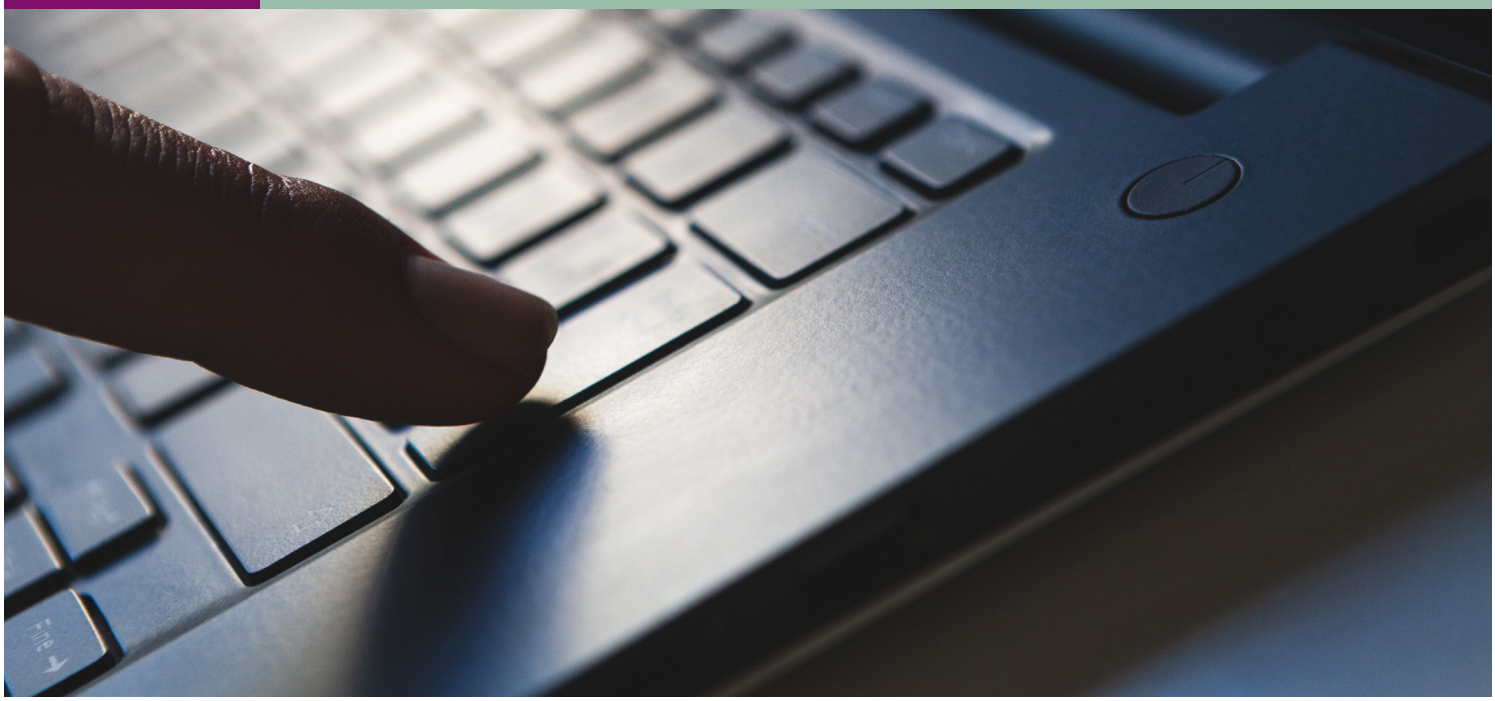
WHITE PAPER

Data Integrity – UV WinLab Enhanced Security (ES) Software for UV/Visible Spectroscopy



Introduction

The FDA defines data integrity as "completeness, consistency, and accuracy of data. Complete, consistent, and accurate data should be attributable, legible, contemporaneously recorded, original or a true copy, and accurate (ALCOA)".[1] ALCOA itself has evolved to ALCOA Plus, which incorporates two of the fundamental definition terms as stated by the FDA; complete, consistent, enduring, and available.[2] Compliance with 21 CFR Part 11 is mandatory for pharmaceutical companies and their suppliers to sell products into the United States, and also applies to other related industries.

PerkinElmer's UV WinLab™ Enhanced Security (ES) software platform for UV/Visible spectroscopy provides structural requirements and features to assist with the needs for ensuring data integrity and compliance. It affords the system owner the ability to comply with regulations and incorporate features into the validation plan to exhibit compliance. The purpose of this document is to demonstrate how UV WinLab ES meets the technical requirements for 21 CFR Part 11.

