

Accelerating Delivery of Compound Profiling Data to Enable Faster Discovery Decisions

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ABSTRACT

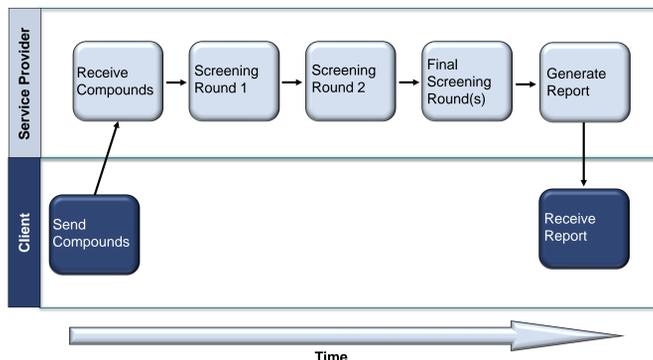
Life Technologies, now a brand of Thermo Fisher Scientific, offers compound screening and profiling services for over 800 validated biochemical and cellular assays. In an effort to accelerate lead discovery and medicinal chemistry timelines, demand for outsourced services that quickly deliver high quality screening data has increased. The recent release of new Accelerated Data Delivery™ capabilities for the SelectScreen® Services provides scientists access to real-time data through a secure online portal. Traditional screening and profiling services required full completion of a project before data could be delivered to a client. Today, clients can access data incrementally as it becomes available; with up to 80% of data typically available within 2 days of project initiation. Faster availability of profiling data allows medicinal chemists to make decisions and initiate downstream testing earlier and makes the outsourced experience more akin to in-house screening being performed in a lab next door. Additional online capabilities allow scientists to search and access past project data and view data in clear heat map or grid formats; thus simplifying data analysis.

INTRODUCTION

Outsourcing core functions of drug discovery such as compound screening and profiling have become an increasingly popular strategy. Commercial screening services provide clients access to a broad portfolio of validated assays and established capabilities and offer cost and logistical benefits over in-house operations. This approach, however, presents an accessibility challenge for scientists who are accustomed to the convenience of walking "next door" to check the status of their project and preview screening data as it comes off the reader. Traditionally, clients of compound profiling services don't see any results until all data pass QC specs, repeats are run, and a report is generated and delivered (typically 5-15+ days). Often the vast majority of the data is completed after the first round of screening, but the delivery of this data is delayed on account of a few repeats which require additional screening rounds.

To expedite clients' discovery decisions and medicinal chemistry efforts, the goal of this project was to develop a convenient mechanism that would enable all clients access to their passing data in real-time with the same confidence in the quality and security of the data that the SelectScreen® services are known for.

Figure 1. Traditional Workflow for a Kinase Profiling Service

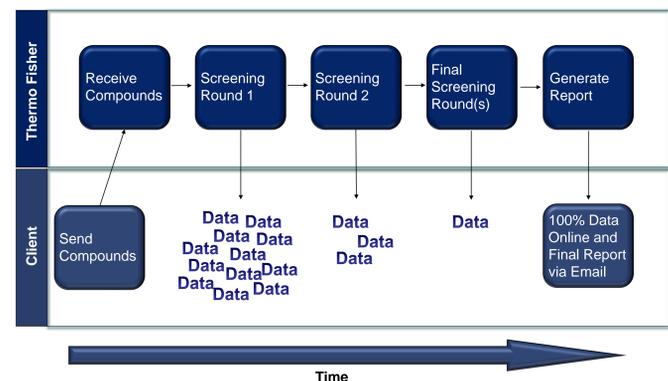


The traditional workflow for a kinase profiling service requires the full completion of a project before data can be delivered to the client.

