



Application Note AN-RS-013

Determination of Container Contents

Simple, Guided Method for Materials ID with Raman

Identification of unknown materials in the field can be a complicated affair, especially in critical situations. It is imperative to know as much as possible about the substance quickly, yet with caution. Safety is at a premium when dealing with unknowns. Is that material toxic? Will a laser beam ignite it? Is there immediate danger to the environment? The nearest expert is far away, but the crisis is here and now—what can you do?

For both speed and safety, identification of unknown materials through containers is essential. Together, the handheld Mira DS Raman analyzer with the intelligent Universal Attachment (iUA) gives the user

Content ID capabilities with a single touch. When the iUA is attached to Mira DS, the Content ID Operating Procedure activates automatically, providing the user with easy guided workflows. Content ID distinguishes the contents of the container from the container material and provides identification of both. This application note demonstrates the use of the iUA combined with Mira DS for determination of container contents, including the guided workflow and examples of Content ID spectra and results. Get safe answers in seconds with no sample contact, using a Mira DS with iUA.

INTELLIGENT UNIVERSAL ATTACHMENT

The intelligent Universal Attachment (iUA) combines three focal lengths into one Smart Tip that simplifies sampling with Mira DS.

Users can safely and easily measure unknown materials through thick or thin barriers, or even on the surface:

Surface <1 mm focal length

Bag ~5 mm focal length, for sampling through a thin barrier, bag, or bottle

Bottle ~8 mm focal length, for sampling through a thicker plastic or glass bottle, for example

Clear display of contents and container material

The iUA is a redesigned tip which offers additional functionality. Rotate the iUA, and Mira DS communicates the best use of that position for direct, simple materials ID (example shown at right). Just press the tip against the unknown material, touch "Acquire" and the system does all the work, providing answers in seconds.

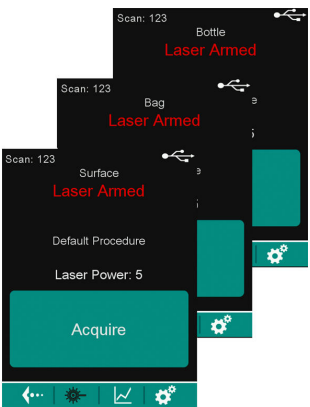


Figure 1. Intelligent iUA 3-position onscreen communication

When the iUA is attached to Mira DS, the Content ID Operating Procedure (OP) automatically becomes active on the device, and can be selected by touching "Change Procedure" and choosing the Content ID operating procedure:

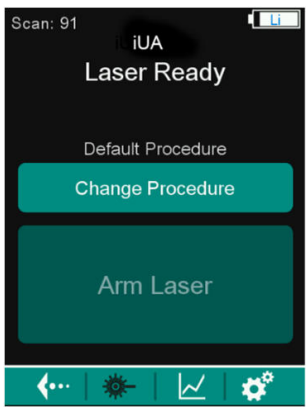


Figure 2. Mira DS iUA Home Screen

Once Content ID OP is specified, Mira DS takes the user through a very simple, two-step guided workflow (example shown at right). Position the iUA below the fill line, on the outside of the container, for the first acquisition. Position the iUA above the fill line for the second acquisition. Mira DS will optimize, average, match, and report results for both the container and its contents automatically within seconds (example shown in Figure 4).

