



PRODUCT NOTE

FT-IR and FT-NIR Spectroscopy

Key Features:

- Create simple workflows for improved productivity and consistency
- 21 CFR Part 11 compliance features such as Audit Trails and Electronic Signature
- Touchscreen, Tablet or PC operation – for both lab or at-sample measurements
- Combines data collection, system testing and analysis - ideal for non-specialized operators
- Create easy-to-use dedicated analyzers with full FT-IR and FT-NIR capability and maximize your return on investment

Spectrum Touch ES Software: Simplifying Workflows in Regulated Environments

Introduction

In a pharmaceutical QA/QC environment, FT-IR and FT-NIR can be used for a variety of different applications, from raw materials identification (ID) to final

product formulation verification. Most of these tasks are performed on a daily basis, often multiple times a day. For such tasks that involve the same steps on a daily basis, automating a number of the steps makes the user's life much easier. It was for this reason that PerkinElmer developed Spectrum Touch™ software. The software gives users in less regulated environments, such as industrial and food, the ability to automate a full IR workflow down to a series of easy push-button steps such that the user has no need to be an expert in FT-IR or FT-NIR. It also means that the user can receive results as a simple pass/fail or single-number-based answer, rather than requiring a large amount of analysis. Furthermore, the software is also optimized for portable touch-screen devices to facilitate mobility around a manufacturing environment.

This software was originally not designed with features to help comply with the U.S. FDA 21 CFR Part 11 regulations and, as such, could not be used in a pharmaceutical QA/QC environment. For this reason, we leveraged our experience with the industry-leading Spectrum 10 ES and Assure ID ES software platforms, combined with our Spectrum Touch workflow GUI, to create Spectrum Touch ES, the first IR automated workflow software optimized for touch-screen devices that assists pharmaceutical companies in complying with 21 CFR Part 11.

Automating Workflows

One of the most common uses of FT-IR and FT-NIR in a pharmaceutical environment is for raw materials ID testing. This is the regulatory-mandated testing to verify that drugs produced at pharmaceutical companies are composed of verified ingredients. In the U.S., the FDA mandates testing 100% of active pharmaceutical ingredients or APIs and 1/3 of excipients that arrive at pharmaceutical receiving bays multiple times a day. As it stands today, laboratory-based IR software can involve a number of steps to complete this, whereas some simplified solutions, such as those on handheld molecular spectroscopy solutions, either are not fully 21 CFR Part 11 compliant or the instrument itself is not accurate enough to discern failing ingredients. This is where Spectrum Touch ES comes in, allowing a user of either a:

1. Spectrum Two N™ FT-NIR with a probe in a receiving bay, or
2. Spectrum Two™ FT-IR or Frontier™ FT-IR/FT-NIR in a lab

to automate the process down to simply entering sample information (not necessary if combined with a barcode reader) and then following simple on-screen instructions to execute each analysis step, ending with the results displayed as in Figure 1. Figure 1 shows that the material in question is most likely povidone and that the sample has passed the raw materials ID test. This measurement is completed in less than one minute, allowing the user to quickly move to the next sample. The user can also have Spectrum Touch ES generate a report in a customizable format and/or can export results to a LIMS system.

21 CFR Part 11 Compliance

Compliance with 21 CFR Part 11 is mandatory for pharmaceutical companies and their suppliers to sell products into the United States. Although the criteria for compliance with 21 CFR Part 11 is quite extensive, the main facets that must be adhered to are:

1. Logins
2. Permissions
3. Electronic signatures
4. File protection
5. Audit trails

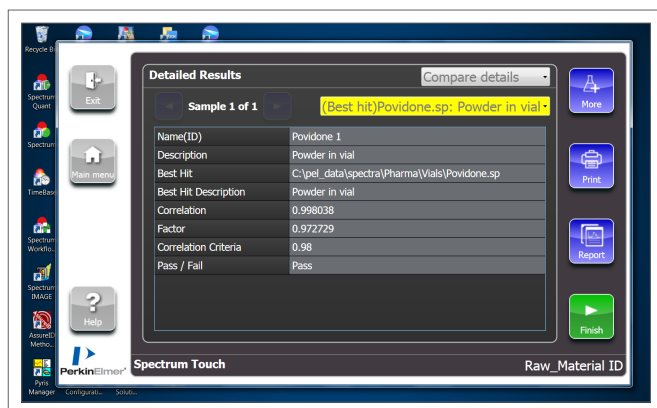


Figure 1. Spectrum Touch ES results screen showing a pharma raw materials ID pass.

