



Allergan Inc. is a global specialty pharmaceutical company traded on the NYSE. The company employs more than 9,000 people worldwide and operates world-class discovery and development facilities and state-of-the-art manufacturing plants. Allergan's product line includes ophthalmic, dermatology and neurological pharmaceuticals.



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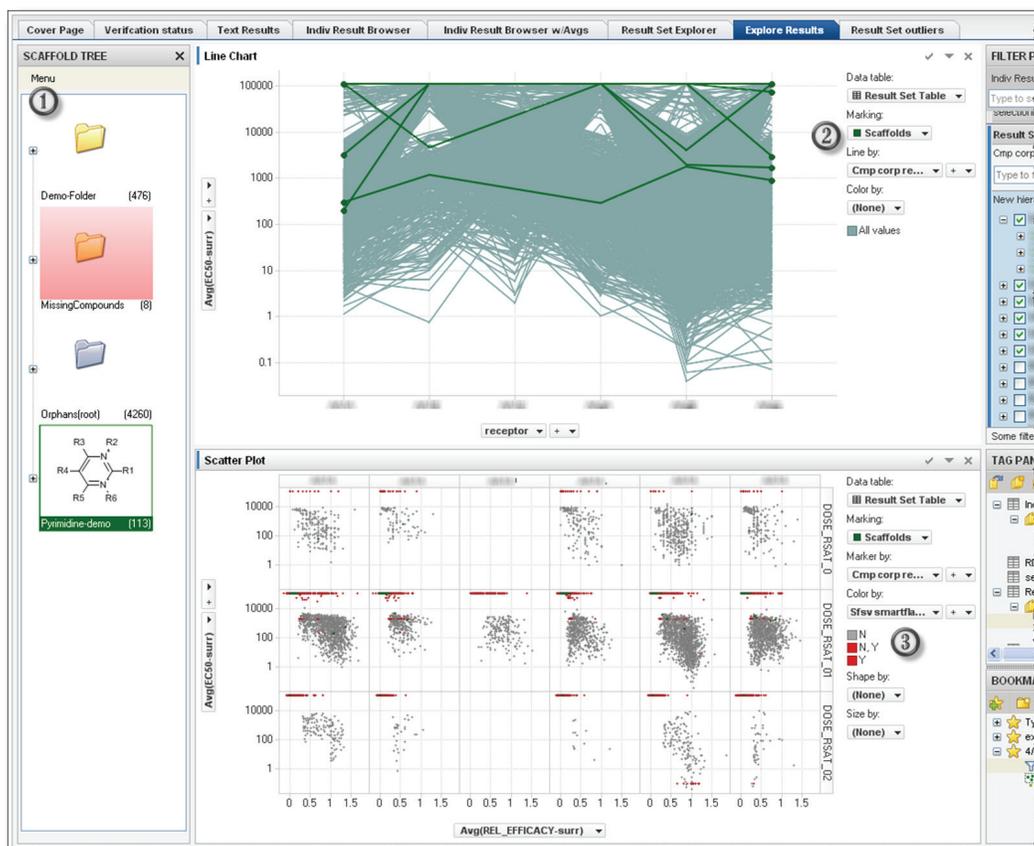
Robert Cain, Principal Scientist, Allergan

TIBCO Spotfire Analytics Enables Allergan Scientists to Overcome the Multivariate Data Analytics Challenges of Drug Discovery

Allergan's Research Informatics Group supports drug discovery relating to medicinal chemistry, biology, and drug safety and evaluation. The group is embedded within a discovery research team of medicinal chemists, biologists, and pharmacokinetics and toxicology scientists conducting research related to small molecule therapeutics.

The scientists' job is to predict the potency of a compound, as well as its efficacy and possible side effects. They also need to predict how the compound will be metabolized, what sort of bioavailability it will have, along with various kinds of toxicity. To perform their analyses the scientists need to relate chemical structure to a wide range of assay results. The assay results are always equivocal, meaning they always need to be able to see the results and drill back to the data to make sure that they're valid and predictive.

The Research Informatics Group's mandate is to help scientists perform these analyses. The group helps them solve the tough analytical problems characteristic of computer driven assays that produce large and complex multivariate data sets.



- ① The scaffold tree is a custom panel that integrates SARVision with Spotfire. This allows assay results to be correlated to your structure analyses. (other features: custom renderer with alignments and R-tables)
- ② Note the results are marked by the scaffold marking scheme
- ③ When surrogate results are used they can be clearly marked (in red here).

