



A-Mode: Customizable Library Capabilities for Advanced Users with the TacticID®-GP Plus Handheld Raman System

Background: The release of the TacticID® Plus builds on the existing modes of operation and library capabilities of the TacticID family. The TacticID Plus (Table 1) contains an **N-Mode** for direct Raman measurements of samples. TacticID-GP Plus users can create their own custom N-Mode spectra to complement the supplied libraries from B&W Tek. TacticID Plus also contains **T-Mode**, which is a measurement based on surface-enhanced Raman spectroscopy (SERS). T-Mode requires the use of the TacPac™ adapter and a SERS paper substrate for analysis of narcotics found either at low-concentration or with fluorescent cutting agents. The T-Mode searches a pre-configured library with factory-defined settings that a user cannot access to change.

TacticID Plus model	N-Mode	T-Mode	A-Mode
N	No library customization	Yes	No
GP	Includes library customization	Yes	Yes
BAS	Includes library customization	Yes	Yes

Table 1. Modes of operation for TacticID Plus models

In addition to the N-Mode and T-Mode, TacticID-GP Plus model now contains an **A-Mode**, which gives advanced users the option to customize their individual library spectra for spectral search range and hit quality index (HQI) threshold. This tool allows users to isolate a specific peak (or sets of peaks) that may act as an indicator for detection of a material. A-Mode is especially useful for forensics laboratories who may want to expand their SERS detection to new designer drugs specific to their geographic region, and also has the potential to benefit such applications as food safety, product contamination, biomarker detection, and detection of illegal pesticides.

On TacticID® Plus, only an Administrator-level user may create new A-Mode libraries. Multiple libraries may be created. A-Mode has its own Operation Preset setup so that multiple A-Mode libraries may be selected to search. Each library entry has its own HQI threshold that the system will use as its “Match” or “No Match” criteria.

Applications example: A widespread public health crisis occurred in 2008 in China, when it was found that milk and infant formula powders had been

adulterated with the industrial chemical melamine to boost protein content. The level of melamine in contaminated powdered infant milk formulas was found to be as high as 2,560 mg/kg (~0.25% w/w), although the safe limit for melamine in infant formulas is 1.0 mg/kg according to the United Nations [1]. The contamination resulted in the death of six infants and illness of at least 300,000 others [2]. Since then, researchers and industry have taken steps to find analytical techniques that can quickly screen for melamine in consumer products.

Experimental: A supersaturated solution of melamine (~300 mg/mL) was made with 1 mL of acetone to acquire an A-Mode library spectrum with a SERS paper strip. Three samples of “contaminated” powdered infant formula were prepared with melamine contamination (0.5%, 0.2% and 0.1% w/w). A blank sample of infant formula without any contamination was also made. Approximately 50 mg of the contaminated sample was added to 0.5 mL of acetone to extract the melamine. A paper SERS strip was dipped into the sample solution, then loaded into

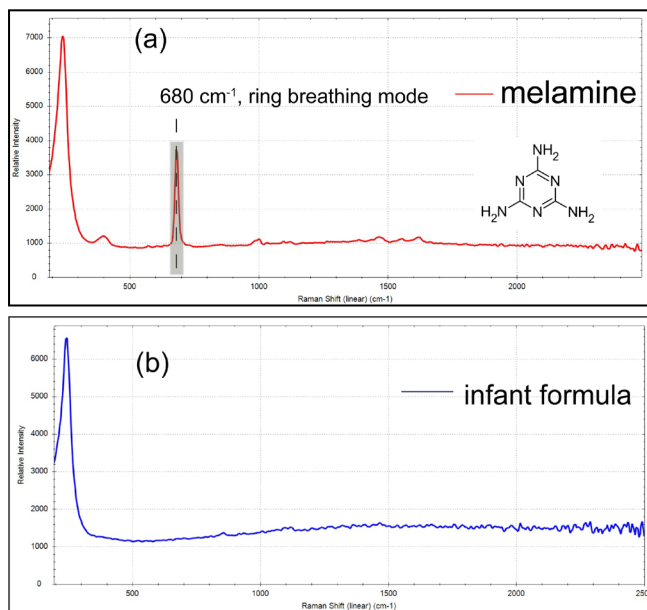


Figure 1. (a) SERS spectrum of melamine and (b) SERS spectrum of infant formula with no apparent SERS peaks. The gray area of Fig. 1a represents the spectral search range set for the A-Mode library spectrum. The rest of the range outside the gray area is not considered in the calculation for matching.



the TacPac adapter for measurement with the TacticID-GP Plus. A laser power of ~30 mW was used for SERS measurements.

