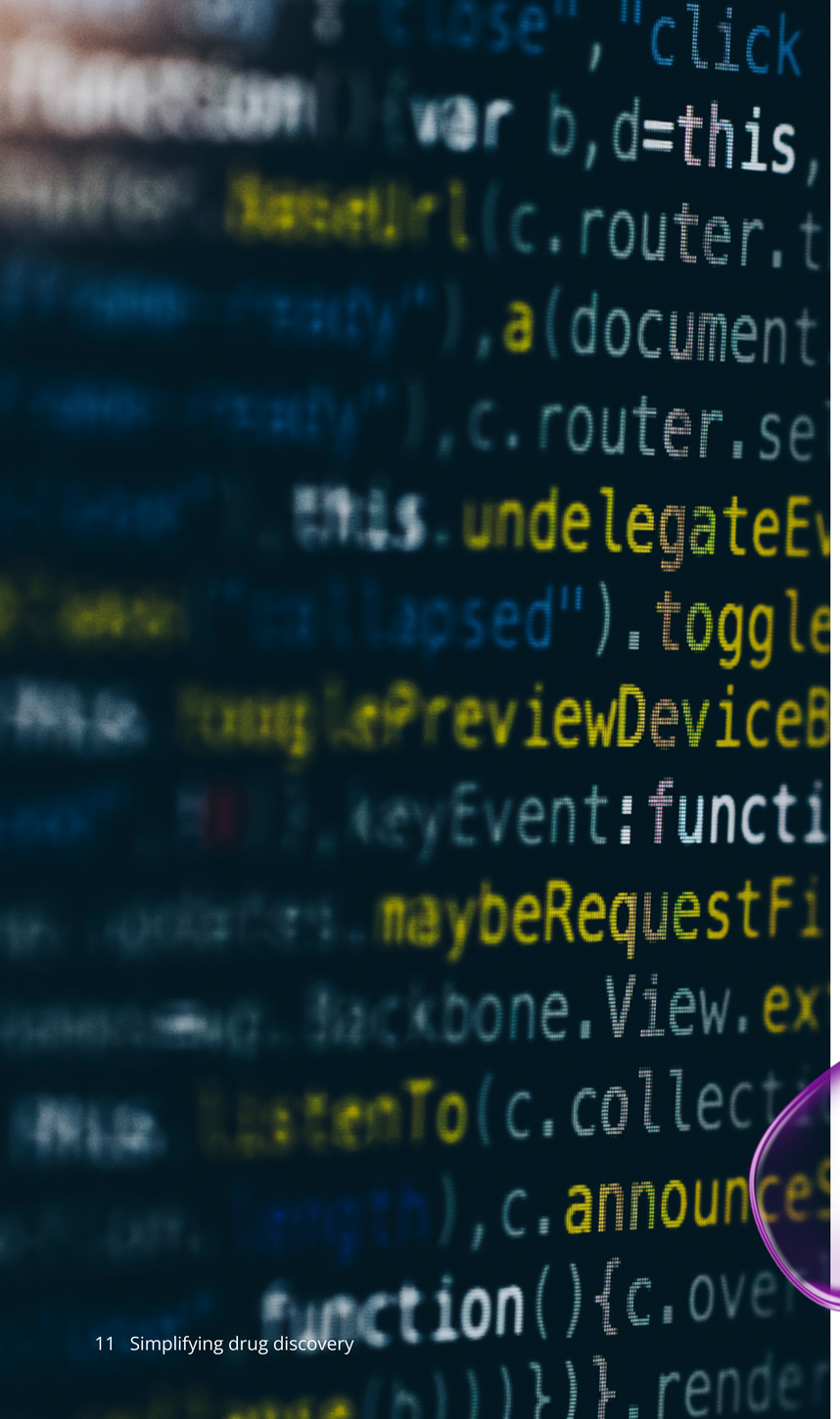
By providing standardized and traceable data analysis, Pluto can reduce bioinformatics bottlenecks and provide reliable and reproducible results.

Pluto's collaborative and connected platform facilitates progression, allowing drug developers to share results and solve problems together.

Pluto's personalized medicine capabilities:

- Disease pathway enrichment analysis
- Patient stratification based on molecular subtypes
- Decision tree analysis for treatment selection





d. Data security

Drug developers face unique data storage and security challenges. Data generated from patients is highly sensitive and developers must ensure that it is stored securely. Patient data breaches are a major ethical concern and can lead to loss of reputation, legal consequences and financial losses. Intellectual property (IP) is another data consideration for the pharmaceutical industry. If data linked to IP is breached, developers can face legal consequences and potentially substantial financial losses and market share. Having an appropriate data storage and security infrastructure in place is also a common part of meeting regulatory requirements for product approval and commercialization.

Bioinformatics platforms built with security in mind can provide drug developers with peace of mind regarding their data storage. Secure platforms can be used to store patient and IP-associated data. This approach helps to mitigate the risk of data breaches, protecting drug developers against legal action and loss of reputation or finances. Having a bioinformatics platform that complies with regulatory requirements can also streamline the approval process and enable developers to accelerate product commercialization.

