



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.

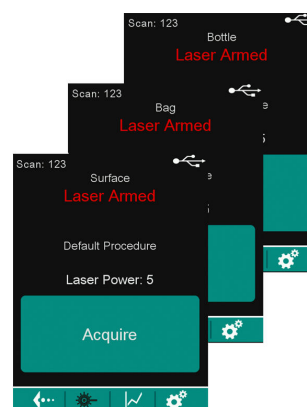


Figure 1. Intelligent iUA 3-position onscreen communication

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:

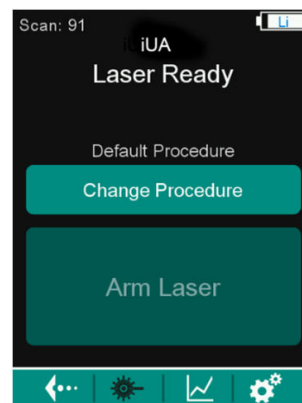


Figure 2. Mira DS iUA Home Screen

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**).

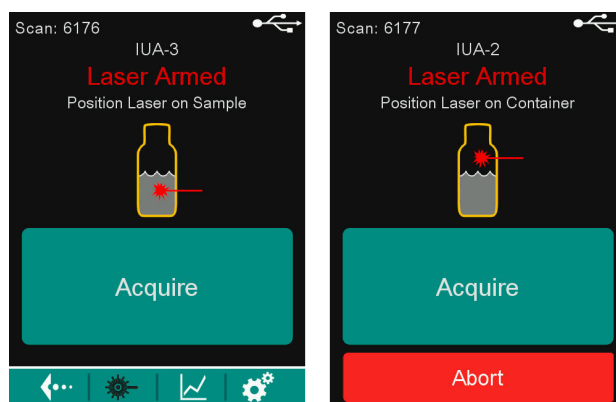


Figure 3. Content ID Workflow

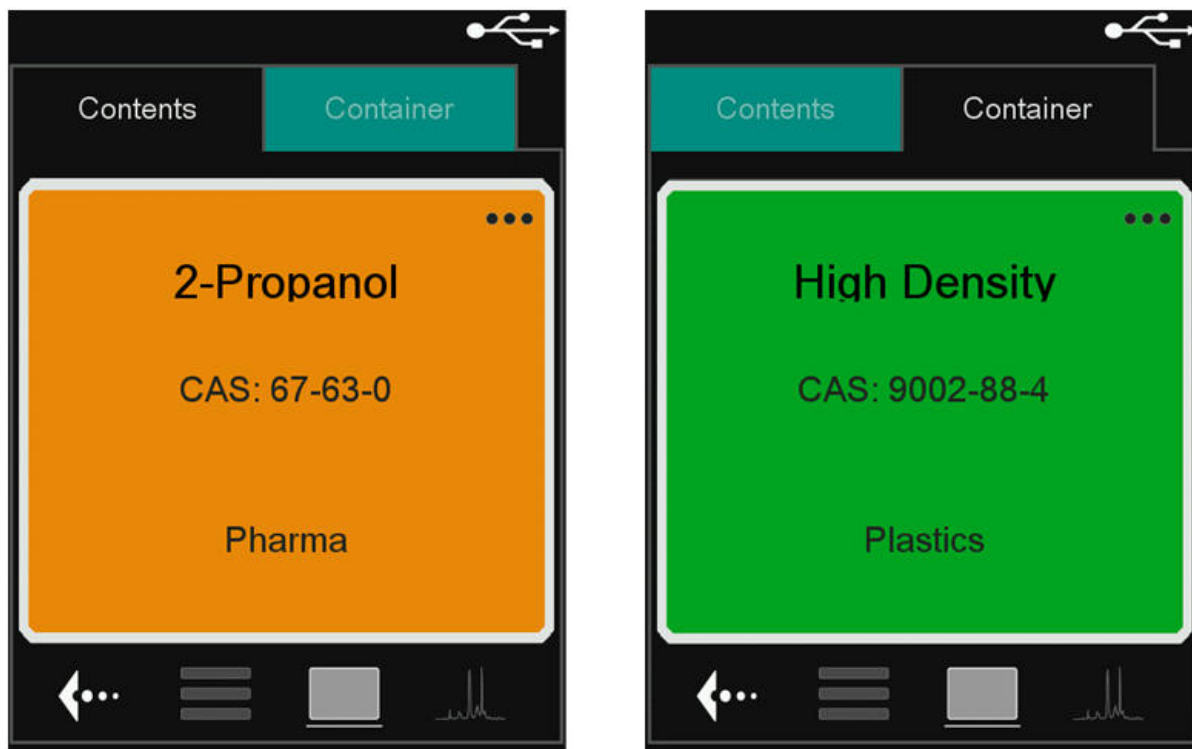


Figure 4. Content ID Results

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.