Logins

21 CFR Part 11.10 (d) highlights that compliant software systems must be 'limiting system access to authorized individuals'. This means a unique User Name and Secret Password is required for all authorized users. For Spectrum Touch ES, Figure 2 shows that logins are required for all key functions in Spectrum Touch ES such as starting a macro, saving or printing results, and running system suitability checks.

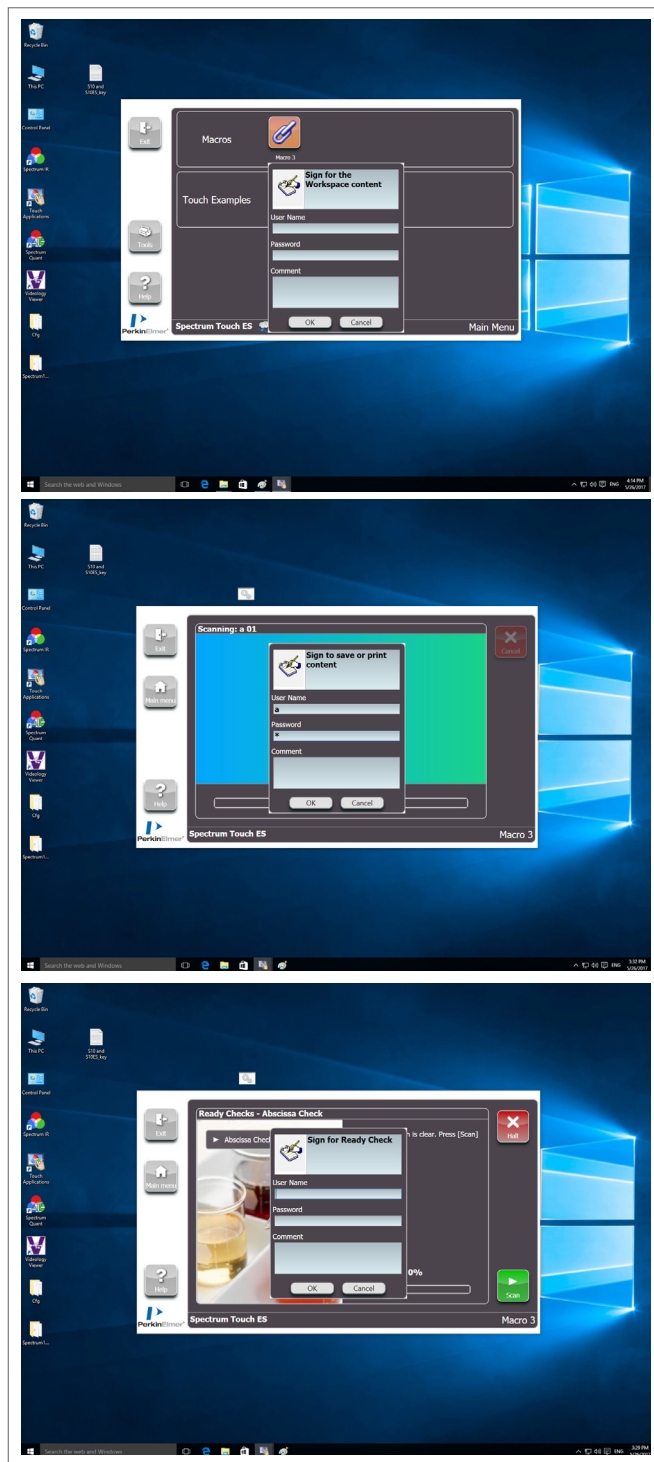


Figure 2. Spectrum Touch ES login screens.

21 CFR Part 11.10 (g) emphasizes that the software must ‘use authority checks to ensure that only authorized individuals can use the system, electronically sign a record, access the operation or computer system input or output device, alter a record, or perform the operation at hand.’ At installation, Spectrum Touch ES has a default set of authorization groups. A Spectrum Touch ES administrator can alter the permissions of the accessible functions for these groups and add new groups to the system. This allows the application to be customized to their way of working. Members of the Administration group may access administration tasks, maintain the system, and allocate areas of access to individual users. Figure 3 shows how an administrator can grant different user groups different permissions:



21 CFR Part 11.100 (a) states that 'each electronic signature shall be unique to one individual and shall not be reused by, or reassign to, anyone else'. In Spectrum Touch ES, this means that each electronic signature is linked to a User Name and user names are unique and cannot be reassigned.