UV WinLab ES

UV WinLab ES provides tightly controlled setup, collection, and reporting of UV/Visible data to meet the technical demands of 21 CFR Part 11 compliance (Figure 1). In addition, the software has an easy-to-use workflow-driven interface to lower the training requirements for non-specialised operators. Most functions within UV WinLab ES are identical in standard (Std.) and ES versions. However, the main differences are related to:

- Logins
- Permissions
- Electronic signatures
- Protection of records
- Working with audit trails

UV WinLab ES is compatible with the LAMBDA™ 25/35/45, LAMBDA 365, LAMBDA 20/40, and LAMBDA 650/750/850/950/1050 instruments. It is also compatible with Windows® 7, 8 and 10 operating systems. UV WinLab ES stores data in a secure, encrypted database for ease of data management and archiving, and supports latest instrument testing methodology (USP <857> (2016), Ph Eur 5.2 (2005)). The software provides multi-level user access and supports electronic signatures.

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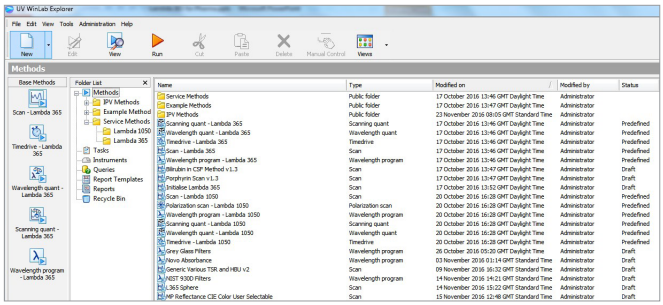


Figure 1. UV WinLab Explorer.

Software Logins

Unique user names and passwords are required for all authorized users to access UV WinLab ES, and cannot be reassigned. The instrument Service Mode is also under password control and only available if logged in as a service user. Users can be setup by the Administrator in the software.

Two password login modes are available (Figure 2):

- PerkinElmer login ➞ logins (user name and password) are created for each UV WinLab User and remain unique within the system, even after a user has left the company
- Windows® login ➞ login is controlled by the login to the Windows® OS, meaning only one password to remember

For technical compliance with 21 CFR Part 11, the login security includes administrator-definable features such as password expiration and failed login detection and lockout. All access or attempted access to the system is logged in an audit trail. Users are limited to a specified number of unsuccessful login attempts. If the administrator-defined number of unsuccessful PerkinElmer logins is reached, that user is locked out for a certain period (defined by the administrator) or once they have been unlocked by the administrator. The UV WinLab ES administrator can allocate a new temporary password, which the user is forced to change on its first-time use (i.e. their next login). Due to the high degree of security in UV WinLab ES, it is highly recommended that more than one administrator be created in case the administrator is absent or forgets their password. If a user is locked out whilst using the Windows login, the company IT administrator will need to unlock their account and/or provide them with a temporary password.

Permissions for Users and User Groups

UV WinLab ES enforces authority checks using authorization groups. Each group has its software access rights defined by the selection of permissions (Figure 3). At installation, the software has a default set of authorization groups (Administrator, Database Manager, Method Developer, Supervisor, Analyst, Approver, Reviewer). However, a UV WinLab ES Administrator can create custom groups as required. Individual users are assigned to one or more pre-defined groups.

