Data Integrity within Material Analysis Using the Rigaku Progeny Handheld 1064 nm Raman Analyzer

How to preserve data integrity with versatile handheld Raman technology.

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INTRODUCTION

In the world of pharmaceutical raw materials analysis, the global compliance landscape is complex and demanding. Various pharmacopeial monographs and chapters provide specifications of a material and the tests that need to be performed to ensure it conforms with the specifications. Specifications are stringent and can vary from country to country, making for a complex landscape.

The data generated to characterize a material must comply with the principles of ALCOA+: Attributable, Legible, Contemporaneous, Original, and Accurate. A key component of all regulations is that data integrity must be preserved through all stages, from acquisition to storage and backing up, and including report generation. In particular, it is important to implement robust protocols to prevent the data from being changed (on purpose or inadvertently) after it is generated.

This article highlights the specific capabilities and features of the handheld Rigaku Progeny® 1064 nm Raman analyzer, which are most valuable for safeguarding the integrity of the data collected with this instrument. In addition, this piece highlights the device's versatility and ease of use for generating detailed reports and building spectra libraries for rapid material identification and analysis.

GENERATING THE DATA

The Progeny handheld Raman analyzer provides onscreen Pass/Fail results for materials identification according to the applications set up on the instrument. In most cases, this is

Figure 1: Ensuring data integrity with the Rigaku Progeny® 1064 nm Raman analyzer.

- ***Data*** is collected by the user and is stored on the portable instrument.
- Connect the instrument to your network to back up the ***data***.
- Your SOPs dictate when the instrument ***data*** is backed up to the server.
- ***Data*** integrity is in the hands of the administrator and validated SOP protocol.

done by comparing the Raman spectrum generated by the analyzer with the reference spectra in the library. This portable Raman spectrometer comes equipped with an onboard library of over 12,000 items. In addition, users can quickly create their own libraries with materials specific to their requirements or add scanned spectra to any existing library. For regulatory purposes, these spectra should always come from traceable samples, such as acquired standards or characterized retains.

An onboard proprietary algorithm performs the spectral comparison and calculates a correlation coefficient (CC). The Pass/Fail decision is based on a CC level set by the organization. It is usually around 0.95, but it can be higher for specific applications, such as polymorph or similar, where a tighter match is needed to separate a subset of materials. At this point, the user can view the spectral data in a variety of formats, including PDF, CSV, TXT, or XML. Other viewing options are available, such as stacking spectra, overlaying previous scan or factory library data, and zooming in via the touchscreen. After reviewing the data, the user can electronically sign off on it. The software also allows for an additional, second signature of the scan reports by an approver or administrator. The user can also take pictures of the samples and their packaging and include them with the reports generated by the analyzer.

SECURING THE DATA

To implement the best security, there must be multiple levels of technical control and user authority on the data's chain of custody, typically Developer, Administrator, and User. To ensure data security, all access to the device itself and its data is user-level controlled and password-protected (FIGURE 1). The user can store the data collected by the Progeny analyzer in its internal memory.

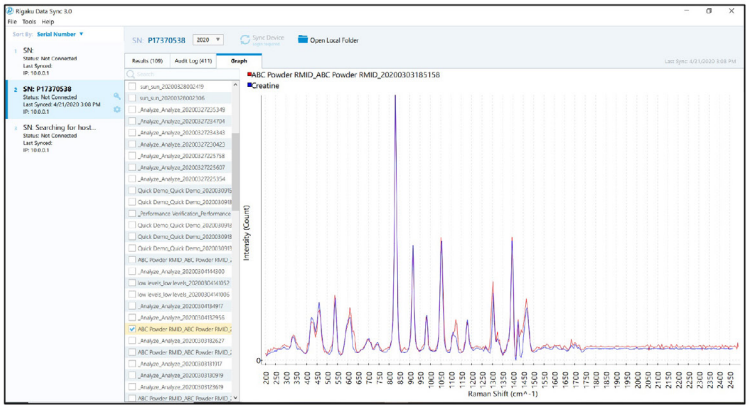
Data backup can occur in two ways. Depending on the SOPs put in place by the user's organization, the user can automatically

Figure 2: How RigakuSync 3™ backs up data to a secure server location.