RESULTS

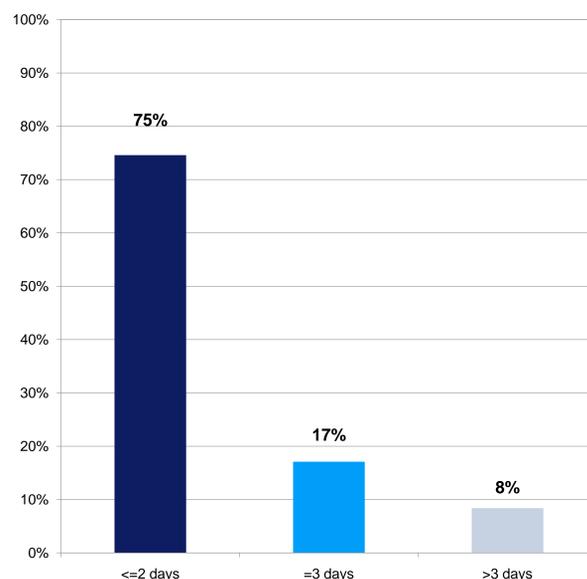
In 2013, the SelectScreen® team built a new online web portal with a secure login to enable customers to place orders and review progress. This portal is easily accessible to all customers requiring only a web browser and therefore was ideal to leverage as a mechanism for providing access to screening data. In April 2014, the functionality of the online portal was extended to enable clients the ability to access real-time data for their biochemical and cellular projects as well as provide powerful capabilities to search and visualize their historical SelectScreen® data. This online tool is easy-to-use and secure. Each client only has access to their own data as confidentiality of this information is critical.

Figure 2. Accelerated Data Delivery™ Workflow of the SelectScreen® Services



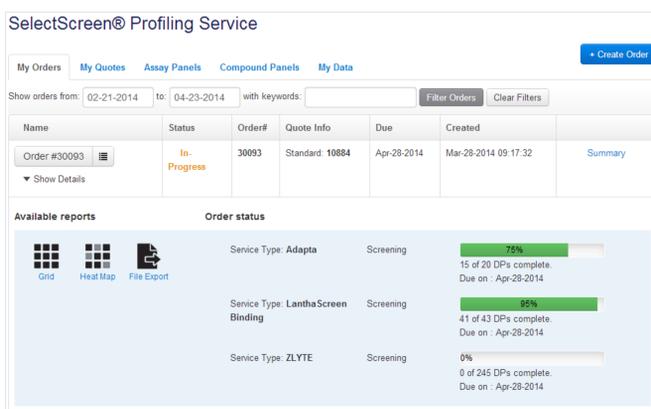
The Accelerated Data Delivery™ workflow enables clients to see data after every round of screening with 60-80% of data typically available within 2 days of project initiation. Email notifications are automatically sent to clients when new data is available with a link directly to the new data. Clients still receive a compiled Excel report with all of their data at the completion of the project. The SelectScreen® team has a 99.6% on-time delivery on over 20,000 projects.

Figure 3. Real-time Data Availability



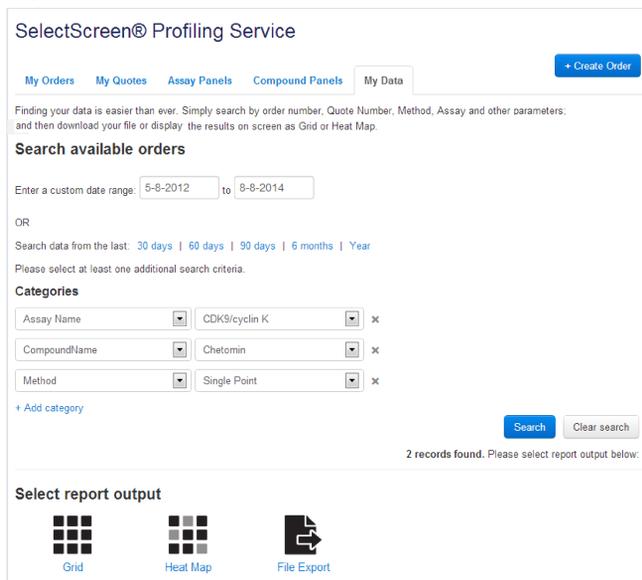
Real-time data measurements were collected between May and July of 2014 for the SelectScreen® kinase profiling service. During this time period, 75% of data was completed and available online within 2 days of the project start date.

