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A Complete Data Integrity Solution for Quality Control Laboratories using Mass Spectrometry

Leo Wang and Hua Dong
Software and Informatics Division, Agilent Technologies

Agilent Technologies

Introduction

Data integrity regulatory enforcement has evolved dramatically since 2013. Both technical and procedural controls are required to meet current regulatory guidelines. Compared with procedural control, technical controls are preferred to maintain data integrity.

Residual solvent analysis (RSA) is a common quality control activity in a pharmaceutical QC laboratory to evaluate the content of residual organic volatile chemicals in pharmaceutical products. Adding mass spectrometry for RSA greatly improves the method sensitivity and provides the capability to screen more than 50 solvents in a single run.

Here we present a complete data integrity solution for mass spectrometric applications using OpenLAB CDS with advanced technical control features to facilitate the generation and management of regulated records, and to reduce the burden on extensive procedural control measures, while improving laboratory productivity.

Experimental

Residual solvent analysis (RSA) is performed using an Agilent GC/MS with a headspace sampler. Data is acquired and processed by OpenLAB CDS software.

Samples containing residual chemicals with concentrations higher than the USP<467> limits (and confirmation with mass spectrometry) are flagged and reported.

Unknowns found are searched against a spectral library for identity confirmation based on acquired MS signals. Reporting for Unknown Analysis and MS Library Search can be easily performed with pre-defined report templates with optional customization.

Once identity is confirmed, a residual chemical analyte with a concentration above the threshold is calculated using the embedded Custom Calculator.

All electronic records, including raw data, sequence/result set, acquisition methods, processing methods, processed results, reports, along with audit trails can be reviewed and approved electronically with e-Signatures.
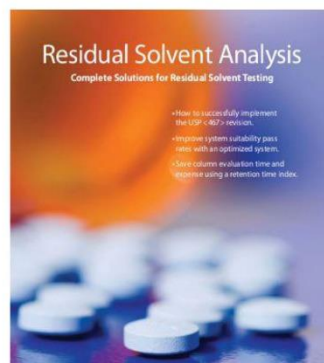

Figure 1. OpenLAB CDS provides a compliance solution for data integrity in pharmaceutical QC labs using mass spectrometry

Results and Discussion

Workflow Automation

Figure 2 illustrates a typical GC/MS chromatogram for residual solvent analysis, where organic solvent analytes were separated by gas chromatography and detected with both FID and MS detectors.
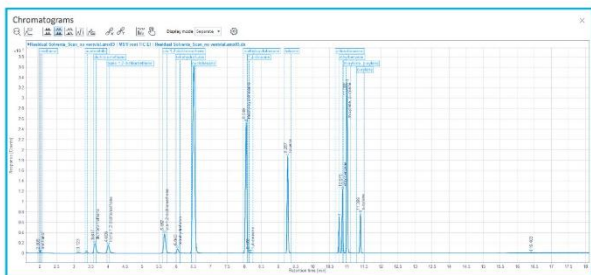

Figure 2. Example Chromatogram for residual solvent analysis with GC/MS

In high throughput laboratories, the complete sample analysis can be performed in an unattended manner where data acquisition, analysis and reporting are completed automatically.

User, User Group and Privilege Management

In a regulated environment, the user role and privilege control is a critical part of the compliance technical control features.

OpenLAB CDS provides comprehensive yet flexible management of users, user groups and user privileges. User privileges and access can be segregated and defined to specific instruments, specific projects, specific type of data sets and specific activities.
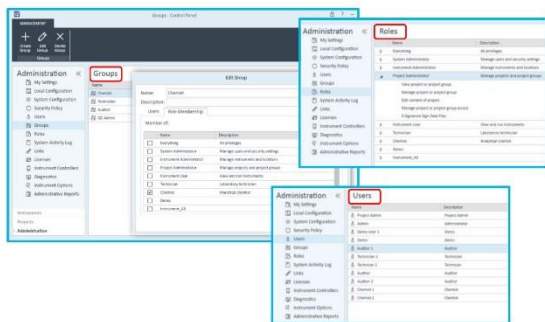

Figure 3. OpenLAB CDS provides central and flexible management for user, user group, user role and privileges

Activity Log and Audit Trail

Another key requirement for technical control features for a regulated laboratory is the capability to record and track all activities and changes that happened in the system. In OpenLAB CDS, System Activity Log records all activities per system, and comprehensive audit trails keep track of generation, transfer, process, modification and other changes for regulated records..
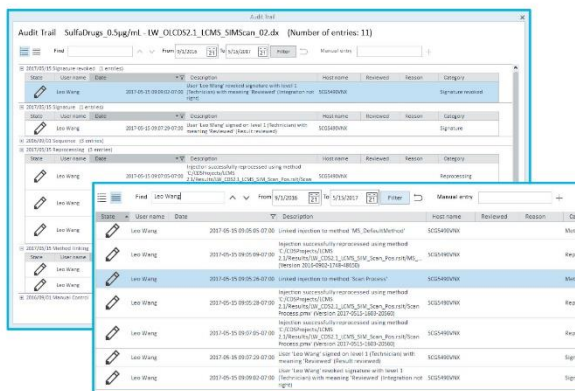

Figure 4. Audit Trail Review

Audit trail entries can be viewed by categories or list, search and filter functions are also available to quickly identify entries of interest.

