

WHITEPAPER

How to Optimize **In Vitro** and **In Vivo** Data Analysis in Drug Discovery



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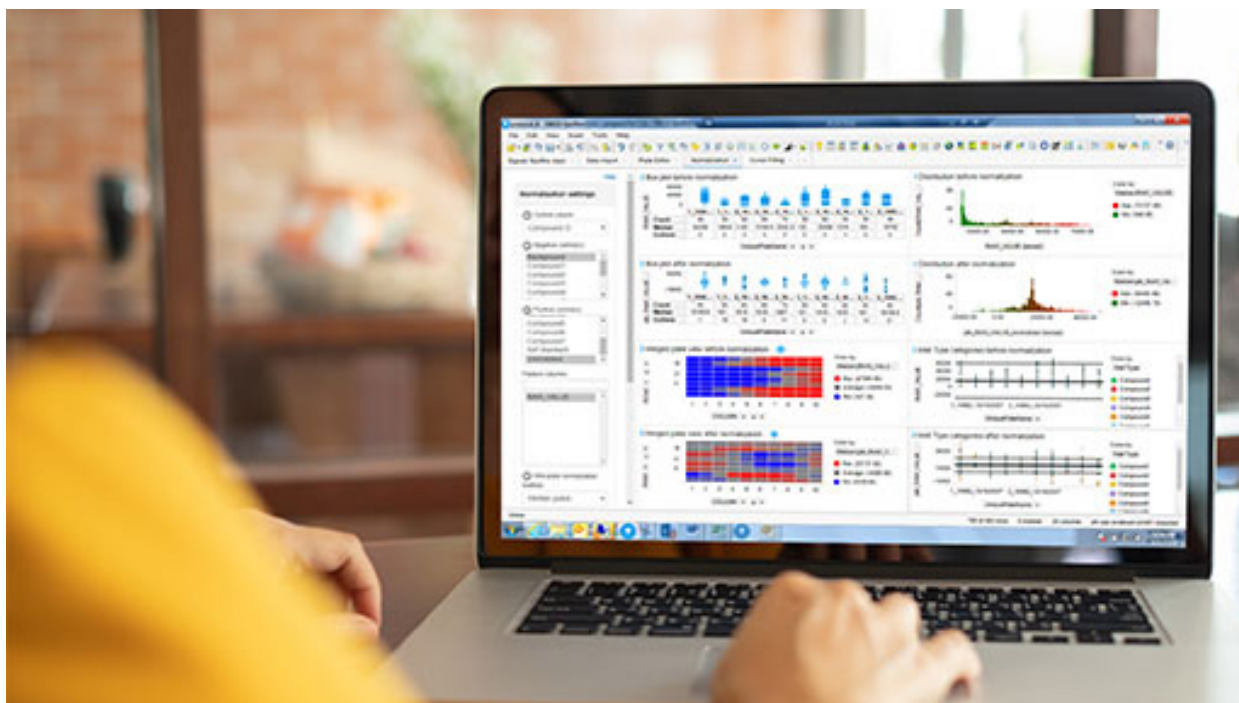
Assay development, high-throughput screening (HTS), and in vivo testing are some of the first steps researchers take to evaluate the effects of potential drug candidates on cellular, molecular, or biochemical processes. Assay quality, and the quality of data collected, influences the effectiveness of the drug discovery steps to follow.

Collaboration between early and later stage analytical teams throughout the drug development process is all about data analytics and efficient sharing of key analytical results generated using many different innovative and specialized analytical technologies. Too many times, accessing those various data types to enable an efficient data-driven collaboration is hindered by traditional, inefficient, and rigid data analysis tools leading to a disconnect between analytical teams, and more importantly, missing key analytical insights and opportunities. For example, the ability to put into perspective results obtained by Mass Spectrometry and other analytical techniques alongside SPR and High Content Screening to characterize a target can be extremely useful for evaluators.

To ensure the highest quality of both the assays and the data, researchers must focus not only on the assay itself, but also the data transformation and analysis workflow. The process of evaluating and investigating millions of compounds requires multiple measurements across multiple laboratories, and historically, multiple software systems.

The instruments used during R&D generate high volumes of diverse data. But until recently, scientists have lacked full visibility into the data as the new drug candidates step from target validation, to lead generation and refinement, and on to preclinical research.