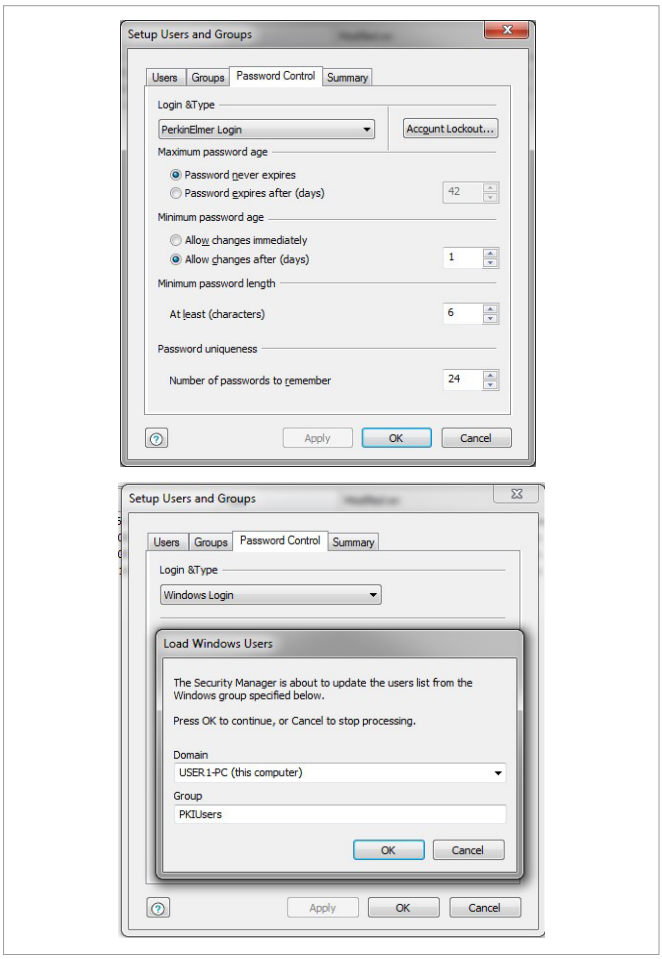


Figure 2. Setup PerkinElmer login (top) and Windows login (bottom).

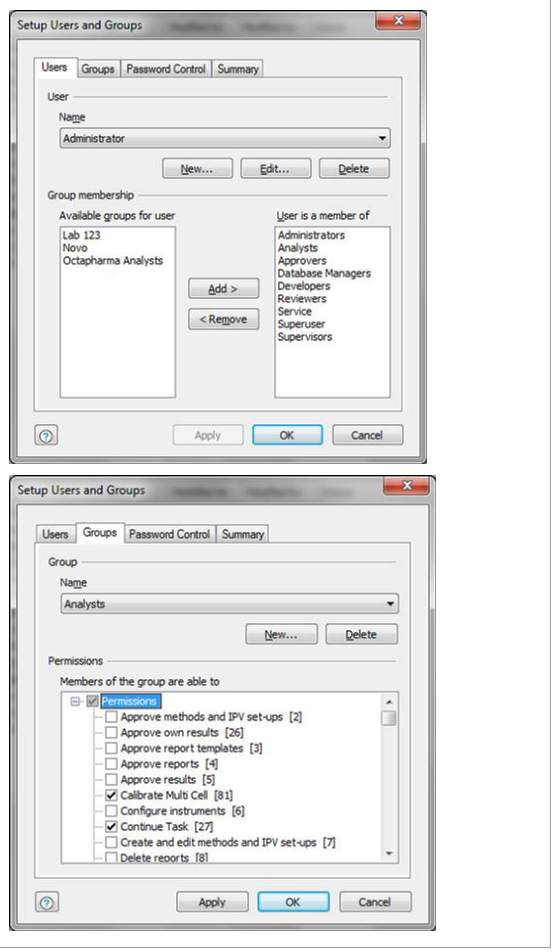


Figure 3. UV WinLab ES User and Group setup and permissions.

Only UV WinLab ES Administrators can alter the permissions of the accessible functions for these groups, add new groups, maintain the system, and allocate areas of access to individual users. The groups to which a user belongs can be toggled and define the areas of software they are permitted access to (Figure 3). This allows the application to be customized to the laboratory's most effective workflow according to their specific analytical requirements.

Electronic Signatures

A Signature Point is a point in the software which requires an electronic signature, usually when a specific action (e.g. method locking, saving etc.) is performed. The list of Signature Points in UV WinLab ES is pre-defined (Figure 4). Administrators in UV WinLab ES can configure these Signature Points individually, or the same settings can be applied to all Signature Points. Where appropriate, signature events can only be applied if the correct analytical sequence has been observed. As an example, data can only be approved if an approved method and report template have been used to generate the data.

If a signature is required, the audit trail will record the user name, date and time when the signature happened, as well as a comment and/or pre-defined reason. Signatures can only be entered by using a user name and accompanying password in the dialog box which automatically appears. The Administrator can decide whether the signature point requires a comment and/or a pre-defined reason. These pre-defined reasons are displayed as a drop-down list at the time of signing. Figure 5 shows examples of available signature dialog box configurations.

The electronic signature log can be incorporated into the analytical report as a way of ensuring data integrity.

