Electronic Laboratory Notebook as a tool to Facilitate Scientific Data Analysis and Review in Regulated and Non-Regulated Bioanalysis

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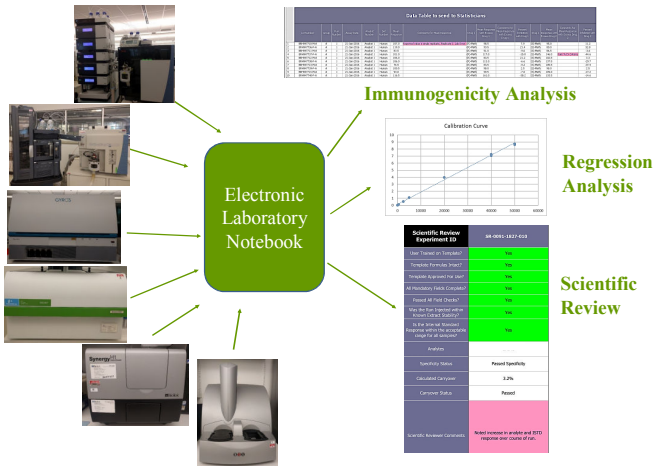
Purpose

To illustrate the utility of the Electronic Laboratory Notebook (ELN) in facilitating scientific data analysis and review in regulated and non-regulated bioanalytical studies.



Regression Analysis

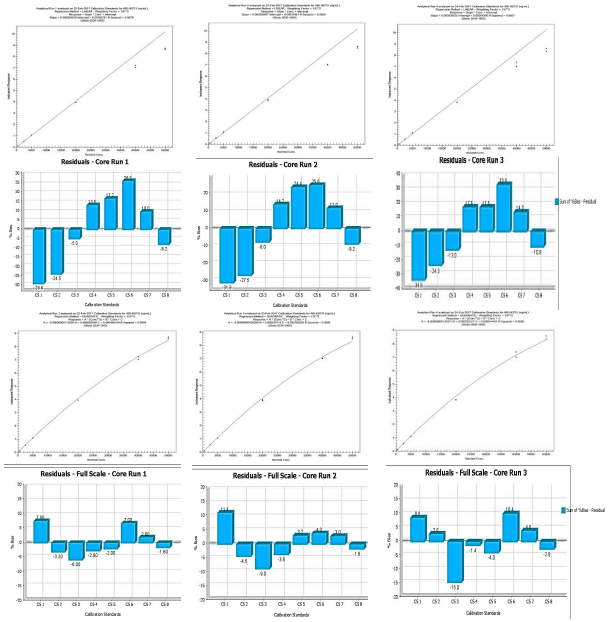
Links data from Watson for core runs and determines residuals allowing for selection of best fit by a regulatory-acceptable pre-defined methodology.

Linear Fit Calibration Curves

Linear Fit Residuals

Quadratic Fit Calibration Curves

Quadratic Fit Residuals

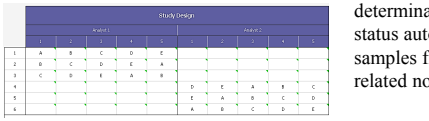


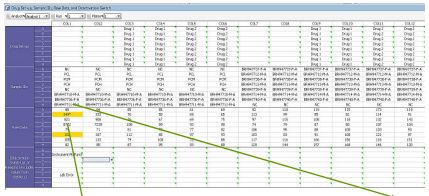
Methods

Since 2011, an Oracle-based ELN (IDBS E-Workbook 10.1.3) has been the backbone of operations at AIT Bioscience. The validated templates and workflows allow real-time electronic data collection and quality control checks. The variety of templates and workflows serve regulated and non-regulated work for both small and large molecule bioanalysis. This work describes the additional benefits of the ELN in streamlining and facilitating scientific data analysis and review.

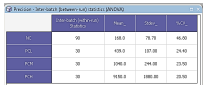
Immunogenicity Analysis

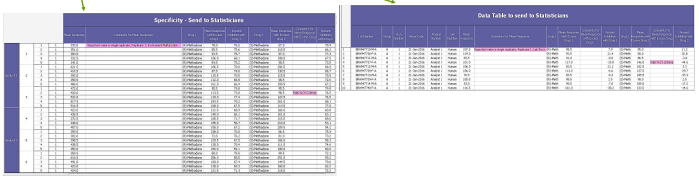
Uses analyst-defined experimental design to calculate all data needed for statistical determination of cut-point. Deactivation status automatically omits deactivated samples from analysis and carries through related notes.





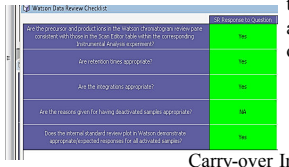
Automated calculation of ANOVA precision statistics for entire experiment.



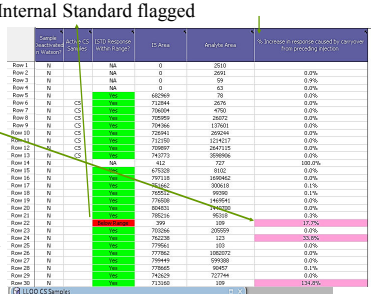


Scientific Review

A combination of manual review of the chromatography for MS transitions, retention times and integrations along with automated determination of extract stability, specificity, carry-over status and sample impact, and internal standard response.

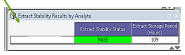


Abnormal Internal Standard flagged

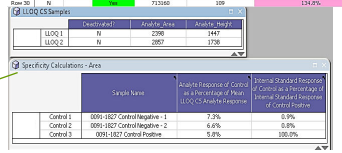


Carry-over Impact calculated by sample

Extract stability checked against the validation.



Specificity automatically calculated.



Results

A key to the successful use of an ELN in the bioanalytical lab is ensuring the flexibility to operate in both regulatory and non-regulatory environments and provide real-time quality control checks. Previous communications focus on the design and structure of our ELN to meet this need.

With the front-end quality control in place, efforts turned to the organization and turn-around time for back-end scientific data analysis and review. Workflows and templates have been created to facilitate 3 major tasks in data analysis and review. Each of these back-end processes rely on direct datalinks from multiple instrument platforms (TSQ Vantage and TSQ Quantiva mass spectrometers, MSD and Biotek plate readers, and PE Gamma Counter) to Watson LIMS.

1. Regression analysis tool for method validation: Imports all validation runs and performs root mean squared analysis for both linear and quadratic fitting with multiple weightings to find the optimal regression.
2. Immunogenicity analysis template: Allows for the collection of confirmatory and domain ADA cut points data. Generates descriptive statistics and presents complete dataset in a format compatible with statistical software.
3. Scientific review template: Calculates carry-over, internal standard statistics and extract stability compliance and flags outlying results.

Having all of the required data imported and the cumbersome calculations handled by these templated workflows frees up the scientific staff's time to focus on critical assessment of the data. Furthermore, it simplifies auditing and reporting of the results.

Conclusion

By providing real time quality control in the lab as well as streamlined scientific data analysis and review using Watson LIMS data links, the ELN is a powerful tool for high quality, audit-ready bioanalytical data.