Without full access to data, analysis quality and efficiency suffers. This leads to missed opportunities, extended drug discovery pipelines, or even costly late failures of drug candidates.



Digital innovation has the potential to transform early stages of drug discovery by allowing researchers to view and compare data across functions. And they can accomplish this task with one platform.

A single research data management platform built on modern architecture allows global research teams to holistically view and analyze all data produced in their labs, allowing for more streamlined, yet more comprehensive, decision making. Rather than wrangle data from multiple unconnected software systems, researchers can work from a unified platform that integrates all results from every raw data format and screening technique.

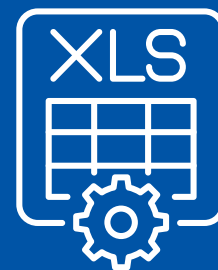
Having all in vivo and in vitro assay data in one place leads to better insights—insights that can lead to the identification of more leads and, ultimately, the discovery of more viable drug candidates. As these candidates move through preclinical research, the likelihood of safer therapies for patients increases.

Historical Challenges with Assay Development Data Analysis

Scientists spend years in the lab testing hypotheses to find molecules that may later cure a debilitating rare disease or an aggressive form of cancer. Their limitations lie not in their imagination or critical thinking skills, but in the tools they use to do their jobs. Archaic hardware, software, and processes slow down assay development and introduce opportunities for error.

- **Manual Processes.** Researchers use multiple instruments, ranging from imaging systems to Surface Plasmon Resonance (SPR), and more. These instruments come with dedicated software to access the data produced by the instruments, some with limited ability to analyze the output. At any time during a research project, a scientist has to be able to combine results from multiple software systems to determine whether to conduct more experiments or move the project to another stage of the overall workflow.

All instruments produce data that needs to be formatted, reformatted, and joined with potentially multiple data outputs from the same or other instruments. It also needs to be analyzed before it gets handed off to the next team. All this information determines what candidates will progress to clinical trials. Getting to that point is a time-consuming, labor-intensive process, sometimes up to weeks or months.



Digital innovation has the potential to transform early stages of drug discovery by allowing researchers to view and compare data across functions. They can accomplish this task with one platform.

“Every time data comes in from an instrument, it comes in an Excel format, text files, or some other format which scientists have to parse into a spreadsheet and add equations, and metadata to start analyzing their experiment results,” says Dr. Christof Gaenzler, Global Product Director Screening Analytics, PerkinElmer Inc. “They repeat this process every time they come up with new data. There is often no automated process. The data is not searchable. You can’t use it to run further analyses, and you can’t share how you arrived at your conclusions so others can repeat your data analysis. When you move through the drug discovery phase, you often have to run analyses on a larger scale. This means that data analysis not only has to be flexible, but it has to be robust and repeatable across all steps as well.”

PerkinElmer Signals VitroVivo is a single platform that can handle complex and high data volumes produced by instruments of any kind. Powerful analytics tools and pre-built templates help scientists eliminate all the time spent building analyses so they can focus on higher-value tasks. And the analysis stays consistent and repeatable from the early assays throughout the drug discovery workflow a project takes.

- **Siloed Software Systems.** Researchers often have no effective way to bring disparate datasets from multiple instruments together to derive a conclusive analysis. Instead, they go through an inefficient transformation of data for individual analyses. They develop their own systems or must rely on Excel or an Excel-like platform, which only meets some of their needs. Traditionally, scientists also have no efficient way to transfer data between groups. Using spreadsheets or pdfs, teams can’t truly interact with each other’s data to conduct meaningful analysis or gain insights.

Cloud-based software has advanced to the level that organizations can replace spreadsheets with a single platform that handles the full scope of assay data processing. Independent research areas, once decoupled due to rigid silos and an inability to seamlessly transfer datasets, become integrated and collaborative.

This single platform allows users to search across all assay and screening data instantly. They don’t have to manipulate data from a spreadsheet. And they don’t have to wait to receive the data.

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- **Processes in Parallel.** The non-linear research process is becoming more and more condensed to save time. For example, in vivo and High Content Screening (HCS) are occurring simultaneously. This is why many aspects of the research process are happening in parallel.