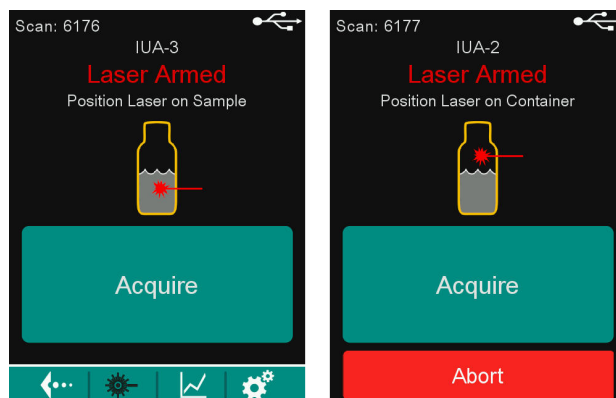


Figure 3. Content ID Workflow

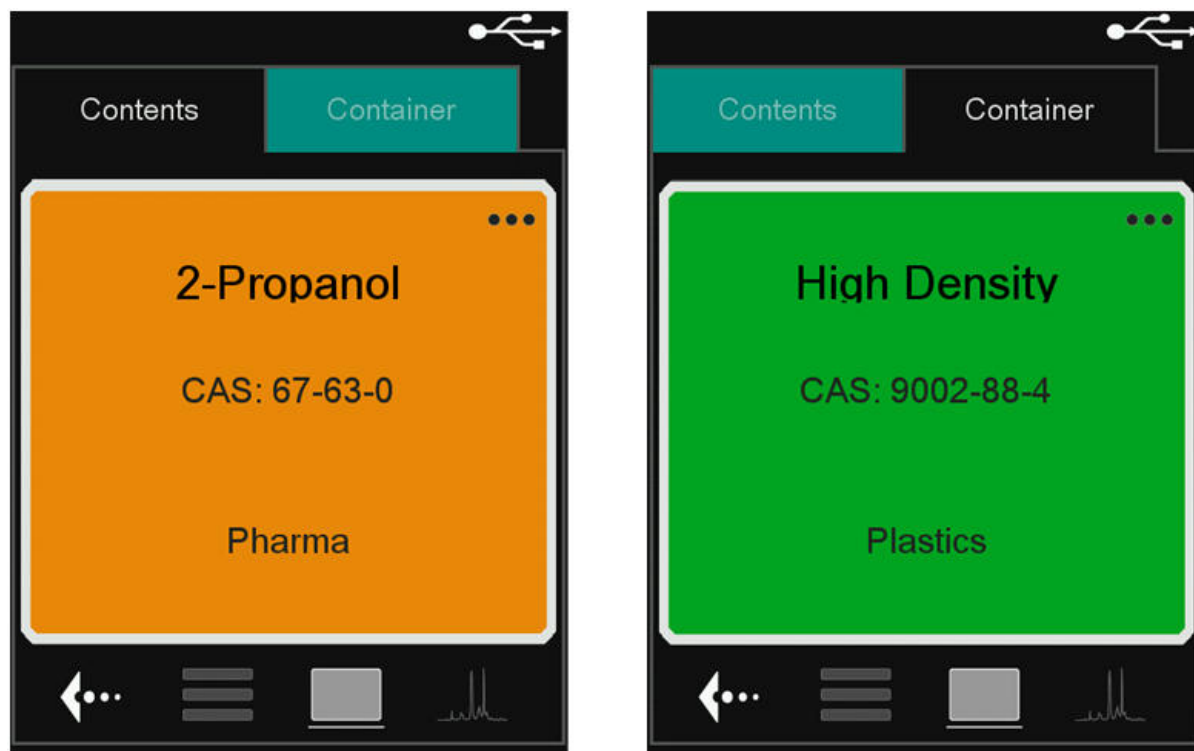


Figure 4. Content ID Results

CONTENT ID EXAMPLES

The powerful combination of Smart Acquire, iUA, and proprietary algorithms in Mira DS provides astonishing results. Consider:

- through-barrier testing
- confident analysis of mixtures
- accurate identification of major constituents in the presence of contaminants

The first example below demonstrates Content ID of a liquid mixture (cough syrup), primarily composed of ~30% w/v glycerin (glycerol) with active ingredients, through a brown plastic bottle.

