

Creating Custom Libraries

Detection of Binary Explosives with Mira DS

Mira DS handheld Raman System

In the ongoing battle against terrorism, there is a very real demand for instruments designed for the detection of novel explosives. The 2016 United States Bomb Data Center Explosives Incident Report includes over 12,000 combined explosive recoveries and suspicious package incidents.

Detection of threatening materials requires robust and sophisticated instruments capable of safe, instantaneous field-analysis of unknowns. In an environment where there is an ever-evolving threat of explosives made from commonly available chemicals, explosive libraries must be customized constantly to include newly targeted materials.

Mira DS from Metrohm Raman is the perfect solution for detection of explosives in the field. This handheld Raman instrument is

equipped with sophisticated analysis algorithms and a suite of safety features for first responders who need the identity of a potential hazard... **NOW!** Mira DS and its software can be customized to respond to emerging hazards: this note describes procedures for creating custom libraries of binary explosive precursors to be used in library comparison and mixture matching routines on Mira DS. With these tools, unknown substances can be identified with color-coded warnings for fast action in critical situations.

Introduction

Figure 1 shows the Raman spectra of two well-known binary explosives, which contain signature peaks from their common precursor: ammonium nitrate. Binary explosives present a unique challenge for law enforcement agencies: they are combinations of common and inexpensive chemicals that are legal in their pure forms. Ammonium nitrate is an excellent example: this compound is well known as a fertilizer and can have mundane uses like instant cold packs. However, when mixed with aluminum, fuel oil, or nitromethane and subjected to detonation, it becomes a powerful improvised explosive. This makes ammonium nitrate an excellent candidate for inclusion in a custom library designed to identify specific explosive precursors with instant information that permits quick response to potential threats.

Actual entries from Mira DS Raman spectral library for illicit materials will be used to illustrate procedures for creating custom libraries with MiraCal DS.

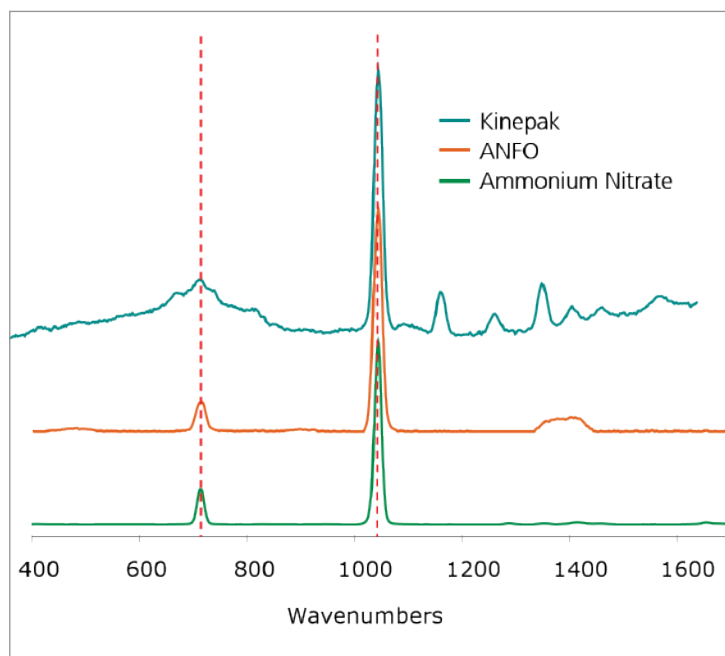
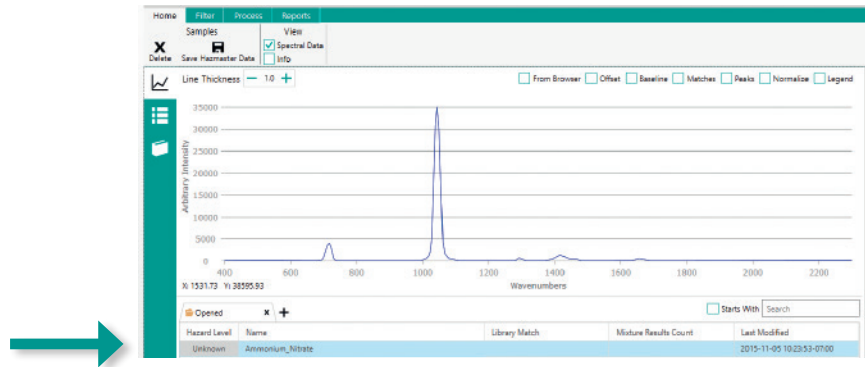


Figure 1. Two binary explosives and their common precursor.