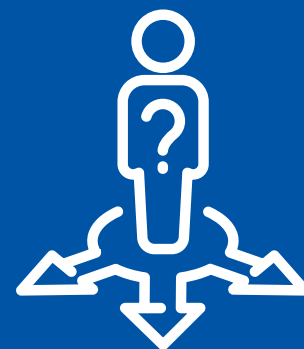
A software platform allowing an entire research group to capture and analyze data and collaborate in one system is the only way to overcome working in isolation and producing data and information silos.

- **Outdated software.** Traditional instrument software often performs a given task as its only job . This limits scientists' capabilities to analyze the experiment results in context.

In addition to an inability to search data, scientists can't access historical data. They can't easily review what worked and didn't work in the past to inform today's research.

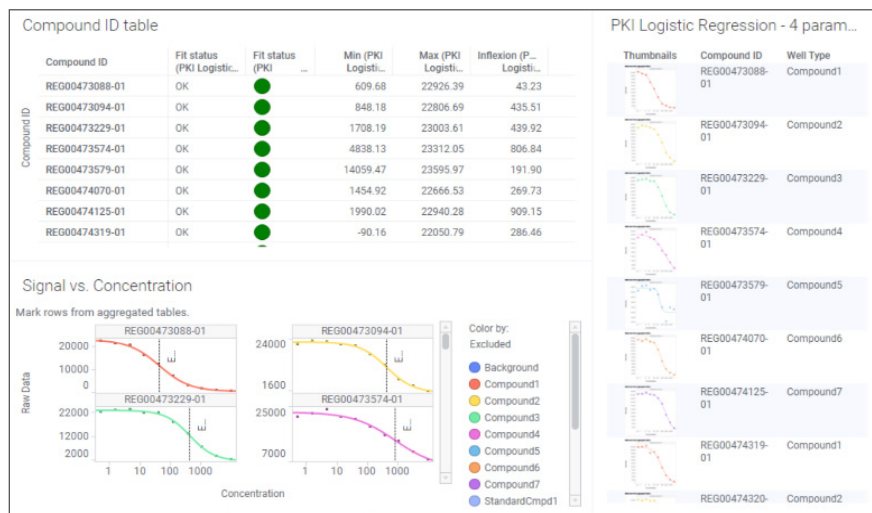
As science advances and experts learn new techniques, rigid software limits their ability to use those techniques. "It's not easy with existing tools to create a new data analysis workflow," says Dr. Gaenzler. "Even changing an existing data analysis workflow takes a lot of time, resources, funding, and potentially custom development. As science grows, existing software cannot grow with it at the same pace."

Cloud-based lab data management and analysis solutions have the flexibility to grow and adapt to scientists' needs. These solutions can address any data format and can be configured to specific lab workflows.



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The Single Platform Solution



A single data management/analysis platform resolves many of the inefficiencies that have hampered drug discovery over the past decades. Cloud computing makes this type of platform possible

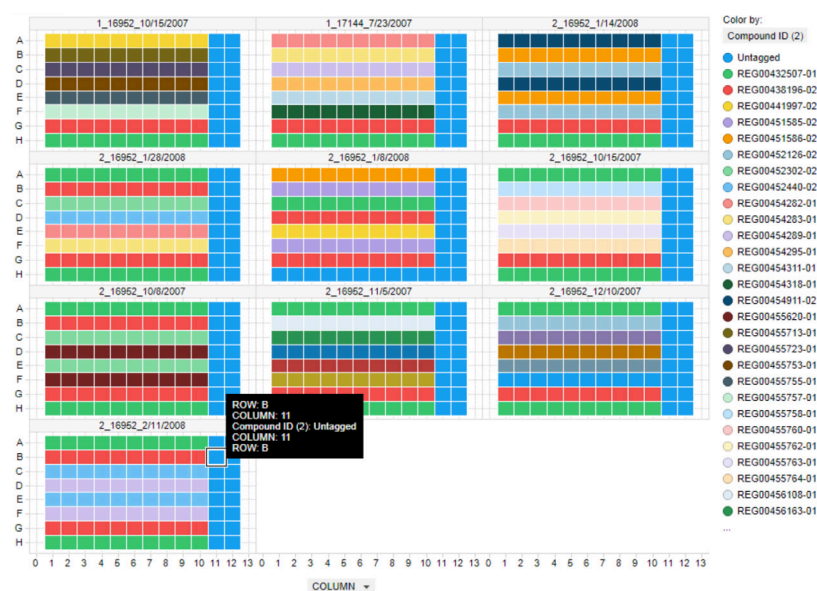
By seamlessly sharing data across the drug discovery continuum, scientists have access to the specialized tools they need, while also gaining the ability to conduct meaningful analysis of that data in a few clicks, no time-consuming manual processes.

