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Effective Data Management in the Analytical Laboratory

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Introduction

It is very common to support security and data integrity in chromatography data system (CDS). This situation is slightly different for other analytical instruments such as spectroscopy equipment and electronic balances because they are not as many as HPLC and GC in the laboratory and they are often standalone system. A separate data management system is implemented in the software to store, backup, retrieve and archive data for each instrument to comply with regulations.
As having separate data management system increases maintenance cost, a unified data management system is required.

A solution for this requirement is to support a generic data management interface in the analytical data system to realize unified access control and data integrity for various instruments.
This system also enables the user to make summary report from various instruments and to connect to the LIMS system through single interface. As a result, it decreases human errors and total operation cost.
In this presentation, it is shown how the unified analytical data system achieves effective data management in the laboratory.

A Demand for data integrity in the Laboratory

In March 2015, MHRA issued a guidance on data integrity "MHRA GMP Data Integrity Definitions and Guidance for Industry March 2015".
Data integrity is fundamental in a pharmaceutical quality system which ensures that medicines are of the required quality.

Data integrity requirements apply equally to manual (paper) and electronic data. Manufacturers and analytical laboratories should be aware that reverting from automated / computerised to manual / paper-based systems will not in itself remove the need for data integrity controls.

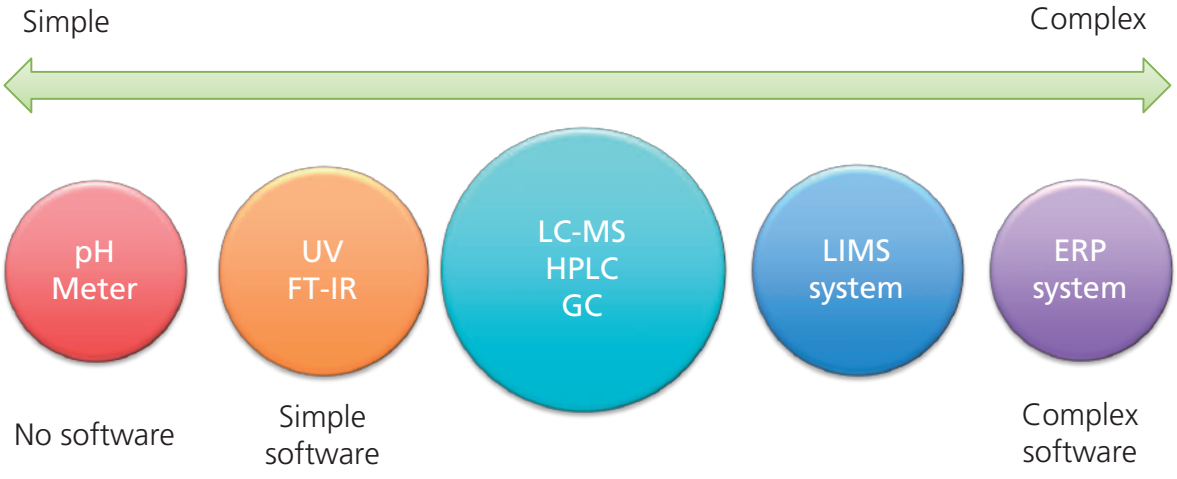

Figure 1. Data criticality and inherent integrity risk

Validation effort increases from left to right in the diagram above. However, it is common for companies to overlook systems of apparent lower complexity. Within these systems it may be possible to manipulate data or repeat testing to achieve a desired outcome with limited opportunity of detection (e.g. stand-alone systems with a user configurable output such as FT-IR, UV spectrophotometers).

Designing systems to assure data quality and integrity

Care must be taken for all phases in the life of the data.