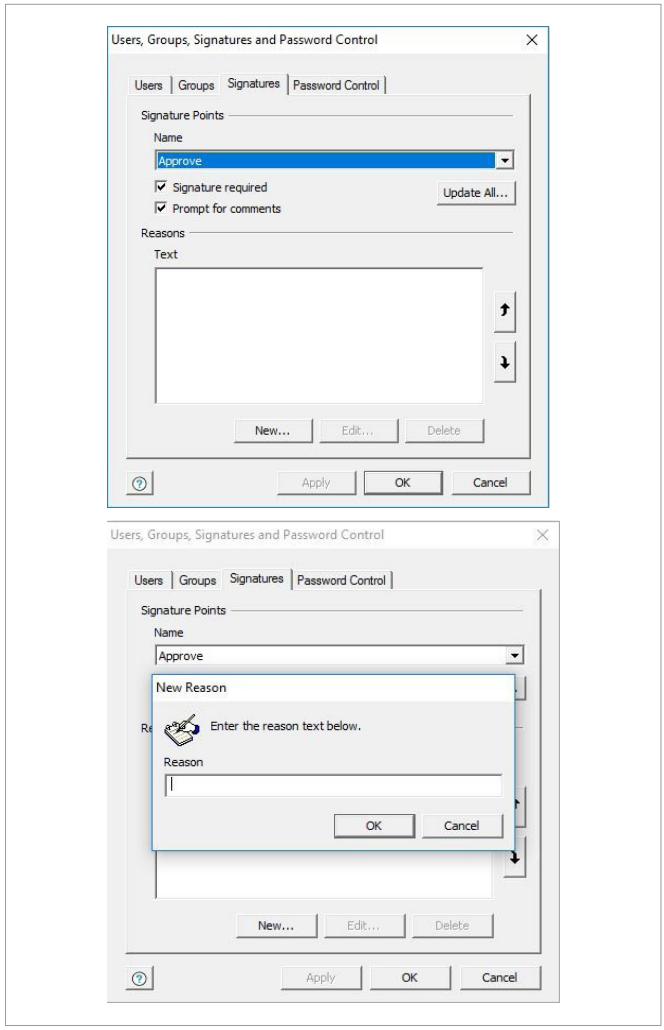


Figure 4. Configuring settings for individual Signature Points.

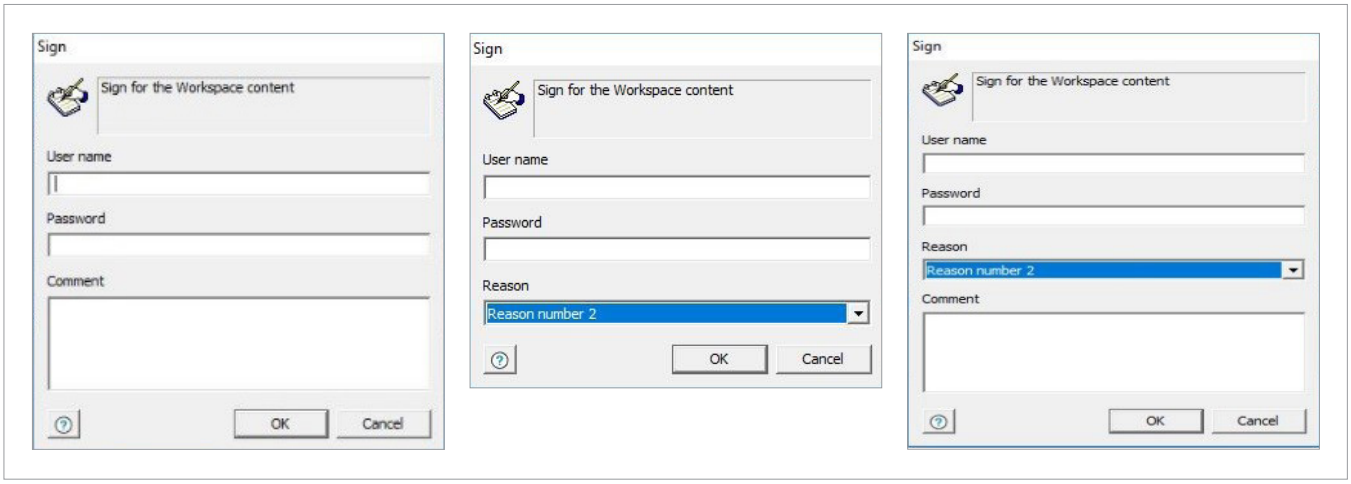
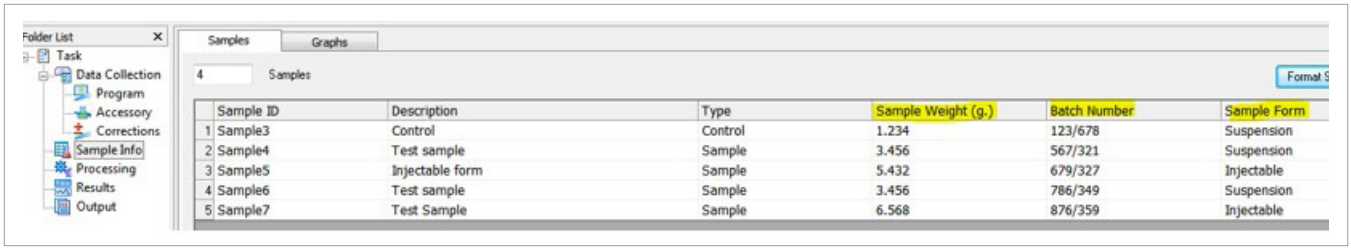


Figure 5. Signature dialog box configurations.