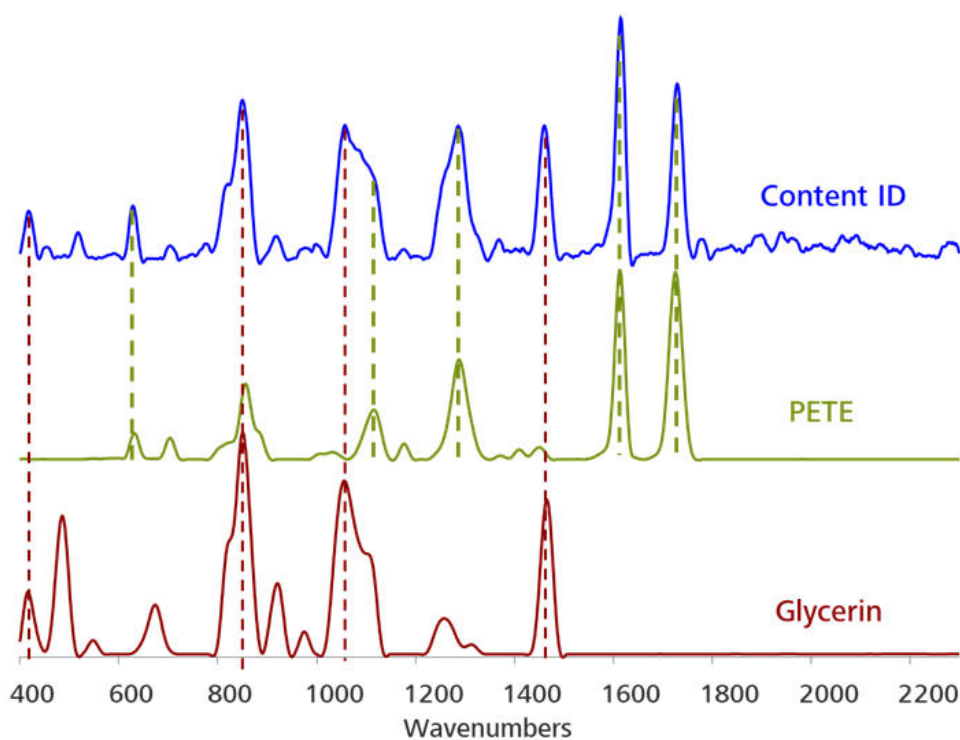


Figure 5. Library spectra of Glycerin and PETE overlaid with Content ID, to demonstrate the ability of Mira DS to solve complex spectra.

Using MiraCal DS, the results show that glycerin had a spectral weight of ~41% in the Content ID result. PETE was identified within the Illicit library with a library

correlation coefficient (HQI) of 0.99. The actual Mira DS screenshot results are found below.