- Metadata derived or obtained from various instruments such as HPLC, GC, MS, NMR, UV, FT-IR, TOC etc.
- Documents such as SOP, work sheet and laboratory notebook created by Excel, Word, PDF etc.
- Pictures and Images for memorandum

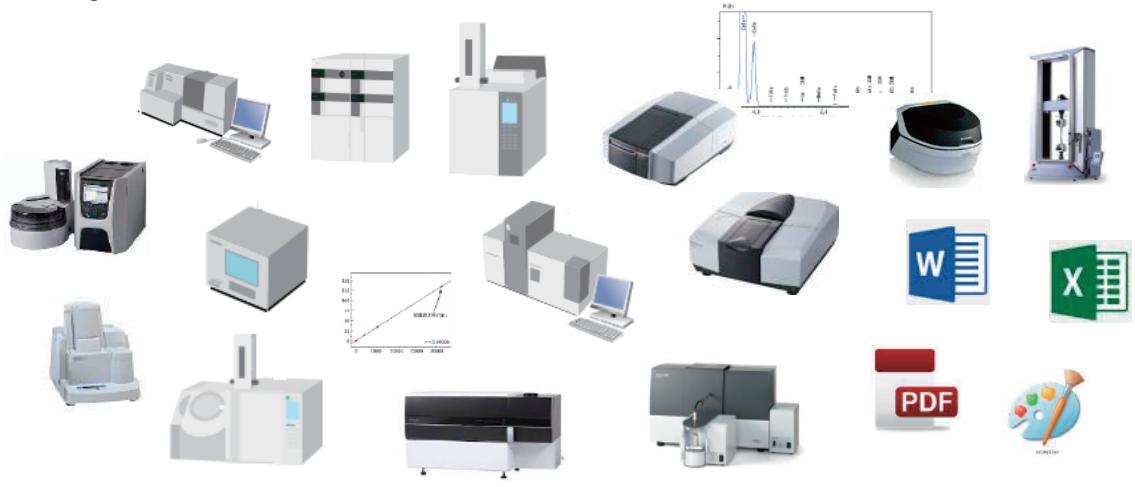

Figure 2. Various instruments in the laboratory

Recording through processing (including transformation or migration).
The procedures for destruction of data should consider data criticality and legislative retention requirements.
Archival arrangements should be in place for long term retention (in some cases, periods up to 30 years) for records such as batch documents, marketing authorisation application data, traceability data for human-derived starting materials (not an exhaustive list).
Additionally, at least 2 years of data must be retrievable in a timely manner for the purposes of regulatory inspection.

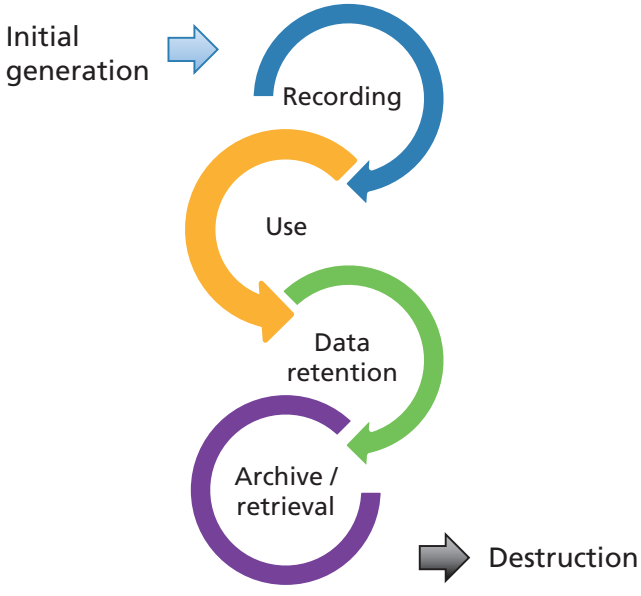

Figure 3. Data lifecycle management

Generic data management interface

- Generic data management interface provides functions of user access control and registering metadata from any instruments to the database.

