

Overview

Modern Ultra-High-Throughput Screening (uHTS) generates data in a wide variety of formats. Each assay screened may require a different method of analysis which presents a challenge in being able to quickly analyze and monitor assay data.

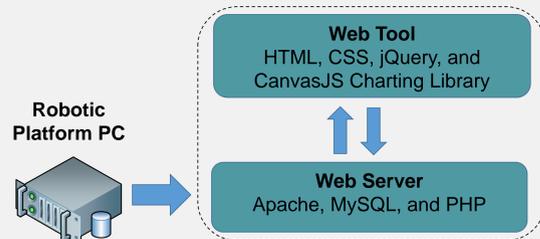
In this poster, we present a web-based tool for monitoring concurrent HTS assay results that has been developed in-house at the Scripps Research Molecular Screening Center. This tool automatically and continuously monitors assay results from the Scripps uHTS platform in real-time to provide automated alerts and access to web-based data visualizations and uHTS QC measurements in a graphical format. This web-based utility includes assay plate heat maps, scatterplot charts, and whole run QC measurements that can be accessed by any workstation or mobile device with a modern web browser. Specific results from any assay plate can be shared with any colleague via a custom URL generated with a single mouse click. User controllable parameters can also be set to generate real-time email alerts when specified assay QC measurements go out of range. This critically important feature allows robotic operators to be notified in real-time if there are any problems with assay results.

Background Implementation

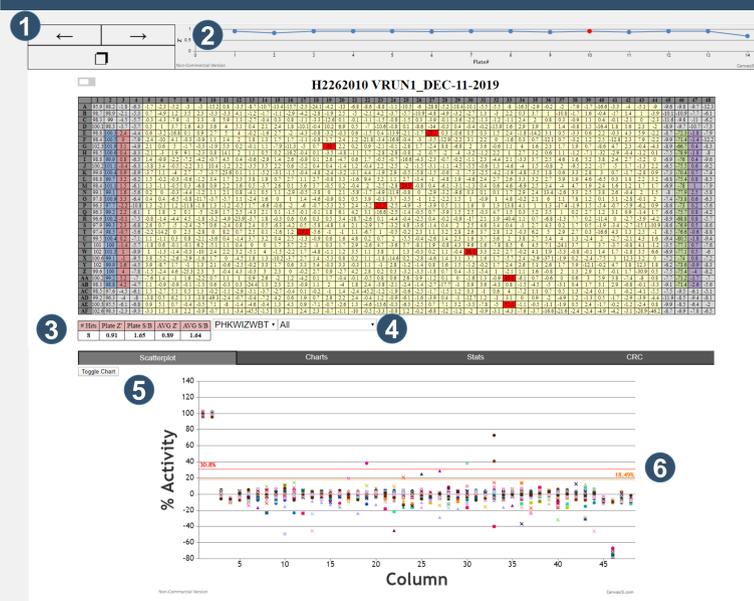
As assay plates are executed, report data from each microplate reader on the Scripps HTS platform is transferred to a central file repository and registered in the Scripps corporate LIMS. During this process, basic assay statistics are calculated to perform a preliminary verification of the quality of the data, with results stored in a local MySQL database. Any data which fails user-defined QC parameters triggers an alert to the robotic operator.

A custom developed web interface allows real-time review of assay results at any lab PC or via mobile browsers thanks to a responsive web design.

Scripps Assay Monitoring System

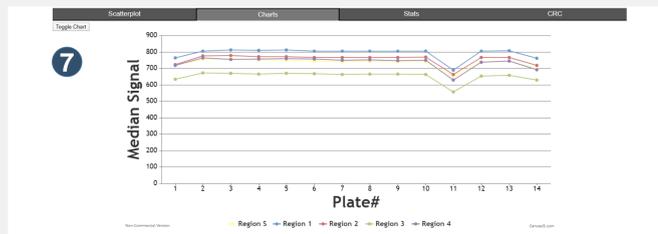


Main Functionality



- 1 Plate data can be navigated using the arrows at the top of the page. The button below copies a link of the currently viewed plate to the clipboard for easy sharing.
- 2 An line chart keeps track of the Z' of the plates for the currently selected assay. To quickly navigate to a particular plate, the data points on the chart can be clicked.
- 3 # Hits, Z', and signal window stats are available for each plate and an average for the day.
- 4 Results can be filtered by assay name and date dropdown menus. By default, data from the 10 most recent assay plates is shown on the page.
- 5 Data is shown as a scatterplot on the chart. The scatterplot can be toggled between row and column view.