Figure 4. Real-Time Data and Project Status



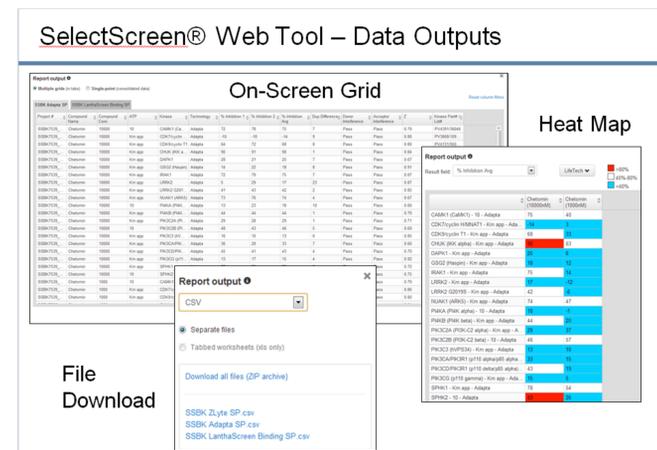
The online portal displays the progress of current orders and enables access to real-time data as it is completed by the screening team. At any time, this data can be visualized through an on-screen grid or heat map or downloaded as an export file. When the work for a given service type and order number is complete, the emailed Excel report can also be downloaded from the web portal.

Figure 5. Powerful Search Capabilities



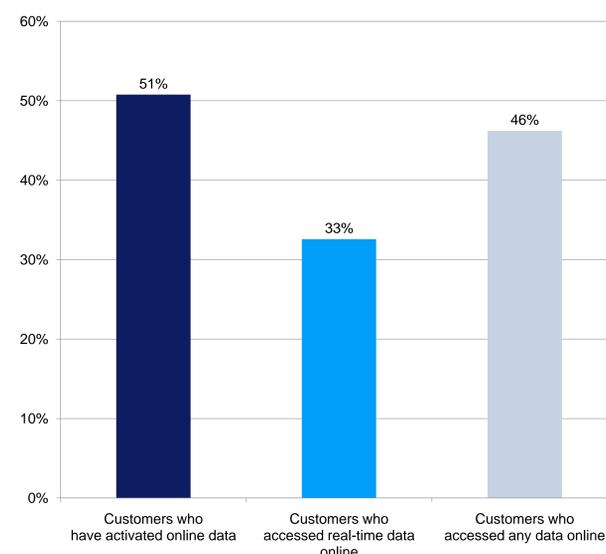
The online portal includes a powerful new interface for clients to search their current and historical SelectScreen® data and output to an on-screen grid, view in a heat map, or export to file(s).

Figure 6. Data Accessibility Options



Clients have the ability to view data directly on screen, view a heat map (single point and 10-point titration data), or download the data in CSV or XLS format.

Figure 7. Client Usage of Online Data



The majority of SelectScreen® clients have already enabled this new technology.

CONCLUSIONS

The launch of a powerful, first-to-market capability around Accelerated Data Delivery™ through the enhancement of the SelectScreen® web portal enables customers the ability to access real-time screening data and expedite their discovery decisions. This new workflow has demonstrated that an average of 75% of data is published within 2 days. Four months after the launch, over half of SelectScreen® clients have signed up for online data with the majority using it to access real-time data during the course of a project, suggesting a strong desire for early viewing and interpretation of data.

"I used the data on demand service for the first time this week. Just wanted to [give] feedback that I think it's a fantastic addition to the service – data turnaround over the last 18 months or so before the new system was already very fast and reliable, but this online service is excellent."

"I just wanted to leave you a quick note to let you know I really, really like the new e-mail notifications I'm getting that announce partial data availability. Thank you to you and everyone else who contributed to this new online data system!"

Multiple display options provide flexibility for clients and a powerful search feature enables clients to query their historical SelectScreen® data. The web portal allows all clients the ability to access real-time data with simply an internet browser. An API is also available for customers interested in automating the data upload directly into their database as it is published by the SelectScreen® team.

TRADEMARKS/LICENSING

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