Cloud-based solutions have allowed businesses across other sectors to share and compare data across departments—a healthcare system can share patient data among primary care doctors, specialists, and radiologists. A pharmaceutical company can streamline its supply chain to get products distributed faster. Why not streamline drug discovery?

A data management and analysis platform optimizes workflows. Scientists aren't limited by their software. And their IT teams don't have to build and maintain custom tools for every new technique. The platform adapts to scientists' needs and fosters collaboration.

A single platform eliminates time-consuming, inefficient tech transfers. There's no recreating of analyses to suit disparate systems. When moving from assay development to HTS to in vivo testing, workflows remain consistent and repeatable.

How Signals VitroVivo Optimizes In Vitro and In Vivo Data Analysis



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There's a reason scientists had to rely on inefficient, outdated software and cumbersome workflows. They had no choice.

With the launch of the PerkinElmer Signals VitroVivo Platform, drug discovery teams can collaborate on one scalable platform. Protocol hand-over and collaboration among scientists, labs, and groups is enabled, ensuring no result or data point is overlooked and all can contribute meaningfully to the progress of drug research.

Scientists can do more with their data in far less time without using disparate, rigid systems. The power and speed of modern, modular architecture, combined with the interactive data visualization and analysis platform TIBCO Spotfire®, makes it happen.

Automated Processes

In a single platform, labor-intensive analysis-building goes away. Users can automate assay development, screening, and in vivo testing workflows. The Signals VitroVivo platform includes an embedded app store that allows scientists to quickly go from data import to curve-fitting, without having to manually wrangle data. They can daisy-chain these apps together and/or move them around to create a protocol custom to the lab's workflow.

The apps configure themselves and allow the user to input parameters on their own—a significant time and cost-saver. “This feature puts the problems of rigid software into the past,” says Dr. Gaenzler. “To solve those problems often required contracting with an external service that took six months or more to build a custom application for a new scientific technique. Now with Signals VitroVivo scientists can do it themselves.”

No longer do scientists have to reinvent the wheel when moving from assay development to HTS. Within Signals VitroVivo, analyses built during assay development become a reusable protocol in the screening stage. When scientists get back months of their time, it trickles down to accelerate the entire discovery and development process.

Break Down Silos

Within a single platform, the data processing pipeline gets built in parallel with the data model. Instead of collaborating through an Excel spreadsheet, a hand-over happens instantly within a platform of consistent data, metadata and data models.



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The platform integrates results from every raw data format and screening technique, including HTS, HCS, and SPR.

Historical, Searchable Data

In addition to workflow limitations, scientists have lacked the ability to easily find information about past experiments and the way the results were analyzed. The ability to access historical data not only prevents them from repeating experiments, but it helps to interpret the current experiments. It also supports the creation of new ideas, improving scientists' ability to uncover "hits" that lead to viable drug targets—and have confidence in the hits they find.

Signals VitroVivo allows users to compare current analysis with historical data in minutes. Applying normalization methods consistently across data sets, analysis can reveal new insights and trends to optimize assay development.

Endlessly Scalable

Cloud-scale informatics solutions handle vast amounts of information fast. Modern architecture allows scientists to analyze millions of data points in seconds. The platform scales horizontally as needed. Thousands of end users can work in parallel on their individual analyses no matter how complex or big the data are.

Powerful Analytics

Signals VitroVivo is based on the flexible, extensible TIBCO Spotfire analytics platform. This allows for configurability and interoperability with third-party and open-source libraries.

But unlike monolithic bespoke applications, the platform is modular. Task-specific applications provide modules of scientific functionality that can be composed into self-documented, reproducible, versioned data-processing protocols. New functionality can be readily added without expensive custom feature development.

In other words, Signals VitroVivo makes data FAIR (findability, accessibility, interoperability, reusability) as defined by a group of researchers in an article published in [Scientific Data](#). The platform follows [FAIR principles](#) and workflow.