- 6 The scatterplot showcases two cutoff lines used to determine which wells are considered "hits." The orange line is three standard deviations away from the mean for the currently viewed plate, while the red line is three standard deviations away from the mean of all compound wells in the assay.

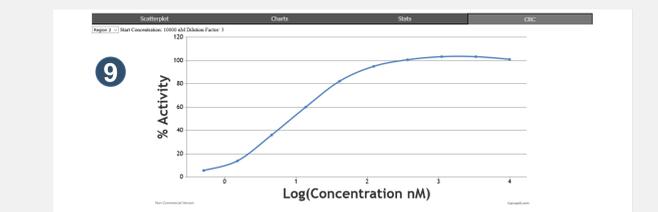


- 7 The charts tab offers a view of the average and median statistics for each plate in a day split up into pre-defined regions. This allows for plate-to-plate tracking of assay statistics.

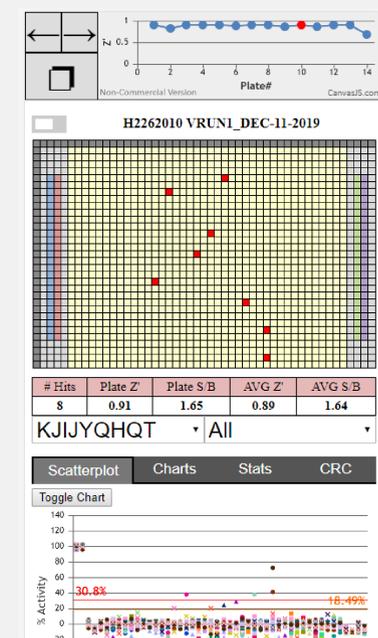
- 8 The stats tab offers similar data to the charts tab but in table format. Plate barcode, signal window, and plate Z' can also be tracked here on a plate-by-plate basis.

Plate#	Plate Z'	Plate S/B	AVG Z'	AVG S/B
H2262010 VRUN1_DEC-11-2019	0.91	1.65	0.89	1.64

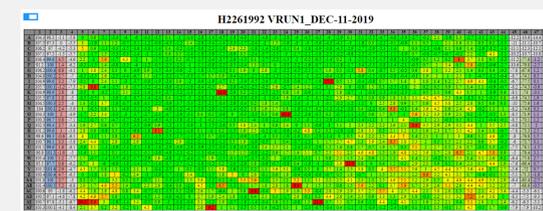
- 9 The CRC tab plots specific regions of the plate as a dose-response curve. The user can specify which part of the plate the dose curve is in, the starting concentration, and the dilution factor.



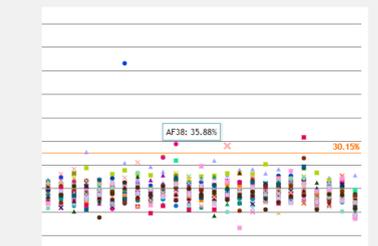
Additional Features



The website is navigable on both desktop and mobile devices. The website layout and buttons shift on smaller screens to better accommodate these devices.



The main data table has conditional formatting options that can highlight in red only wells that are considered hits (more than three standard deviations away from the average), or give a color to each cell based on its value with green being the lowest values and red being the hit cutoff.



Hovering over the individual data points in the scatterplot gives a popup of the well name and the scaled percent activity of the well.

This poster can be viewed online by scanning the following QR code:



Conclusion

Development of these software tools will help enable the Scripps Research Molecular Screening Center to more quickly validate the performance of currently running assays. It also enables automated, real-time assay analysis and error detection for problems with currently running robotic screens that were originally not possible. Assay statistics are easily accessible from any device with a web browser, allowing careful monitoring of assay results in a wide variety of situations.