Electronic Signature (e-Signature)

OpenLAB CDS supports e-Signature workflows. Privileges of applying or revoking e-Signatures can be assigned to specific user(s) or user group(s) that belong to different authorization levels, e.g. technician, supervisor or manager. Meanings of the e-signature can also be defined or customized per regulatory and procedural requirements.
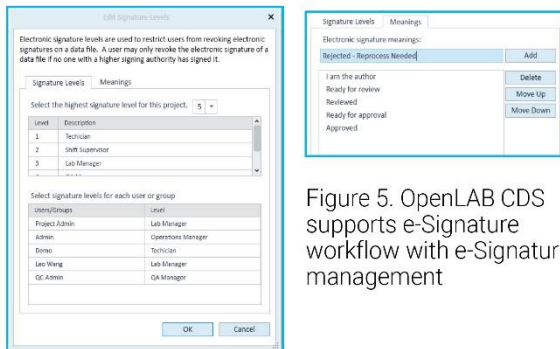

Figure 5. OpenLAB CDS supports e-Signature workflow with e-Signature management
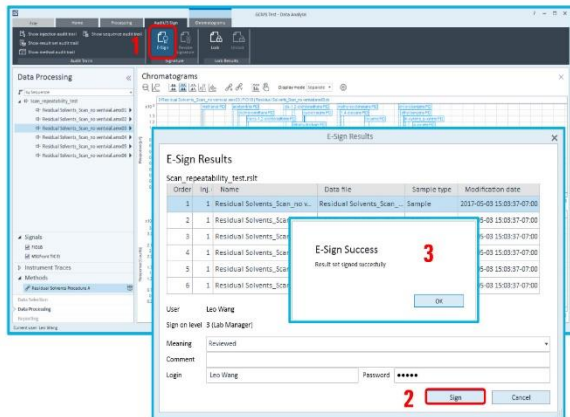
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Results and Discussion

Figure 6. Use of e-Signatures to approve result set

Figure 6 above demonstrates 3 easy steps to approve a result set with e-Signature by authorized users, with the meaning of the signature and review comments. Similarly, e-Signature can be revoked to allow further editing or reprocessing of the data.

Revision Control

OpenLAB CDS tracks the versions of regulated records when audit trail is activated (audit trail for result is activated by default).

For example, Figure 7 below demonstrates the version history of a processing method.
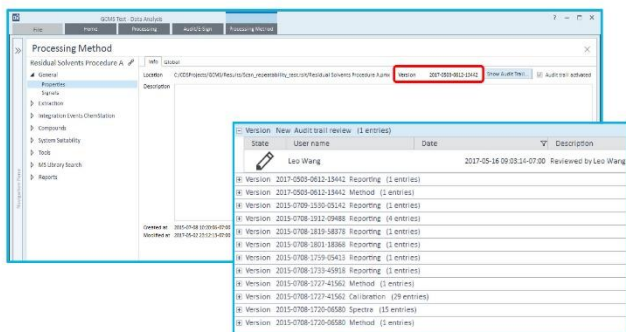

Figure 7. OpenLAB CDS version control

OpenLAB CDS not only tracks the versions of regulated records, but also can provide access to all saved previous versions.

For example, Figure 7 illustrates the versions of a result set from data acquisition, unattended data processing, saving, data review and reprocessing.

Figure 8. Version control with OpenLAB CDS and OpenLAB Server content management

Conclusions

OpenLAB CDS provides a complete data integrity solution for mass spectrometry applications in quality control laboratories via advanced technical control features:

- Secure centralized data storage
- User, user group and privilege control and management
- Comprehensive activity log and audit trails
- Electronic Signatures
- Revision control and access

References

- Support for Title 21 CFR Part 11 and Annex 11 compliance: Agilent OpenLAB CDS version 2.1, Whitepaper, 5991-6492EN, Agilent Technologies;
- Data Integrity and Compliance with CGMP, Guide for Industry (https://www.fda.gov/downloads/drugs/guidances/ucm495891.pdf, accessed May, 2017)

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