Entering Metadata

User-defined metadata, such as sample weights and batch numbers, can be entered via the UV WinLab sample data entry table (Figure 6). Numerical data can interact with the equation editor to allow calculations. Sample tables can be imported as, for example, a LIMS generated worksheet (in Excel .csv format). It is also possible to use barcode readers.



	Sample ID	Description	Type	Sample Weight (g.)	Batch Number	Sample Form
1	Sample3	Control	Control	1.234	123/678	Suspension
2	Sample4	Test sample	Sample	3.456	567/321	Suspension
3	Sample5	Injectable form	Sample	5.432	679/327	Injectable
4	Sample6	Test sample	Sample	3.456	786/349	Suspension
5	Sample7	Test Sample	Sample	6.568	876/359	Injectable

Figure 6. UV WinLab sample table demonstrating three user-defined metadata columns.

Protection of Records

UV WinLab ES stores all data in three secure, encrypted databases (Figure 7) to facilitate archiving and data backup. These databases handle system security (logins, passwords, electronic signatures), methods (UV WinLab database), and data and reporting (Communiqué Report Creator). Accurate and ready retrieval throughout the retention period of the electronic records is mandatory for technical compliance and the databases provide the fastest way to access valuable data. Databases can be placed directly on a network, if desired.

Data is saved in the database as a complete data record, thus all information which is associated with an analysis is retrieved with the experimental results. This includes instrument settings, raw spectra, calculations, and the final report.

Additionally, UV WinLab ES features legacy data security. A security checksum is added to spectral data which is generated within its software. Data which has been collected in a non-compliant environment is identified by the system and cannot be automatically used. However, to safely use valuable legacy data, the system administrator can manually inspect and security stamp spectra from other sources. This adds a checksum and allows safe use in UV WinLab ES.

Audit Trails

UV WinLab ES has the following audit trails which capture events and signatures:

- Method/task (data) history (method/task event log)
- Method audit trail for each locked/approved method together with version control
- Sample table (sample event log)
- UV WinLab security – logins, users, groups, signature policies
- Communiqué (report generator)

Within UV WinLab ES, methods can be locked, reviewed, and approved (Figure 8). The locking feature turns on the audit trail. If a method is unlocked, edited and then locked again, this will create a new revision of the method and the earlier version of the method will become "read-only". After the first incidence of method locking, the method can be reviewed and approved any number of times, allowing users flexibility to determine their approach to this through any laid down procedures they may have. An example of an approved method is shown in Figure 9. The Method Event Log (Figure 10) shows the transition from a "draft" to an "approved" method, with relevant date/time for audit trail purposes.

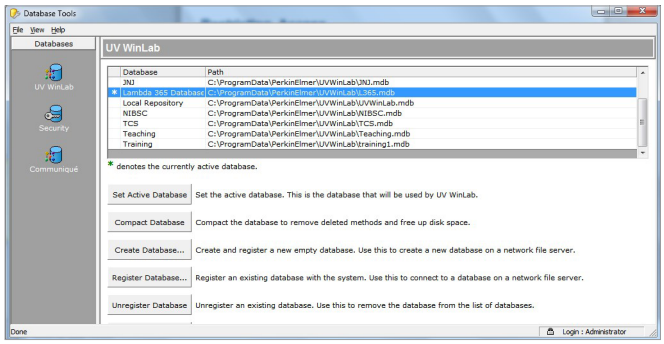


Figure 7. UV WinLab ES database structure.

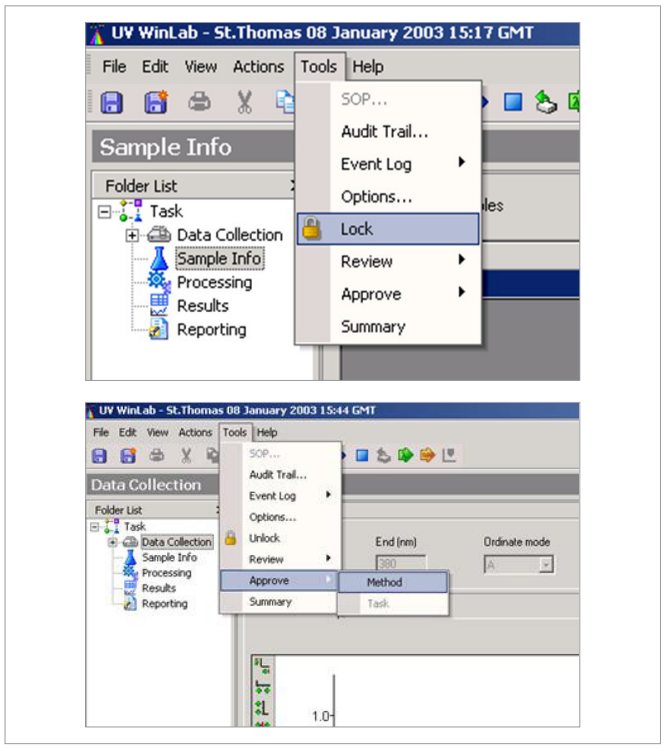


Figure 8. Locking and approving a method in UV WinLab ES.