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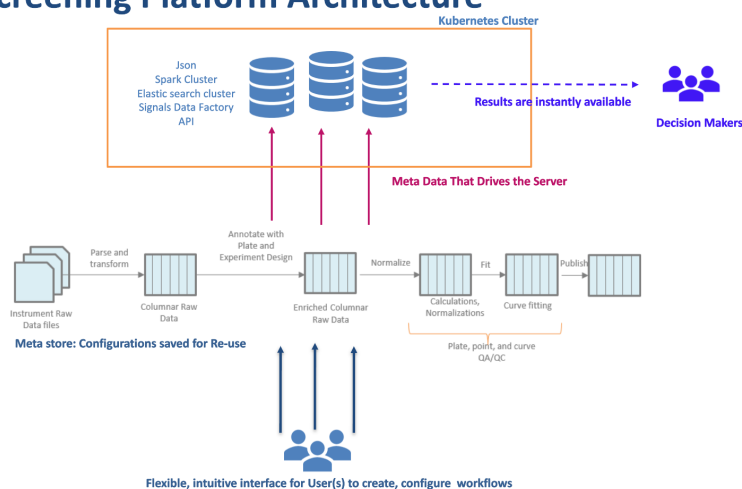
Accepts Anything

Technology should enhance, not hamper, the work of humans. When a scientist wants to use a new technique, tool, or file format, the data platform should enable this function.

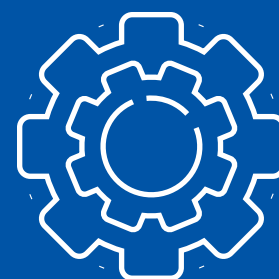
Signals VitroVivo supports all instrument data formats, databases, and web services, either directly or managed through an integration layer. This flexibility directly addresses and resolves the complex challenges that have plagued drug discovery for so long—lack of visibility into the data across workflows.

About PerkinElmer Signals VitroVivo Architecture

Signals Screening Platform Architecture



Signals VitroVivo architecture is modular but tightly integrated. Experiment data can be parsed from raw data files or any other data source from relational databases, object stores and web services. The resulting columnar raw data is combined with metadata about the experiment either manually or again by reading from data sources, e.g. LIMS systems resulting in enriched columnar raw data. This metadata represents the annotations like plate layouts and experiment designs. After these steps the experiment data can be correctly normalized with the built-in calculations or user defined ones. After this data preparation is done, the curve fitting engine can be used to calculate any curve fit and the associated quality control and assurance steps. Plates, curves, or individual data points can be



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knocked-out again manually or again by calculations, supporting the scientist in compiling the most accurate and valuable hit lists and results, e.g. IC50 values and other fit parameters.

Once the results are ready, they can be published to the PerkinElmer Signals Data Factory - a Kubernetes cluster with an Elastic search and Spark engine. The results can be immediately searched and analyzed in context together with all other experiment results available. The query engine is built into a logical search interface where no code is needed to compile and retrieve the data for further analysis, e.g. SAR tables and sophisticated multi-dimensional visualizations. Throughout the end-to-end workflow, the end user never has to code or copy data from one step to the next. The entire Signals VitroVivo platform takes care of data integrity and prevents errors by guiding the scientist through the individual steps of the data analysis.

Conclusion

Across industries, software solutions based on scalable cloud technologies have allowed users without IT experience to query large databases and perform complex data analysis tasks with minimal effort. Signals VitroVivo enables drug discovery scientists to do the same.

A single platform provides the scalability and flexibility this data-intensive area of life sciences truly needs and deserves. As life sciences continue to advance, it now has a platform that can evolve with it.



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Informatics Solutions

About PerkinElmer Informatics

PerkinElmer Informatics offers one of the most comprehensive suites of scientific software in the world. Our powerful informatics solutions are used across a spectrum of industries including Pharma and Biotech, Specialty & Agro-Chemicals, Energy & Petrochemicals, Flavors & Fragrances, Food & Beverage and Electronics. Our future-proof technology enables investigators in Life Sciences to capture and analyze their data from initial research and development of their therapeutics, through biomarker discovery & patient stratifications and ultimately live tracking of their clinical trials.

From our internationally recognized flagship ChemDraw® and E-Notebook applications, to our Signals Research Suite (Signals Notebook, Signals VitroVivo, and Signals Inventa) to our exclusive TIBCO® Spotfire® partnership that brings scientific data analytics to visual life, no scientific company offers a wider range and more powerful suite of scientific solutions than PerkinElmer Informatics.

Contact us for a Signals VitroVivo demonstration today

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