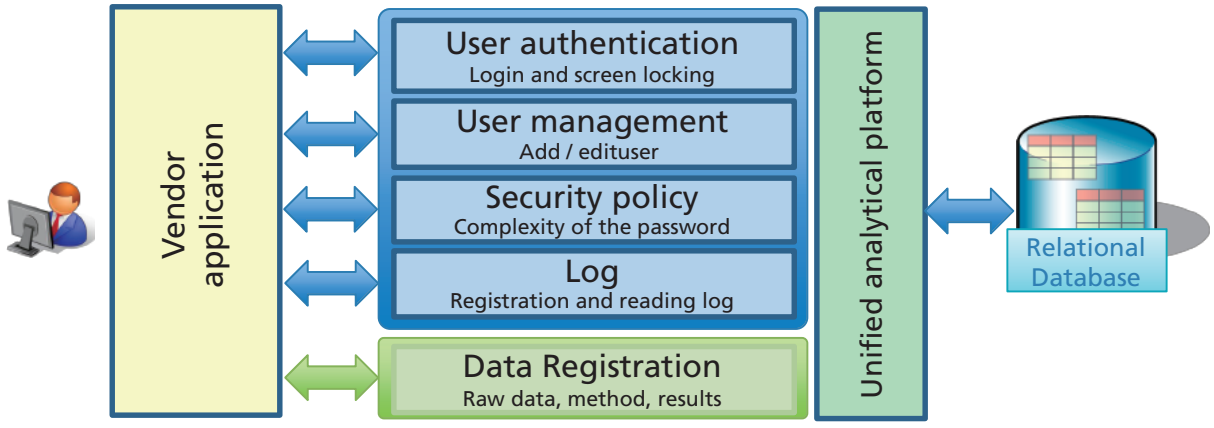

Figure 4. Generic data management interface

- Data is automatically registered to the secured database by the prescribed settings.

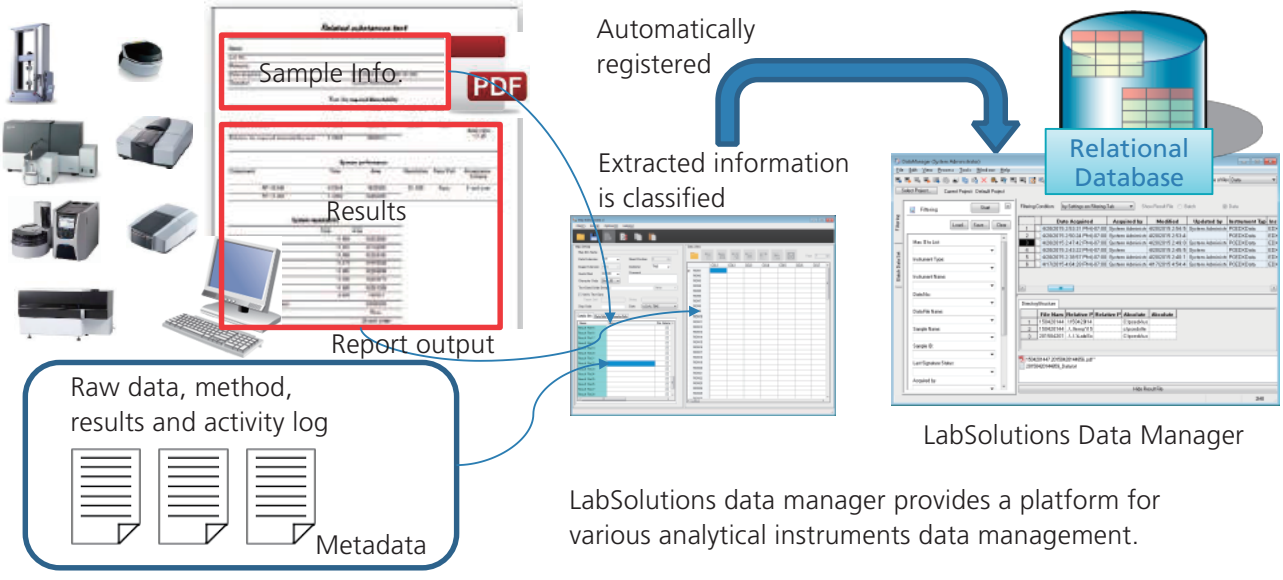

Figure 5. Multi instrument data registration

Unified analytical data system

Unified access control

- Ensures uniqueness of user ID in the network without limitation.
- Grants individual access levels to each user.
- Ensures the historical information of user access level.

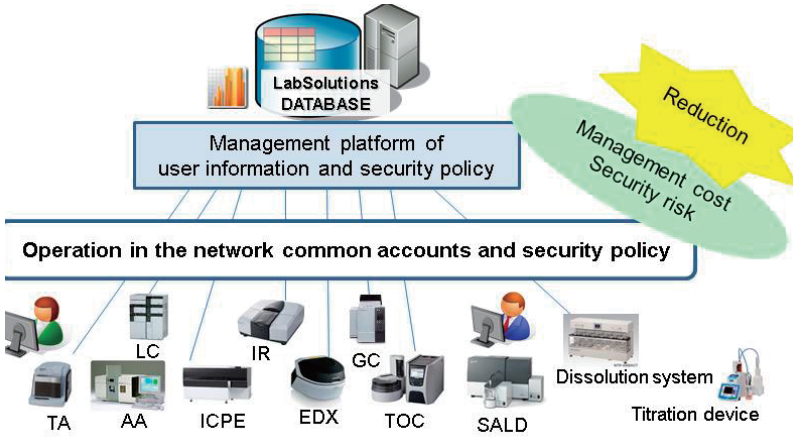

Figure 6. Unified access control

Unified data management

- Review, Archive / Retrieve data on the single platform.
- Reduces the system maintenance cost in the laboratory.