- Connect Progeny to Network PC via USB or WIFI
- Data downloads from Progeny unit into the Data Sync database
- Reports and Data Files are generated and stored in the secure folder location
- Acts as a “hands-off” secure file transfer method for End-User-lockout

Easy-to-use graphical interface allows for quick data reviews, audit trail investigations, and report generation

- Searchable and sortable files
- Create multiple types of reports



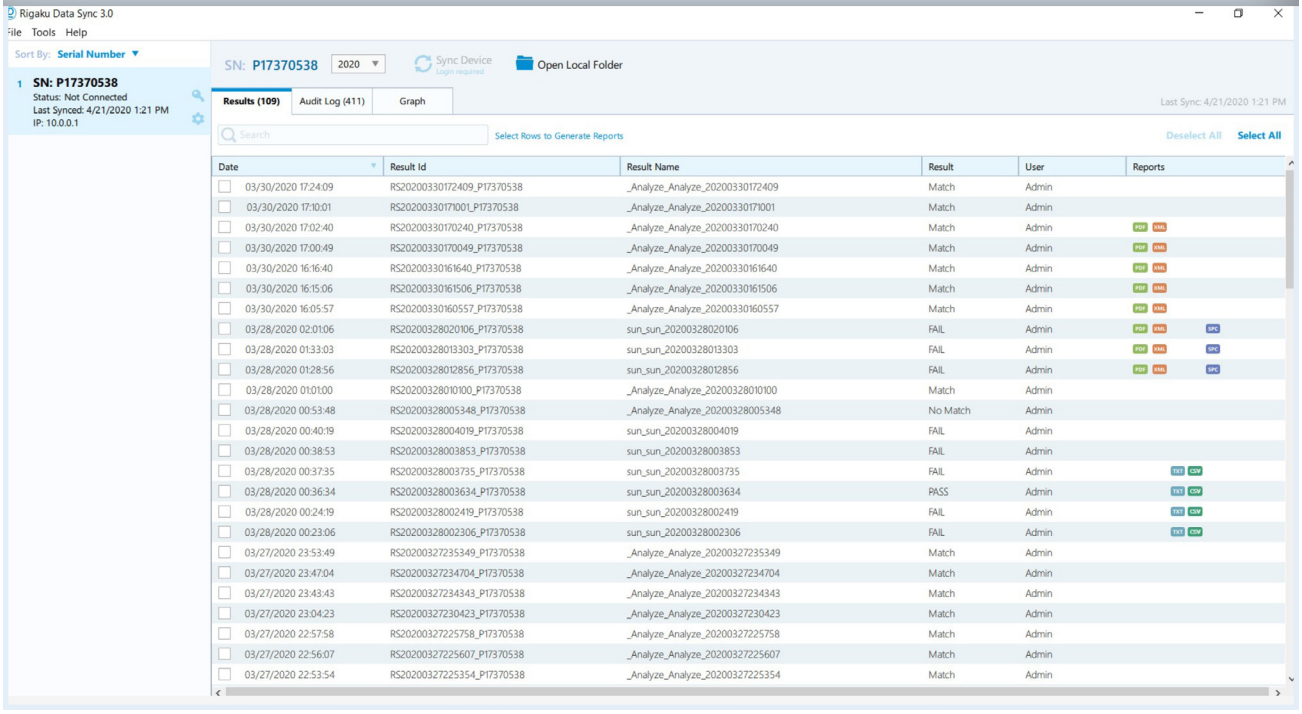
transfer the data to a secure server using the RigakuSync 3™ software that in included with the analyzer (FIGURE 2). The RigakuSync3 software resides on a local PC that has access to a secure server. A secure connection from the Progeny to the PC can be established via USB or Wi-Fi on a secure path to initiate the data transfer. The Wi-Fi connection can go directly to a network router and it allows for transferring the data from a remote location, such as a warehouse or receiving dock. The Wi-Fi network can come from a hot spot or from peer-to-peer networking.

The user can direct data-transfer methods via USB or Wi-Fi connection to a secure PC. A web-based portal can be used to access instrument data storage, and the user’s SOPs should specify a secure location where the user will transfer the data files.
Note that the original raw data can continue to reside on the instrument, if desired. The instrument allows for a significant amount of local scan data storage, but data can be purged, if needed, with the proper authorization. Another useful accessory of the Progeny analyzer is its docking station, which can be set to automatically sync the data when the instrument is docked, if the docking station is configured on a network. The docking station provides uninterrupted stationary operation or data transfer while continuing to charge the analyzer. This accessory also charges the instrument battery and external auxiliary battery simultaneously.