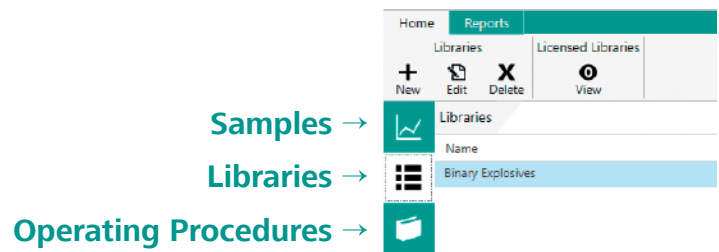
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Procedure

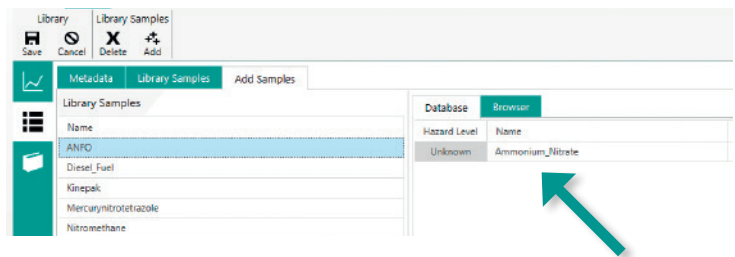
1) Import or acquire spectra of selected materials to MiraCal DS.



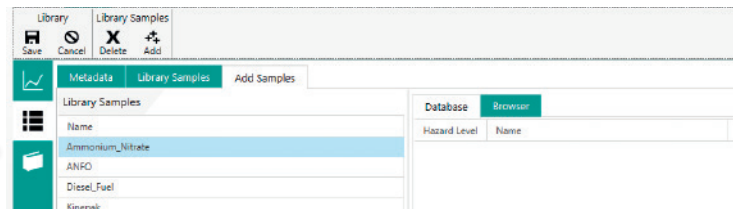
2) Open library tools by clicking on «Libraries» tab, select «New» and assign name.



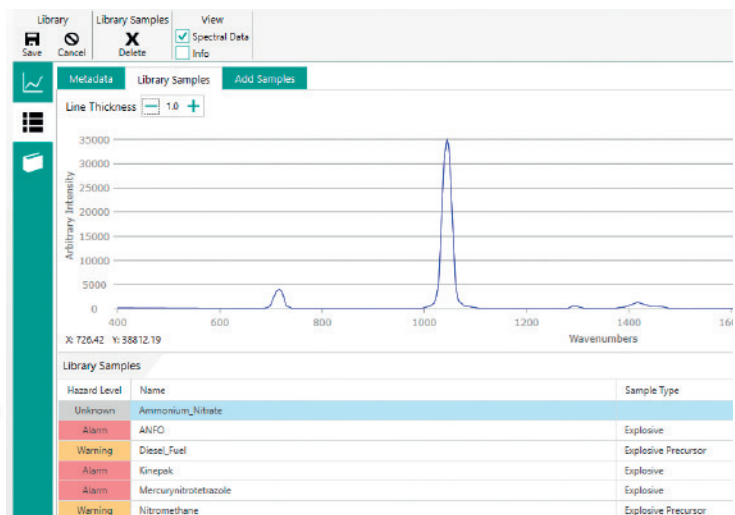
3) Click «Add Samples.» The current library and its entries will be displayed on the left. Imported and Acquired spectra will appear at right.



4) Double-click on samples at right to move them into the library. Save the library.



5) When «Library Samples» is selected, the newest entry is included in a list on the spectral view screen, as seen at right. Notice that there is no metadata associated with the new entry.