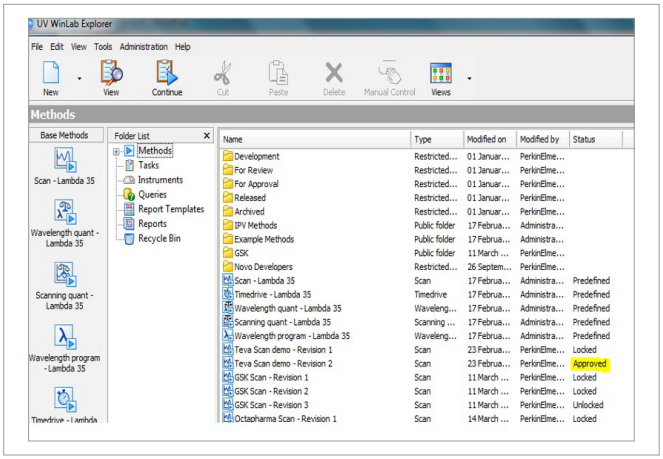
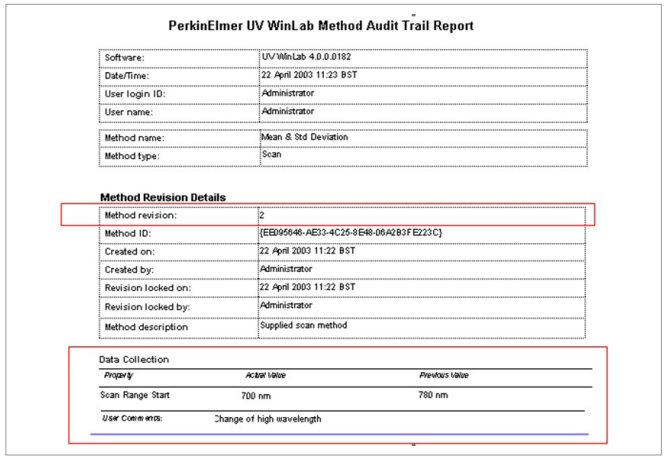


Figure 9. Example of an approved method in UV WinLab Explorer.



PerkinElmer UV WinLab Method Audit Trail Report

Software:	UV WinLab 4.0.0.0182
Date/Time:	22 April 2003 11:23 BST
User login ID:	Administrator
User name:	Administrator
Method name:	Mean & Std Deviation
Method type:	Scan

Method Revision Details

Method revision:	2
Method ID:	{EED95646-AE33-4C25-8E48-06A2B3FE223C}
Created on:	22 April 2003 11:22 BST
Created by:	Administrator
Revision locked on:	22 April 2003 11:22 BST
Revision locked by:	Administrator
Method description	Supplied scan method

Data Collection

Property	Actual Value	Previous Value
Scan Range Start	700 nm	780 nm
User Comments:	Change of high wavelength	

Figure 11. Section of a UV WinLab Method Audit Trail report.

Method Event Log :

Event	Rev.	User Date / Time	User Name	Full ID	Reason	Comment
Approved	2.000	06 October 2016 14:04 GMT Daylight Time	PEService	PerkinElmer Service Personnel	Approved	
Reviewed	2.000	06 October 2016 14:04 GMT Daylight Time	PEService	PerkinElmer Service Personnel	Reviewed for technical content	
Locked	2.000	06 October 2016 14:02 GMT Daylight Time	PEService	PerkinElmer Service Personnel	Ready for review and approval	
Unlocked	2.000	06 October 2016 13:59 GMT Daylight Time	PEService	PerkinElmer Service Personnel	Method unlocked for editing	
Approved	1.000	06 October 2016 13:58 GMT Daylight Time	PEService	PerkinElmer Service Personnel	Approved	Looks OK
Reviewed	1.000	06 October 2016 13:58 GMT Daylight Time	PEService	PerkinElmer Service Personnel	Reviewed for technical content	Reviewed - looks OK
Locked	1.000	06 October 2016 13:58 GMT Daylight Time	PEService	PerkinElmer Service Personnel	Ready for review and approval	

Figure 10. Method Event Log showing transition from draft to locked/approved method, with dates and times.