RIGAKUSYNC 3 KEY FEATURES

This software is at the center of the data integrity structure of the Progeny analyzer. It allows for completely “blind” backup of data in multiple file formats. User authority level can be set to prevent users from changing

Figure 3: Rigaku Sync 3 homescreen.



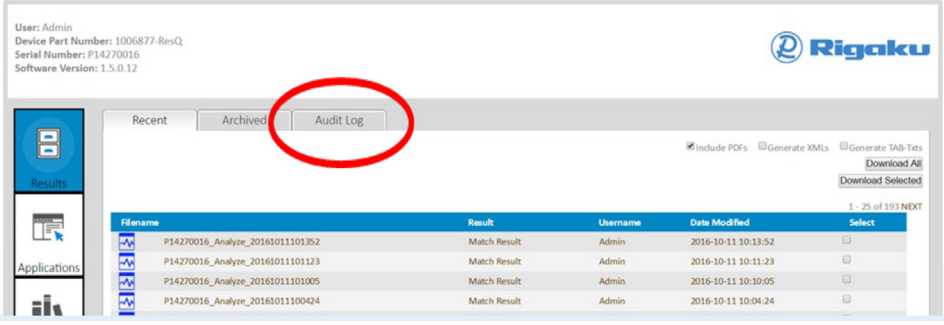
the data, while allowing them to sync the data to the secure location. This feature is essential for maintaining compliance because it prevents operator-level users from having access to results files in any way. The software can be set to automatically transfer files upon connection. End-users cannot make any changes to the data after it is transferred to the secure location by the software, but developer and administrator level personnel have the ability to clear raw data from the device within a selected date range, or choose to keep a permanent copy of the data on the device.

Syncing the data is very fast, as the software syncs only new data. From the home screen, users can select the desired reports and report types to output upon syncing, or they can select and generate them after syncing (FIGURE 3). The screen will display which type files have been created for each scan. These result files include all relevant information, such as scan conditions, match results, CC value, search results, as well as the resulting spectra. In addition, PDF reports can include multi-level (dual) electronic signatures, company logo, and any attached sample or packaging photographs. Finally, if more than one instrument is on the network, the software will display the connected devices on the home screen. The instruments can have different individual security and operational settings. The RigakuSync 3 software can be used for Progeny LT instruments as well.

Alternatively, Rigaku offers a web-based portal option to access instrument data storage. Authorized users can access the portal via a connected PC or device; their access level is determined by their organization's SOPs.

Figure 4: Data backup via web portal (3).

- Complete Original raw data resides on Progeny
- Web Portal Results section also shows Archive File on Progeny
  - Archived tab shows data that previously has been transferred from the unit
  - This data is representative of the permanent data that resides on Progeny
- Web Portal also includes an Audit Log
  - All instrument activities and changes recorded here



Information available on the web portal includes results, libraries, applications, and user profiles. The complete original raw data resides on the Progeny analyzer, and the web portal can show the archive files located there. In addition, the web portal includes an audit log that contains all recorded instrument activities and changes (FIGURE 4).

CONCLUSIONS

A combination of hardware and software features on the Progeny 1064 nm Raman analyzer allows for easily setting up secure data pathways for compliance with a wide variety of regulatory entities. The data collected by the instrument's users is easily backed up to secure locations (automatically if so desired) and cannot be accessed or modified by personnel without proper authorization. The included software also enables easy report generation in a variety of formats through its easy-to-use graphic interface and has powerful database management features.

Running a Batch of Containers with Progeny 1064 nm Handheld Raman Analyzer

The Progeny 1064 nm handheld Raman can be used to conduct identity testing on a batch of containers. Simply select the application and material you're testing. Next, select the batch ID and indicate the number of containers you need to analyze. Click Arm Laser, position the sample over the laser, and then scan the test batches one by one. The instrument will immediately indicate if it passes or fails, and a batch summary will also display with your pass/fail results. Here, the quality supervisor can sign off on the batch or you can rerun specific tests.