This file can now be saved to the library (non-prompting) and further customized. This allows the analysis to be shared. This results will be current. The scaffold tree is saved with the file and easily reloaded with the latest files.

CHALLENGE

It's very difficult to analyze a large amount of this type of data without a graphical visualization technique. Using a tool such as Excel, a scientist could analyze the last few weeks' worth of data but wouldn't be able to put it into proper context, leading to missed insights and lost opportunity.

The Research Informatics Group tracks data for four organizations, more than 100 experimental protocols, 56 categories of experimental conditions and more than 200 types of results – highly multivariate

information comprising more than one million rows (56 GB) of data. Scientists need to be able to perform analyses as quickly as possible because they want to run through their "experiment, observe, analyze, improve hypothesis" cycle as many times as possible to identify the right compounds on a timely basis. Allergan scientists determined that Excel was unable to perform repeatable analyses of structural activity relationships to pick out a set of compounds for follow-on testing.

SOLUTION

The Research Informatics Group's Principal Scientist Robert Cain identified TIBCO Spotfire® software as the visual analytics solution to overcome these analytical hurdles. It provides a highly visual and interactive environment in which the Allergan scientists can quickly summarize, visualize, and filter large, complex datasets.

The Spotfire solution is designed to efficiently support elaborate analytics on a huge variety of data with minimal configuration. A single generic Spotfire file is used as the starting point for new analyses, creating common tables and visualizations that enforce best practices such as proper marking. The user can pull data into Spotfire Analytics from any of more than 100 experiments in the database, representing a huge variety of results.

One file prompts in two steps for the data from selected protocols and types of experiments. The searches are broad – allowing fast in-memory filtering – sometime as many as ten years worth of data is compared. Search results are programmatically displayed in cross tables with the proper column and row headers in a way that is helpful to most scientists.

Spotfire-specific Architecture

Allergan's overall system architecture revolves around Spotfire Analytics and is designed to handle diverse sets of data that are brought into the software in a way that meets the common research needs without intervention. The common requirements are:

- data retrieval and integration
- standardized units of measure
- pivot as needed
- view and search by structure
- view experimental curves
- mixed text with numeric results
- custom multivariate analyses
- collaboration

This is possible because the software understands which columns correspond to experimental conditions, the cardinality of the experimental conditions and which columns correspond to results. This information allows the software to place the appropriate columns on the appropriate axes in the cross tables. This application of Spotfire enables the user to filter the results intuitively. An on-demand table format summarizes the protocol, experimental conditions and assay results that correspond to selected results in the cross table and shows experimental curves and structure.

SARVision Integration

SARVision is a chemical Structure Activity Relationship analysis software tool that assists in the visualization, mining and organization of chemical data. It can quickly identify chemotypes responsible for a given activity. Cain conceived of mashing up SARVision with Spotfire Analytics to form a powerful way to

highlight a chemical substructure and see the results that correspond to it in any Spotfire visualization. He worked with SARVision and Spotfire Professional Services to develop the integration using the Spotfire software development kit.

When scientists are analyzing structural activity relationships they want to see whether a certain substructure corresponds with selective compounds. The Spotfire Analytics/SARVision integration allows them to do this very easily through a custom scaffold panel on the Spotfire interface. Scaffold analysis embodies all of the structural analysis done over months at a time. It's always available to be applied to current sets of data being pulled into Spotfire Analytics. "This is a great example of how customizable Spotfire is," says Cain. "The integration of SARVision's scaffolding with Spotfire's visualizations allows our scientists to correlate chemical structure to activity in a way that no one else can."

RESULTS

Cain notes that scientists don't want to know how their data is organized or transformed; just that it has to be done correctly. Spotfire Analytics allows them to bring together all the data in a large, multivariate data set and make sense from it using the software's interactive interface and filtering capabilities.

As part of Allergan's research analytics program Cain conducts bi-weekly lunch and learn seminars, where he demonstrate new types of Spotfire Analyses. He also maintains a tip of the week blog to promote something novel done in Spotfire Analytics for one group that may have broad applicability.

"Spotfire makes it possible to support a large variety of analyses on disparate data in a way that would be impossible otherwise," says Cain. "Without it, we would never be able to help scientists carry out the number of analyses that we do currently do."



TIBCO Software Inc. (NASDAQ: TIBX) is a leading independent business integration software company and a leading enabler of real-time business, helping companies become more cost-effective, more agile and more efficient. TIBCO has delivered the value of real-time business, what TIBCO calls The Power of Now®, to thousands of customers around the world and in a wide variety of industries.

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