Chemical and Explosives Identification with Tagging

For Thermo Scientific FirstDefender RM and Thermo Scientific FirstDefender RMX

Introduction

The use of vibrational spectroscopy in field instruments, specifically Raman spectroscopy, continues to increase as the method is applied to more safety and security applications.

Thermo Scientific™ FirstDefender™ RM and Thermo Scientific FirstDefender RMX analyzers now include an advanced Tagging feature which enables users to tag items of interest for preferential visual display and enables detection at lower concentration limits, even for complex mixtures.

Background

Raman spectroscopy is actively used for field screening and identification of a wide range of chemicals including energetics, narcotics, industrial chemicals and their precursors. Portable Raman is already widely accepted and deployed by military and civilian first responders on a global scale, often in conflict zones, where it is used for identification of unknown liquid and solid chemicals. FirstDefender RM and FirstDefender RMX analyzers are handheld Raman instruments designed for point-of-use sample identification. The embedded analysis algorithms are fully automated and leverage a chemical library of more than 11,600 solids and liquids. These algorithms are designed to scour a vast library of known materials and determine whether the unknown measurement is consistent with any of the library items. If the unknown spectrum does not match any library spectra, an automatic mixture analysis is performed to determine whether a combination of library spectra explain a significant portion of the unknown measurement. As such, the device algorithms seek to answer the question "What is this?" and can be employed by users with very limited information about the sample being measured. Thus, *identification algorithms* are used to identify a material from many thousands of possible candidates and incorporate no prior information about the potential presence of specific materials.

Another type of algorithm useful in many spectroscopic field applications are those designed for material screening. Screening algorithms are typically configured to detect from a small list of target materials and are designed to determine whether some features in an unknown measurement correspond to one or more target materials. Thus, screening algorithms are much less broadly applicable than identification algorithms; however, they typically provide higher detection rates because they are customized for the detection of specific materials. Said differently, *screening algorithms* take advantage of user expertise regarding the potential presence of certain materials. As such, screening algorithms can be used for applications where enhanced detection may be more important than broad applicability or scenarios where the instrument operator has knowledge about the potential presence of specific materials.

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Figure 1. Result screens highlighting the tag result displays.

Tagging—A combined approach

During the course of a response, field instrument users are frequently presented with information regarding the potential content of a sample from multiple information sources. Traditional identification devices provide very few options to allow a user to incorporate their knowledge, or situational awareness, into the analysis of an unknown sample. To address this unmet need, a new Tagging feature has been added to FirstDefender RM/RMX software version 4.0 and later, combining the company's robust identification and screening capabilities. This approach maintains the broad identification ability users have come to expect—allowing the identification of thousands of pure materials and trillions of potential mixtures—while simultaneously allowing users to configure subsets of the library as "tag lists." A tag list can be tailored depending on the application, mission, or available information, and once created, can be seamlessly transferred from one device to another. Items can be tagged directly on the device, in real-time, without need for any external software. When identified, tagged items are preferentially displayed on the result screen (see Figure 1) through the use of a tag icon ( ). Additionally, mixtures are displayed with tagged substances appearing at the top, regardless of the spectral contribution for that substance.

Additionally, by taking advantage of certain attributes of screening algorithms, tagged substances can be identified at lower concentrations and with higher probability of detection, even in complex mixtures.

Application examples

An "unknown" sample was measured on a FirstDefender RM device that was not configured with a tag list. As seen in Figure 2a, the corresponding measurement (Scan035) is extremely similar to chloroform. Very close inspection of Scan035 reveals the presence of minor peaks that are not attributable to chloroform; however, because the features are so small the device's embedded identification algorithms were unable to determine to which substance they corresponded. As such, the sample was reported as a yellow screen for chloroform (indicating that the unknown is very similar, but not a pure component match for chloroform).