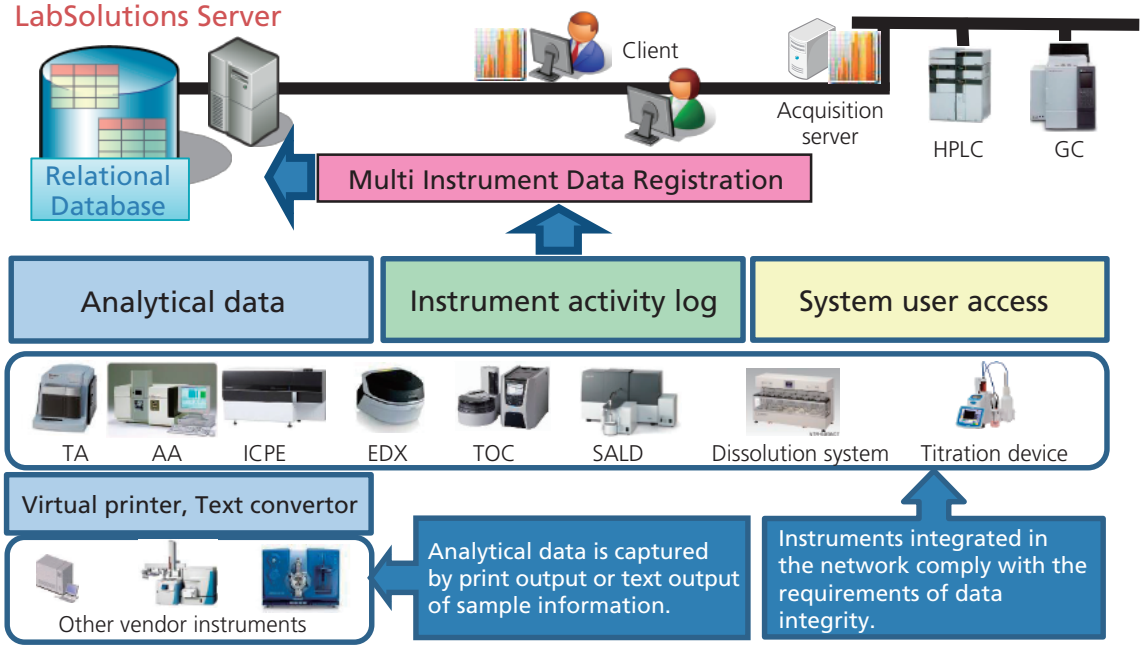

Figure 7. Unified data management

Other benefits of the unified analytical data system

Generating summary report with various Instrument Data

- Various instrument data on the database is integrated, summarized and reported.
- Decrease human-error of gathering and transferring multi instruments data.

