Supporting Novel High-Throughput Assay Development via a Flexible Shiny Dashboard

Jocelyn Sendecki[1], Traymon Beavers[1], Amruta Ronghe[2], Simin Rahighi[2], Steven Jacobs[2]

[1]Johnson & Johnson US, Discovery and Nonclinical Safety Statistics; [2]Johnson & Johnson US, Therapeutics Discovery

Bio

Jocelyn Sendecki has been a preclinical biostatistician with Johnson & Johnson since 2014. Previously, she worked and taught as an adjunct professor at Thomas Jefferson University in Philadelphia and holds an MSPH in Biostatistics from Tulane University School of Public Health & Tropical Medicine and an MS in Statistics from Temple University.

Abstract

Drug development begins with the creation of hundreds or thousands of molecules designed to act against a particular target. High-throughput assays are used to sift through these candidates, identifying and excluding those that carry undesirable characteristics. For example, these can be related to chemistry that is difficult to manufacture or that is known to be toxic.

Our biophysics team has developed a novel promising assay to quickly and simply identify a particular type of undesirable characteristic and asked for statistical assistance in establishing cut-offs in the response that could identify a candidate molecule as having this characteristic or not. Results from commercially available bodies with known activity (desirable vs. undesirable) were analyzed repeatedly over time. This allowed for the construction of tolerance intervals based on the behavior of these standards, against which candidate molecules could be plotted and compared. Results of this new assay were also compared against other established high-throughput screens to determine if this undesirable characteristic overlapped with other unwanted biophysical characteristics.

This was all achieved using a Shiny Dashboard, written in R and deployed through RConnect. This interactive tool allowed the scientist the flexibility to explore the data. Over time, we also added upwards of 20 new commercially available standard molecules for comparison. In particular, {ggplotly} was used to interactively select tolerance intervals to compare against the original standards, each other, and against sample compounds. This simple tool has put considerable power in the hands of the scientist to visualize and evaluate a new tool for advancing the drug development pipeline.