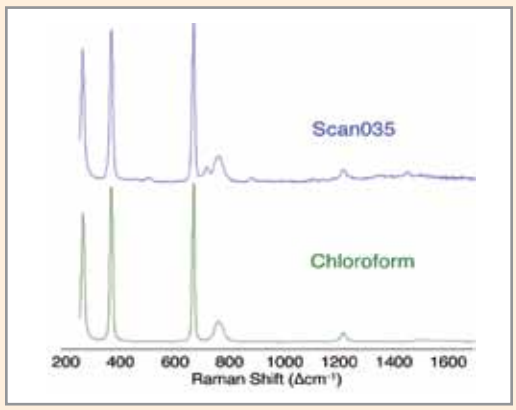

Figure 2a – Scan035 and Library Spectrum of Chloroform

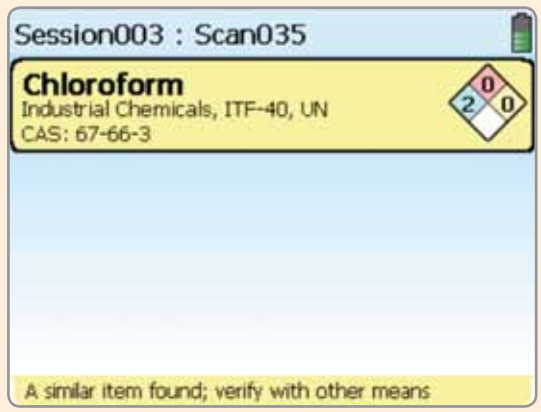

Figure 2b – GUI display; Chloroform yellow screen

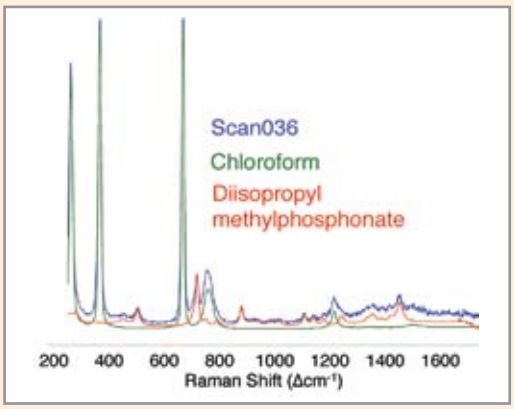

Figure 3a. Scan036 and Library Spectra of Chloroform and DIMP

Figure 3b. GUI display; blue screen mixture containing tagged DIMP

If the user obtained information about the potential presence of other substances after collecting the data associated with Scan035, how might they be able to use this information in conjunction with the tagging feature? Suppose the military or hazmat user obtained information indicating that phosphonates, such as dimethyl methylphosphonate (DMMP), diethyl methylphosponate (DEMP), diisopropyl methylphosphonate (DIMP), or diethyl ethylphosphonate (DEEP) may be present on scene. With this improved situational awareness, the user is able to create a tag list in real time containing these substances and re-measure the sample. As shown in Figure 3a and 3b above, use of this tag list resulted in the correct mixture identification for this challenging example in Scan036. The tag list improves detection performance because it forces the on-board algorithms to carefully check and make a considered determination of the potential presence for each tagged item.

In another set of application examples, "unknown" samples were measured on a FirstDefender RMX device. As seen in figure 4a, the user was especially interested in new synthetic narcotics—they had added and tagged several emerging threats, so that they could be alerted to the presence of an item of interest. Figure 4a highlights detection of 2C-D hydrochloride (a Schedule 1 controlled substance), which is clearly presented as a tagged item. With a clear indication that a tagged substance has been detected, even users unfamiliar with 2C-D hydrochloride have information that can help them escalate as appropriate. Another example is given in figure 4b. In this case, the customs official had tagged a series of narcotics of interest and scanned the contents of a suspicious package. The device returned a blue mixture result, including the tagged narcotic methamphetamine HCl as well as a second mixture component, dimethyl sulfone, a common cutting agent.

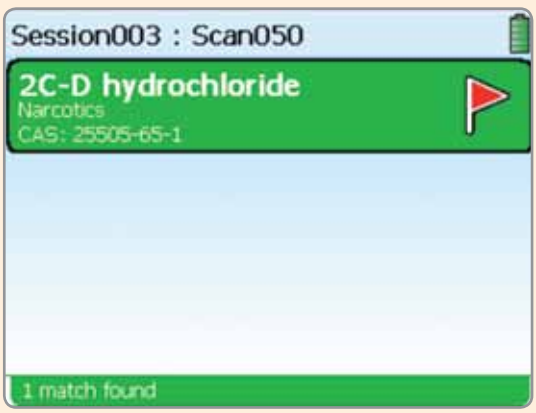

Figure 4a. GUI display; green screen containing tagged 2C-D Hydrochloride

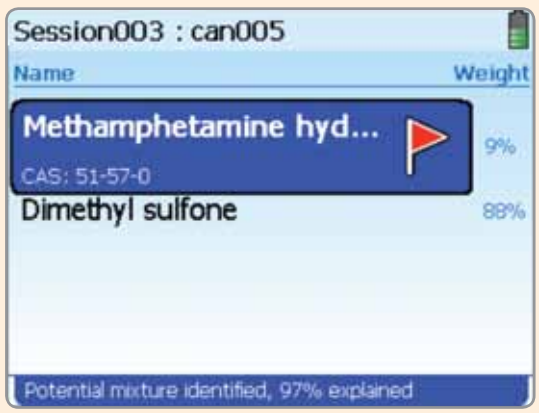

Figure 4b. GUI display; blue screen containing tagged methamphetamine hydrochloride

Summary

Beginning with FirstDefender RM/RMX software v4.0 and later, a new tagging feature has been incorporated, allowing *users to incorporate situational awareness to enhance analysis of priority items. This is done by adding a screening capability within the FirstDefender identification platform.* This approach maintains the broad identification capability users have come to expect from FirstDefender instruments, while simultaneously enabling the ability to screen for a subset of library items.

Key advantages include:

1) When identified, tagged items are clearly identified in the device result screen
2) The enhanced screening capability allows tagged items to be more easily identified at lower concentrations and with a higher probability of detection, even in complex mixtures.

The table below highlights specific customer applications where tagging would be of particular benefit.

Benefit	Potential Customer Applications
Tagged items are clearly highlighted ( ) on the GUI	1a) An *Airport Checkpoint Officer* who is primarily concerned with short list of prohibited items. 1b) A *Security Manager* whose team may not have extensive chemical knowledge, requiring a clear on-screen visual indication of when to escalate an issue.
Tagged library items are more easily identified at lower concentrations and with a higher probability of detection, even in complex mixtures	2a) A *Civil Support Team* called to a potential chemical warfare agent incident who needs to determine whether a threat is present. 2b) A *Customs Officer* who is interested in a small number of specific chemicals dissolved in beverages that are smuggled over borders.

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