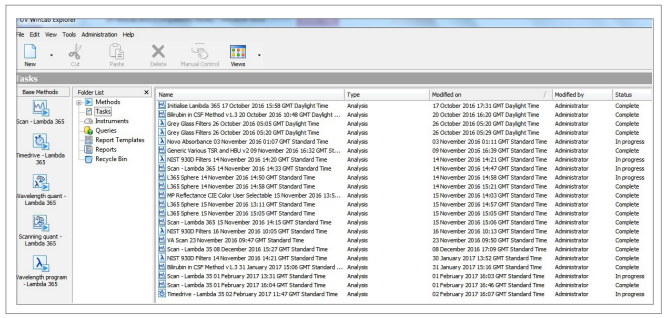


Figure 12. List of 'Tasks' in UV WinLab Explorer.

Figure 11 shows an example of part of the method audit trail. The change in wavelength from 780 to 700 nm has been logged together with comments from the method developer as to why the change was made. The audit trail also shows that this was the second revision of the method.

Within UV WinLab ES, data for a batch of samples stored in the database is saved as a "task" (Figure 12). This is the complete data record for that set of samples, containing the audit trail, user-entered metadata, sample event log, instrument parameters, and signature events. The Administrator can configure users to open the task as static data (i.e. with no reprocessing rights) or dynamic (with reprocessing rights). A task can only be approved if the data was collected using an approved method.

The history of each individual sample is kept in the sample event log (Figure 13). This is stored as part of the task for that set of samples and will contain the date/time of analysis as well as approval history. Any post-run changes in metadata entry are recorded and the previous values are logged (with reason for change, dates and times) for full data traceability.

Login history is fully audit trailed (Figure 14) along with a history of all changes to permissions, groups, and passwords. All access or attempted access to the system is logged, and unsuccessful logins are noted for action by the administrator.

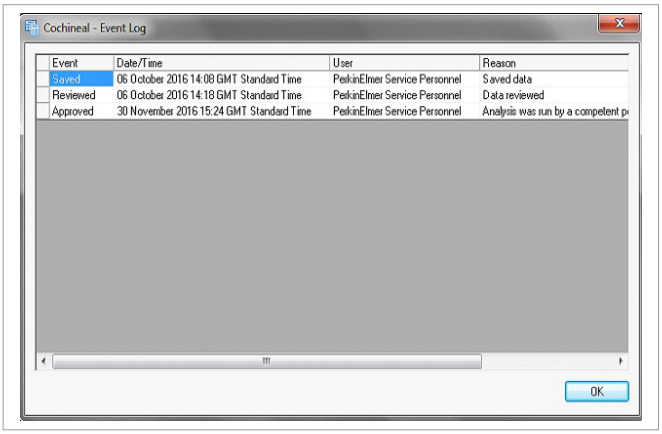


Figure 13. Sample event log.

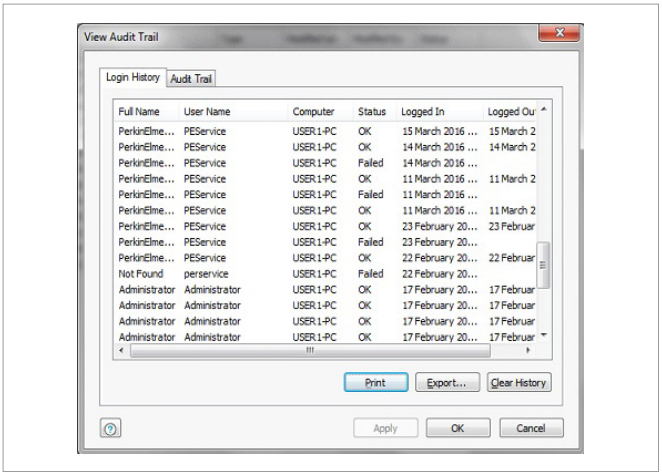


Figure 14. View Audit Trail dialog box showing login history audit trail.

UV WinLab ES includes PerkinElmer's Communiqué Report Generator which simplifies the creation of customized reports using a drag and drop editor. Communiqué features integral 21 CFR Part 11 technical compliance including user permissions and configurable electronic signatures. Restrictions can be applied, to authorized users only, for the creation, review, and approval of report templates and reports. Company logos can be incorporated, along with detailed GLP/GMP information and full interaction with instrumental and system parameters. The date and time of each individual sample can be reported together with the analyst's name (as defined by the login). Date and time formats are fully configurable (Figure 15).

The reporting 'Audit Trail' and 'Event Log' (Figure 16) handles all aspects of reporting, including templates, and report saving and approval.

