Overview

Managing the wide variety of sources and formats of data found in a modern High Throughput Screening lab is an ongoing challenge. As a result, data management software is constantly evolving to accommodate the sheer volume of data and the complexity of information generated. Commercial data management solutions can meet some of these challenges, but they are often expensive and inflexible, performing only a handful of the many tasks needed to manage HTS data tasks effectively and efficiently. Alternatively, developing a custom in-house informatics solution allows software to be tailored to the exact needs of the end-user. To address these issues, we have developed a custom web-based interface known as the HTS Dashboard.

The HTS Dashboard has been architected to be sufficiently extensible to meet future needs, enables rapid development by utilizing the latest open source web technologies and allow users of diverse backgrounds to easily generate sophisticated data sets. The HTS Dashboard interfaces with a number of data sources including HTS readers, corporate LIMS records for compound and plate records, compound management automation, and QC instrumentation such as LC-MS and the Plate Auditor. By providing a unified and user-friendly data interface webpage, utilities can be easily accessed by biologists, chemists, project managers and engineers to assist with a broad array of HTS related tasks including aggregation of data, performing QC checks, generating visual presentations, and exporting data. Further, these capabilities work across the entire spectrum of activities found within a HTS campaign, from pilot screen through primary, confirmation, counterscreen and dose response. The infrastructure which has been developed and deployed within the Lead Identification group at Scripps Florida and its impact on HTS operations are presented.

Software Architecture

The HTS Dashboard unifies a number of data sources through a user friendly web-based interface that is based on open source software frameworks. The frameworks used and their configuration within the HTS Dashboard is shown in the layer diagram below.

Prior to the development of HTS Dashboard, users had to manually curate data using a combination of tools including Microsoft Excel, Microsoft Access and TIBCO Spotfire. The goal of the HTS software utilities was to replace these tools to reduce the possibility of error in manual curation of data and to reduce the amount of time and energy required to curate, validate and organize HTS data.

Conclusion

Integration of these software tools has reduced the time by hours, if not days, of time per assay required to perform QC on HTS data and increased the robustness of processes for aggregating and exporting HTS data. End-users no longer have to manually assemble and then spot check data. This eliminates the chance for errors in reporting HTS data internally and externally.

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