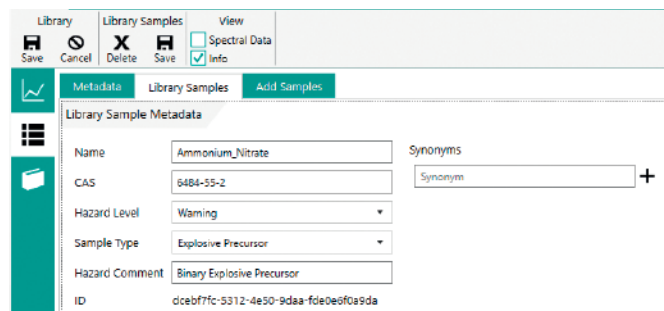


Left click on the new entry, then click on «Toggle View» to open the metadata screen

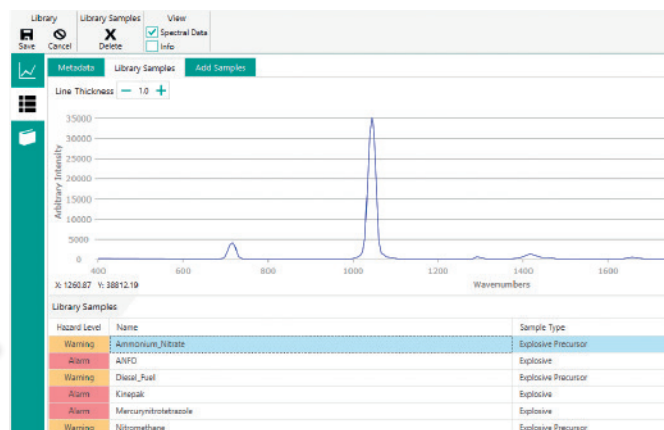
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- 6) Select/ fill in desired metadata, including:
- CAS#
 - Synonyms
 - Hazard Level – determines color of hazard warning
 - Sample Type – e.g. Narcotic, Pharmaceutical, Explosive...
 - Hazard Comment – any additional information

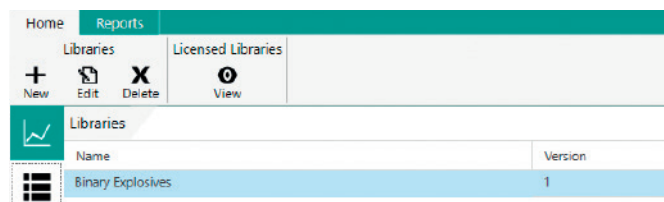
Save the Library Sample data. If the information is not saved before leaving this screen, it will be lost.



- 7) The new entry appears in the spectral view screen, with its metadata. Repeat for each new sample. Save the library when finished.

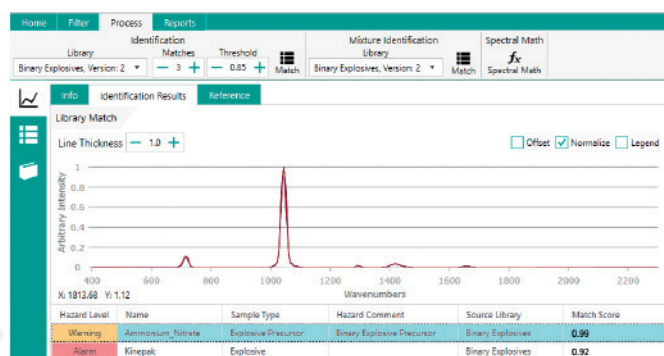


- 8) The new library will now be available for use in with new samples. When this library is enabled in MiraCal DS, new acquisitions and stored spectra are subjected to custom identification and mixture matching analyses.



Name	Version
Binary Explosives	1

- 9) The results of spectral analysis with a custom library can be seen at right. MiraCal DS successfully identified ammonium nitrate through spectral comparison within the new library.



Conclusion

No library, even those available from Metrohm Raman, can keep up with innovative hazardous materials. That's why we offer our users the power to create collections of current chemical concerns, which can be tailored to include recent threats. With custom libraries on Mira DS and

MiraCal DS, Defense and Security professionals have advanced tools for enhanced response to ever-changing threats. **We protect the safety of first responders who protect YOUR safety!**