Secure data storage

Pluto is designed to keep data secure, protecting against risks and data breaches, and ensuring storage compliance for regulatory approval.

By continuing to invest in security, Pluto can take care of data storage, allowing pharmaceutical companies to focus on development and innovation.

Pluto's data storage simplifies security, reducing risks and giving drug developers peace of mind.

Pluto's data security capabilities:

- SOC2 compliance
- End-to-end data encryption
- GDPR compliance
- Individual privacy protections
- Dedicated trust center
- IT and security audits

4
Transforming drug discovery

Drug development is a significant investment for pharmaceutical companies, and drug discovery is one of the most challenging parts of the process. Bioinformatics can help simplify drug discovery and drive success later in development.

By investing in a bioinformatics platform that can organize big data, provide accessible data analysis, drive collaboration and securely store data, drug developers can simplify drug discovery and transform their drug development.

Pluto is a bioinformatics platform designed to provide flexible, collaborative and easy-to-use data analysis. A secure platform compatible with big data technologies, Pluto can help drug developers overcome challenges and simplify drug discovery now and in the future.

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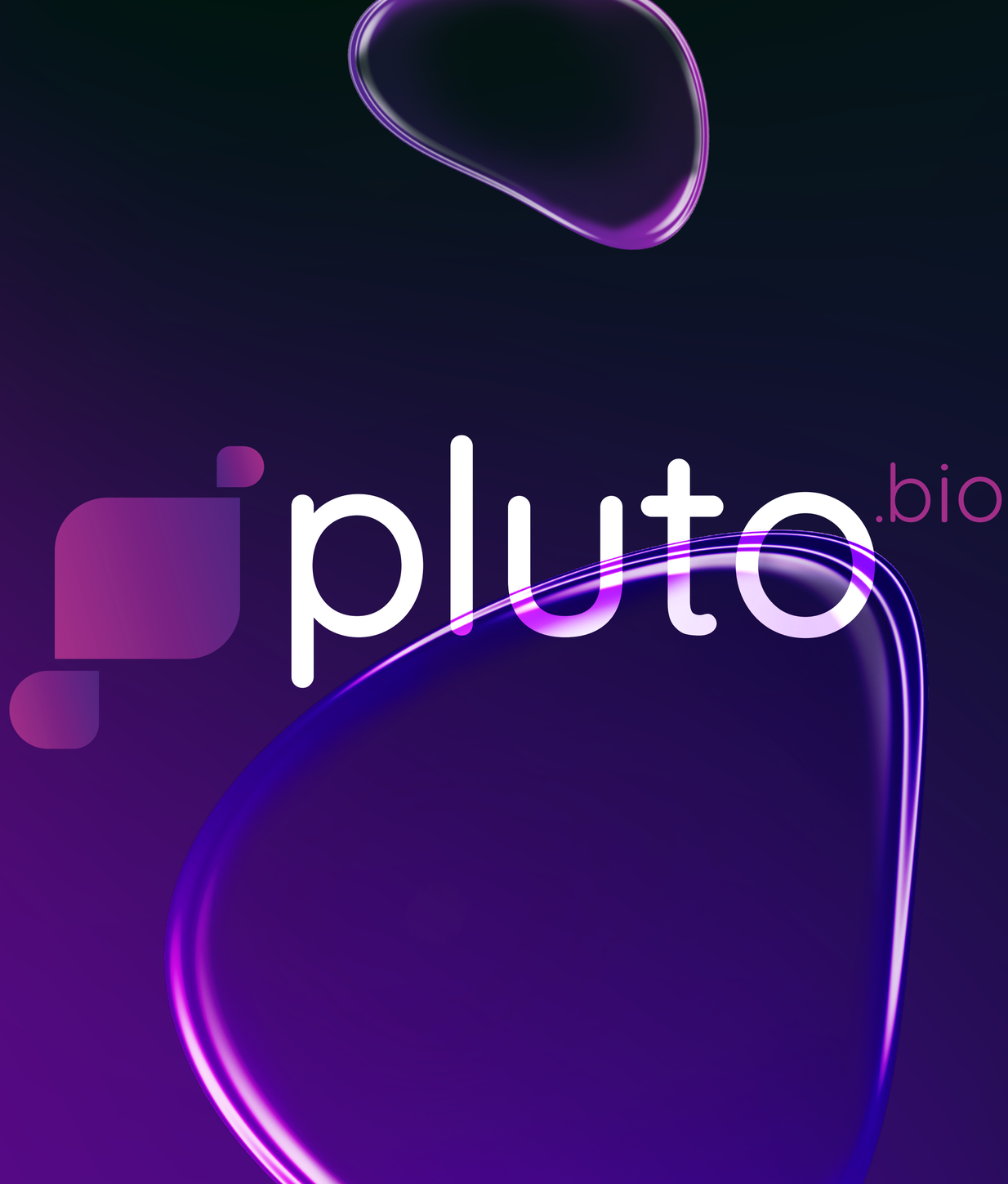
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