Results: Figure 1a shows the A-Mode library spectrum acquired for melamine. A strong peak at ~680 cm⁻¹ attributed to the ring breathing mode of melamine is used as the indicator peak [3]. Figure 1b shows the SERS spectrum of powdered infant formula, which shows no indicators for melamine nor any other significant spectra features. The intense peak at ~240 cm⁻¹ in both spectra is contribution from the paper substrate.

In the TacticID-GP Plus software (Fig. 2a), the search range for the melamine A-Mode library spectrum was set to 664-700 cm⁻¹ (gray region in Fig. 1a) to isolate the indicator peak. The minimum HQI threshold was lowered to 50 to reduce the possibility of false negatives. Figure 2b shows the Match screen when detection of melamine is successful. All three samples of contaminated infant formula matched to melamine with high HQIs (~99).

Figure 3 shows the comparison of the SERS spectrum collected from 0.25% w/w melamine in infant formula to the melamine A-Mode library SERS spectrum. The detected melamine in the infant formula matched to the library SERS spectrum of melamine with an HQI of 99.8.

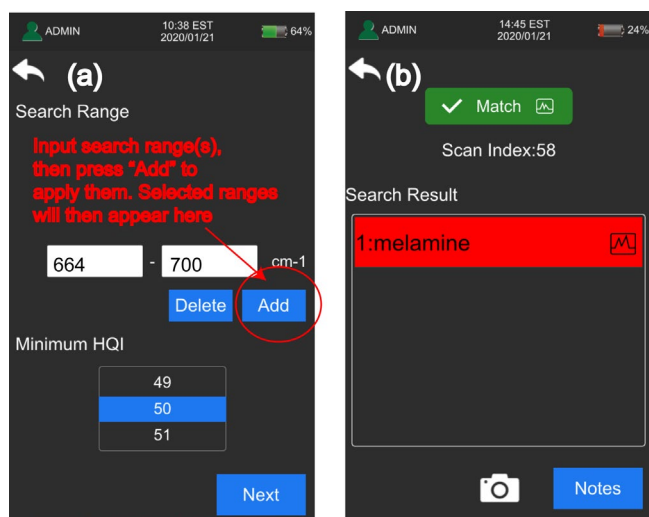


Figure 2. (a) TacticID-GP Plus A-Mode library entry customization for spectral search range and minimum HQI threshold and (b) "Match" screen for melamine using A-Mode

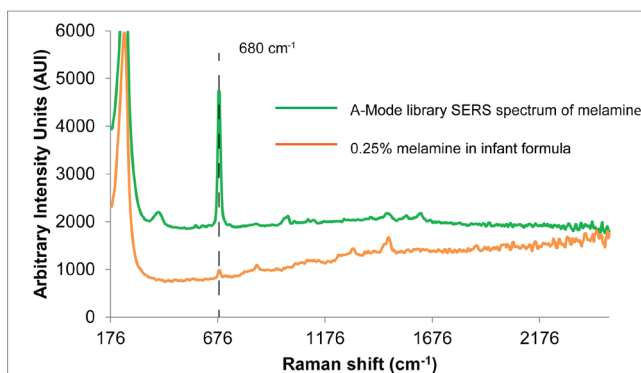


Figure 3. Comparison of TacticID-GP Plus SERS spectrum of 0.25% melamine by weight in infant formula with the melamine A-Mode library spectrum (spectra manually offset for clarification)

Conclusion: A-Mode on TacticID-GP Plus for can be used to create library spectra that can be customized for both spectral range and minimum HQI threshold. In this example, A-Mode was used to allow TacticID-GP Plus to screen for melamine contamination in infant formula powders. A-Mode opens up possibilities for advanced users to tailor the capabilities of the TacticID GP-Plus for their specific application and research needs.

For more information: See Sections 5.5 and 5.7 of the TacticID-GP Plus User Manual for specific A-Mode operation instructions.

References:

1. <http://www.fao.org/food/food-safety-quality/a-z-index/melamine/en/>
2. Huang, Y. The 2008 Milk Scandal Revisited. *Forbes* [Online], July 16, 2014, <https://www.forbes.com/sites/yanzhonghuang/2014/07/16/the-2008-milk-scandal-revisited/#1c6fbe194105> (January 20, 2020).
3. Mircescu, Nicoleta E., et al. "FTIR, FT-Raman, SERS and DFT study on melamine." *Vibrational Spectroscopy* 62 (2012): 165-171.

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