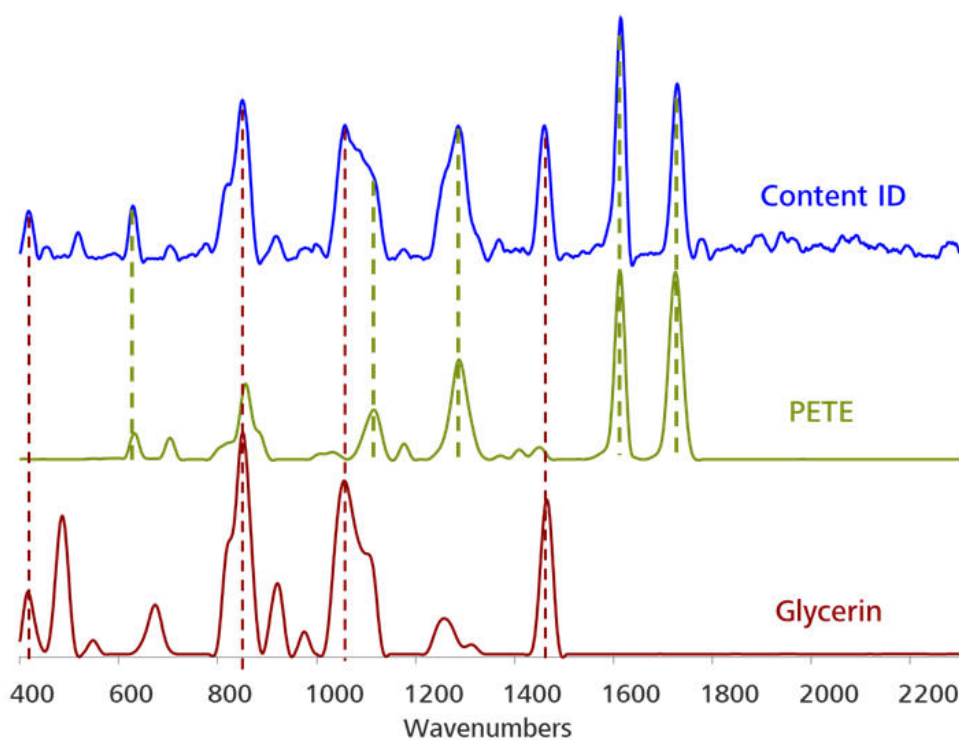


Figure 5. Library spectra of Glycerin and PETE overlaid with Content ID, to demonstrate the ability of Mira DS to solve complex spectra.

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.