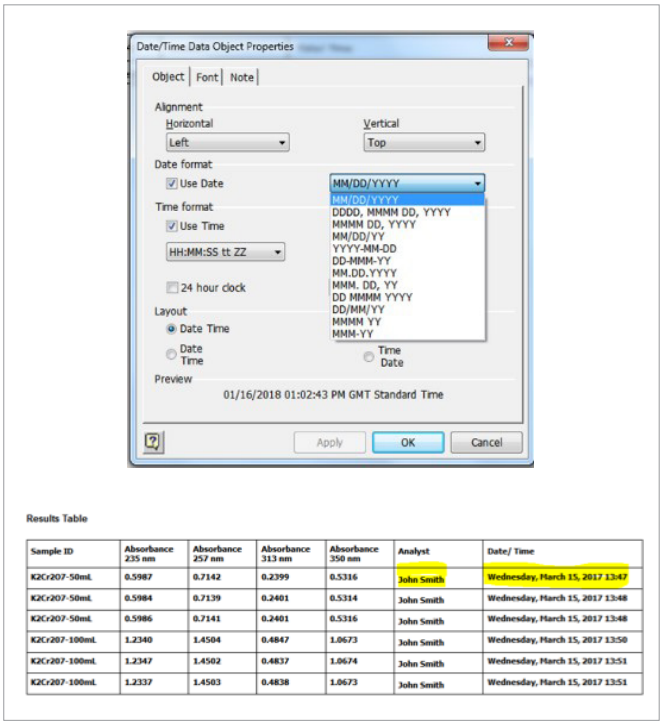


Figure 15. Fully configurable date/time formats.

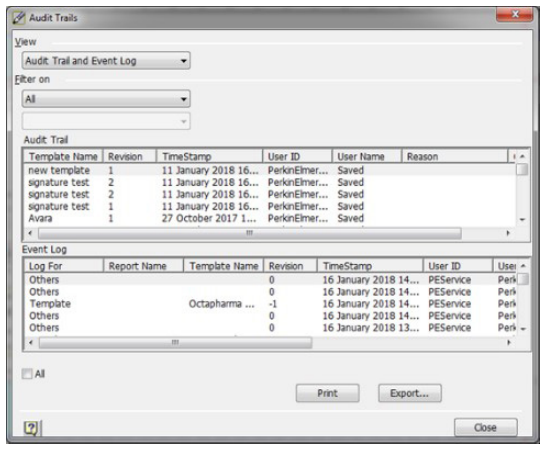


Figure 16. Reporting Audit Trail and Event Log.

Instrument Performance

UV WinLab is supplied with a library of methods for checking instrument performance according to:

- USP <857>
- Ph Eur (2005 addendum)
- JP
- PerkinElmer service procedures
- ASTM stray light

For PerkinElmer's high-performance instruments, there is a collection of Service Methods. There are also additional service methods for some major accessories such as the integrating spheres and the Universal Reflectance Accessory (URA).

In addition, the PerkinElmer OneSource® UOQ program offers laboratories ongoing compliance with continuously evolving regulatory conditions.

The UOQ program includes:

- A protocol which is customizable by the user, including options to test according to pharmacopoeial requirements. When finalized, the protocol is approved and then locked so that changes are not permitted during the testing time.
- Instrument testing by a service engineer according to user defined specifications. Multiple instruments may be tested simultaneously to reduce downtime.
- The UOQ report provides an ultra-secure document including pass/fail results and built-in calculations. This report is 21 CFR Part 11 compliant.
- Digital Archiving of data making it easy to provide information required for audits.

The UOQ program supports FT-IR, UV/Vis, HPLC, UPLC, and GC systems, regardless of equipment manufacturer to allow efficiencies in testing, reporting and review of annual operational qualifications.

Conclusion

PerkinElmer's UV WinLab Enhanced Security software platform for UV/Visible spectroscopy provides additional security and data integrity features for achieving compliance with 21 CFR Part 11. In addition to enhanced access control features, ES software automatically stores data, experimental parameters and audit trail information in secure databases. Actions can quickly and easily be recovered for inspection purposes using the various audit trails in the ES software. Electronic signature points can be added for certain actions, defined by the system administrator, and included in the audit trail. Additionally, the PerkinElmer OneSource UOQ program offers laboratories ongoing compliance with continuously evolving regulatory conditions.

References

1. Data Integrity and Compliance with Drug CGMP: Questions and Answers; Guidance for Industry, Food and Drug Administration, 2018.
2. The 5P Model for Data Integrity, Institute of Validation Technology, 2018. Available from: http://www.ivtnetwork.com/article/5p-model-data-integrity.

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