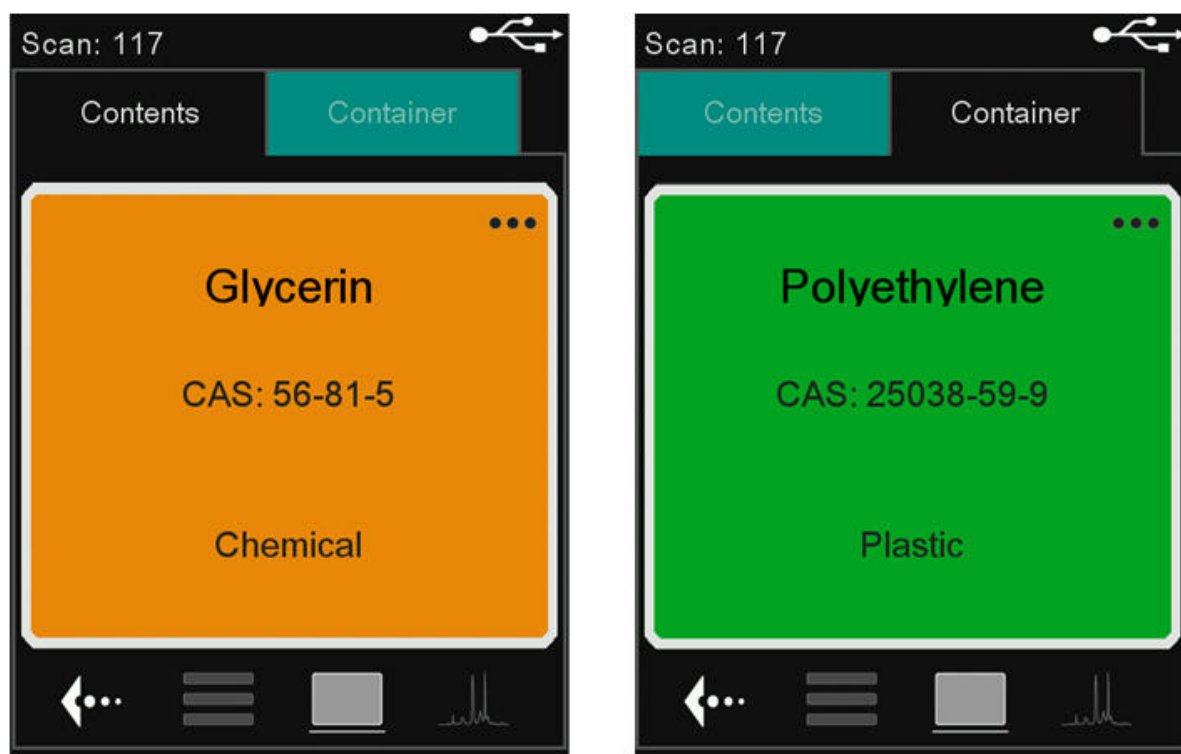


Figure 6. Actual screenshot of Mira DS result displays for cough syrup

A second example of Content ID results is analysis of acetaminophen through its opaque white plastic

bottle (below).

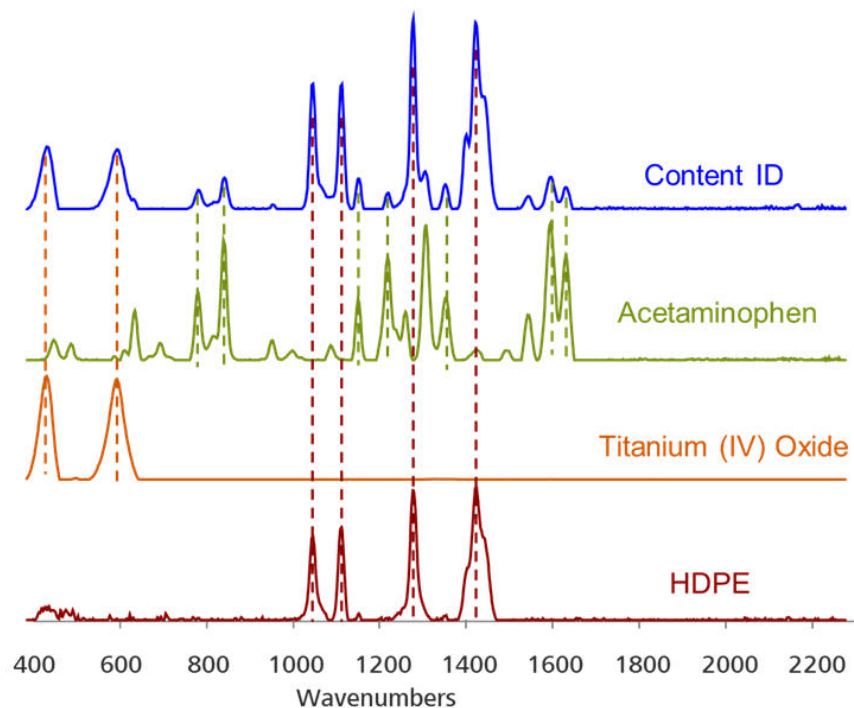


Figure 7. Library spectra of acetaminophen, HDPE and titanium oxide overlaid with Content ID to illustrate Content ID results.

This is a unique example because Content ID, in combination with Mixture Matching on the Mira DS, was able to analyze both container components—the plastic and the coloring agent (HDPE and titanium

oxide, respectively)—in addition to a positive ID of the acetaminophen within. All components were identified with an HQI of 0.99.

Table 1. Mira DS Specifications used for the analyses displayed in this Application Note

Wavelength	785 nm
Range	400–2300 cm ⁻¹
Smart Tip	iUA
Firmware version	8.0.1.136
Software version	1.1.14
Laser Power	5
Integration Time (s)	10.0
Averages	2
Library	Illicit
Threshold	0.96

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CONFIGURATION



MIRA DS Advanced

The Metrohm Instant Raman Analyzer (MIRA) DS is a ruggedized, high-performance, handheld Raman spectrometer used for rapid, nondestructive determination of illicit materials, e.g. drugs, explosives, starting materials, and hazardous agents. Despite the small size of the instrument, MIRA DS is extremely rugged and features a high-efficiency spectrograph equipped with our unique Orbital-Raster-Scan (ORS) technology.

The Advanced package includes a calibration standard, universal attachment for analyses in bottles or bags or for direct analysis, and the right-angle attachment, ideal for running samples on a surface and/or in a bag. Class 3B operation. MIRA DS supports Metrohm handheld Raman libraries.