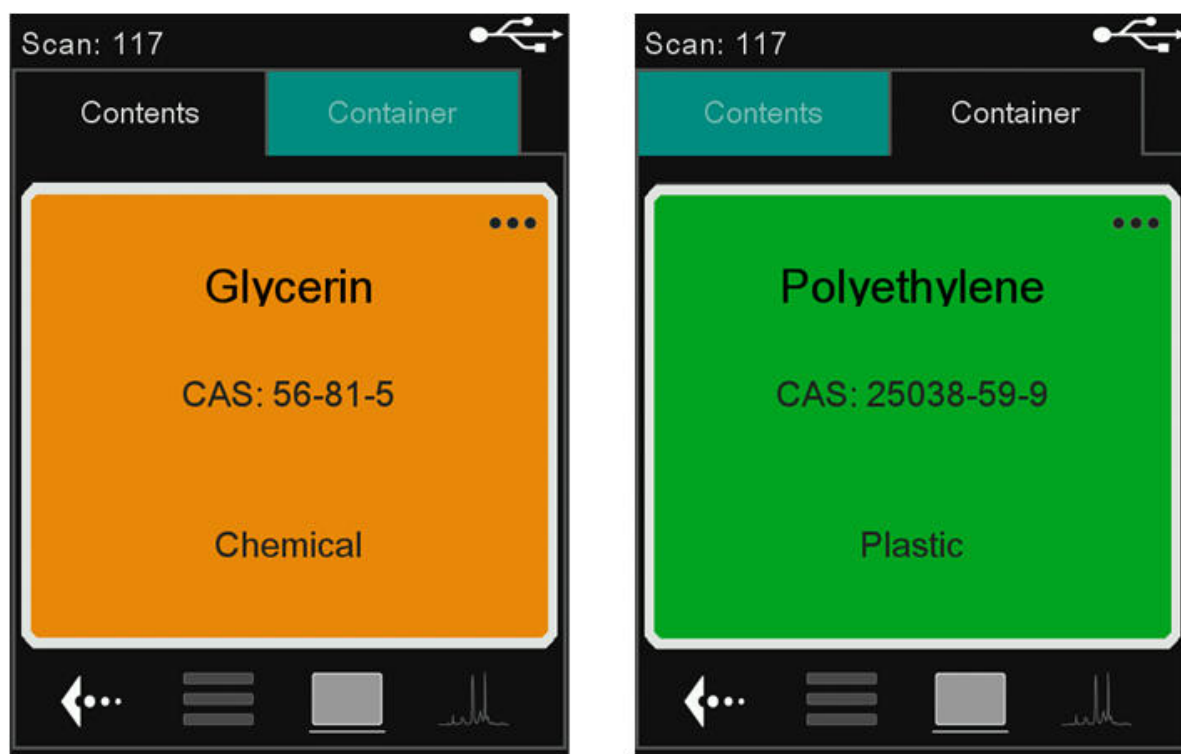


Figure 6. Actual screenshot of Mira DS result displays for cough syrup

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

white plastic bottle (below).

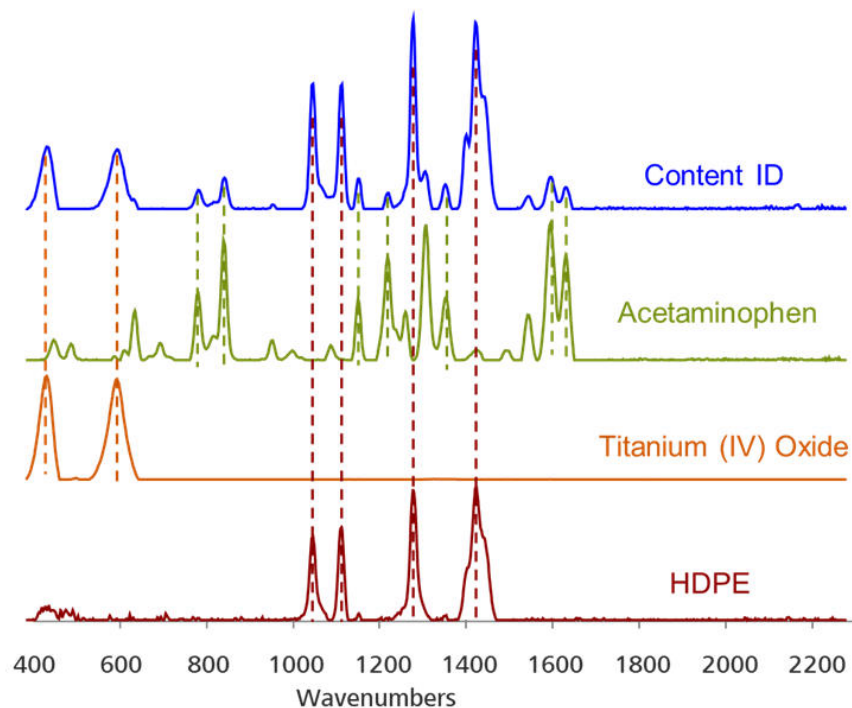


Figure 7. Library spectra of acetaminophen, HDPE and titanium oxide overlaid with Content ID to illustrate Content ID results.

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

Metrohm Instant Raman Analyzer (MIRA) DS 是一款坚固的高性能手持式拉曼光谱仪,用于快速、无损地确定非法物质,例如毒品、炸药、起始原料和有害物质。尽管仪器体积小,但 Mira DS 非常坚固耐用,提供有高效光谱仪,并配备了我们独特的栅格环绕扫描 (ORS) 技术。

该高级套件包括校正标准件、供瓶装或袋装分析或者直接分析用的通用附件以及直角附件,非常适合在表面和/或袋中运行样品。3B 类操作。MIRA DS 支持瑞士万通手持式拉曼功能库。