21 CFR Part 11.10 (c) indicates that the software must have 'protection of records to enable accurate and ready retrieval throughout the records retention period'. In Spectrum Touch ES,

this means that all data collected and generated inside Spectrum Touch ES software will be stored in SQL databases. This data can be reloaded from the database back into the software for review. If data has not been signed for when a power failure occurs, data can be recovered from the software and be signed for and saved.

21 CFR Part 11.10 (e) maintains that the software must ‘use secure, computer-generated, time-stamped audit trails to independently record the date and time of operator entries and actions that create, modify, or delete electronic records. Record changes shall not obscure previously recorded information. Such audit trail documentation shall be retained for a period at least as long as that required for the subject electronic records and shall be available for agency review and copying’.

In Spectrum Touch ES, this means that all data collected and edited within Spectrum Touch ES is retained within the database. All settings, processes, and results created inside Spectrum Touch ES software are recorded in an audit trail stored within the database. Changes to records do not obscure previous entries, changes which will affect signed data will cause a new file (spectra file, equation, macros...) to be created, thus retaining the original. Results or data generated in the software will not be able to be removed or overwritten. The audit trail contains the user name of the user, the user's full name, the date and time stamp when the record was created, modified or deleted, the new value, the old value, and the type of modification (e.g. insert, delete, modify etc.). Audit trails can be viewed, printed and exported for inspection purposes. Figure 4 shows a Spectrum Touch ES-generated Audit Trail.



Creating Methods

Spectrum 10 ES allows users to create Macros or methods that can be carried out by users in Spectrum Touch ES. This allows, typically the administrator, a lot of flexibility to create unique bespoke methods for various different pharmaceutical testing needs. Figure 5 shows a Spectrum Touch ES macro being developed and some typical steps that can be incorporated into the final workflow. In addition to data collection and analysis, individual instruction screens can be easily customized to incorporate local language requirements and illustrations/ photographs incorporated to provide easy, specific on-screen instructions. Furthermore, Spectrum 10 ES allows a lab-based IR solution to be controlled by the more configurable Spectrum 10 ES software platform for final checking while an FT-NIR can be running a Spectrum Touch ES macro in the receiving bay, with the lab system also capable of generating methods for the receiving bay instrument as/when new methods are required without having to learn two separate software platforms.

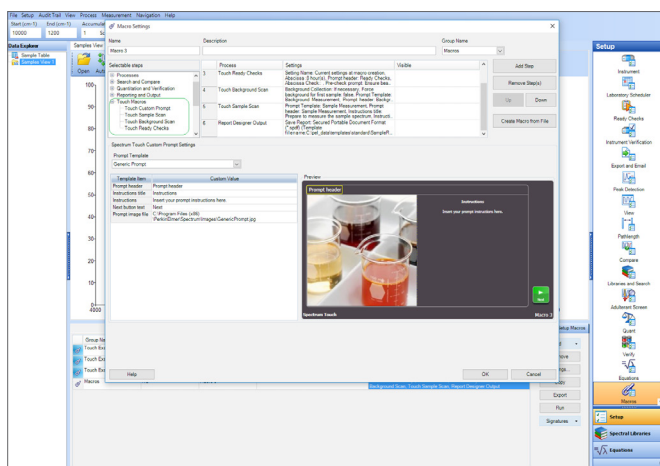


Figure 5. Spectrum 10 ES macro developer screen.

Summary

Spectrum Touch ES is an easy to use, workflow-oriented software platform that allows automation of IR testing workflows in a pharmaceutical-regulated environment. This software allows administrators to limit users' access to non-essential functions (e.g. to limit access to instrument setup parameters), speeding up productivity, reducing the necessary IR familiarity of the users and the risk of operational mistakes. The software being optimized for touch screen devices also facilitates the solution being used anywhere in a manufacturing setting such as on a cart in a receiving bay, while still allowing operation within an environment controlled by 21 CFR Part 11 guidelines.