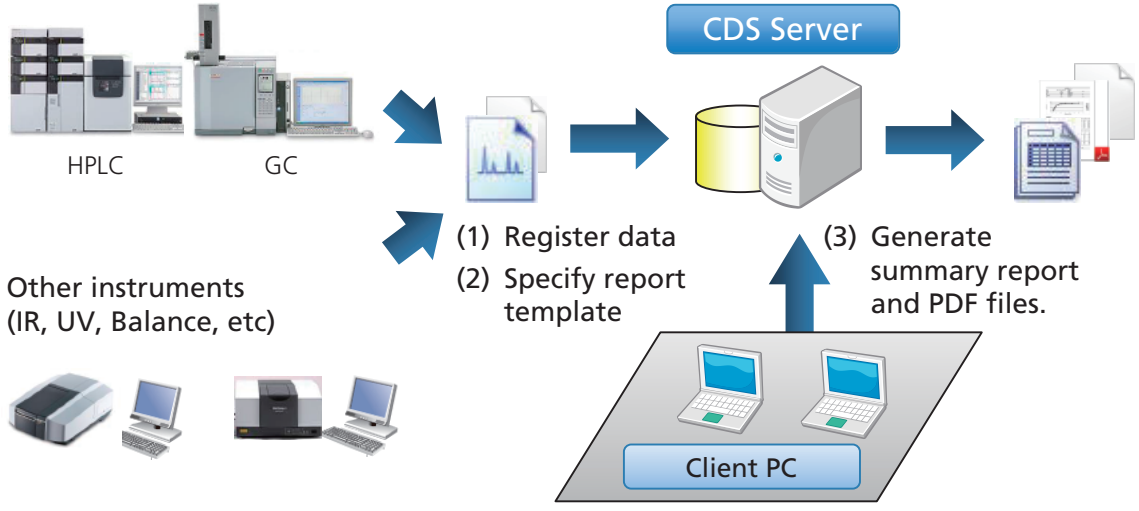

Figure 8. Generating summary report

Single interface to the LIMS system

- Integrate sample data from various instruments.
- Calculate and generate results with formatted data.
- Send results to LIMS system at the specified event.

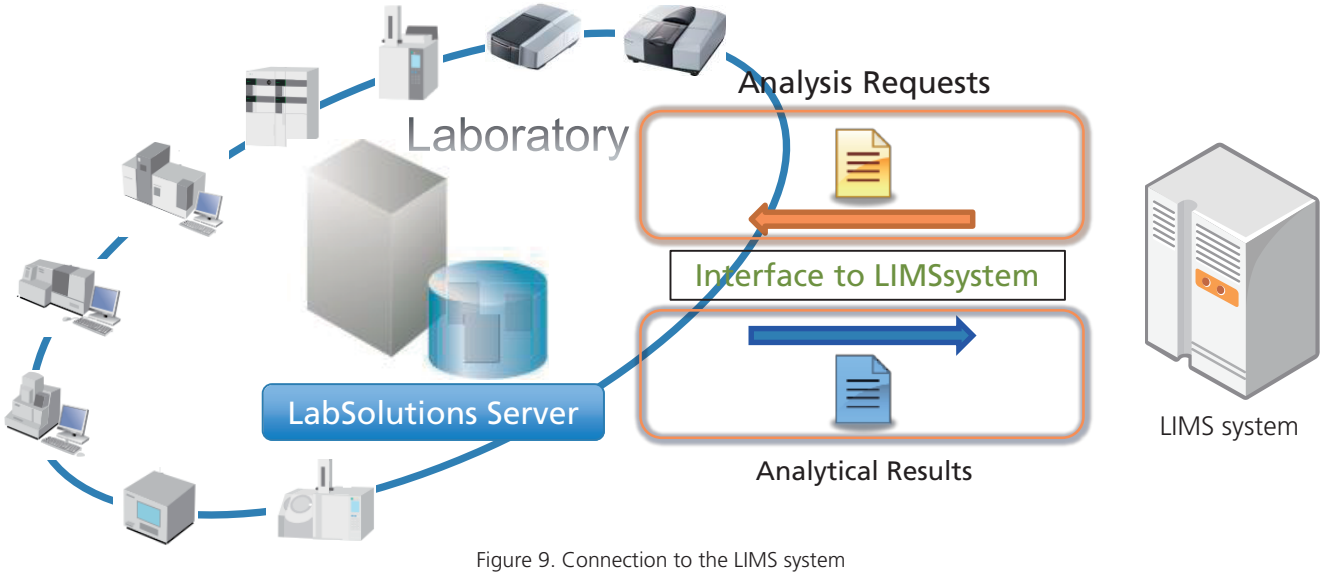

Figure 9. Connection to the LIMS system

Conclusion

- LabSolutions base package offers a unified analytical platform with relational database while maintaining seamless connection of chromatographs and other instruments.
- Access control and data registration functions for various instruments support the requirements of data integrity.
- Metadata including raw data is stored safely in a relational database together with human readable format.
- Summary report from various instruments is easily generated with Multi Data Report function.
- A single interface to the LIMS system for various instruments is provided with LIMS tool kit.
- Generic data management interface for various instruments extends the unified analytical data system and achieves effective data management in the analytical laboratory.

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