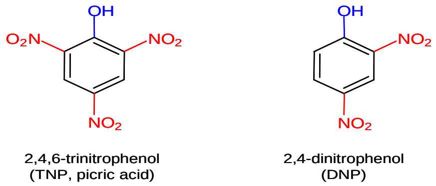
Picric Acid Case Study
The Advantage of High-Precision Algorithms for Material ID

Ahura Corporation's ***First* Defender**™ handheld Raman material identification system is more than a Raman system in a small, rugged package. It also raises the bar in terms of intelligent material identification algorithms. This application brief gives some examples of the level of enhanced information these algorithms can provide to the first responder.

Traditional spectroscopy library search methods often have a relatively high false-positive rate, meaning they will usually return a 'hit' to something in the library, and poor precision, meaning many materials are presented with high hit-scores. The ***First* Defender** DecisionEngine™ algorithms achieve a dramatic improvement in the false-positive rate and precision of spectroscopic search for the first responder by providing an "on-board spectroscopist".

This application note demonstrates how Ahura's ***First* Defender** can differentiate between TNP and DNP. TNP, known as picric acid, is an unstable and explosive nitro compound that can be prepared relatively easily from aspirin by rudimentary synthesis. DNP can also be explosive under some circumstances, but has a history of illicit use as a diet or 'fat-burning' drug, in spite of its high toxicity. Both materials are white-yellow solids.

Figure 1 shows the library spectra and molecular structures for 2,4-dinitrophenol (DNP) and 2,4,6-trinitrophenol (TNP). The similar molecular structure of DNP and TNP leads to similar Raman spectra, but there are also some minor spectral differences between the two. Unfortunately traditional spectroscopy library search software looks for bulk commonalities, rather than discrepancies, so a measurement of DNP is likely to also lead to a very high traditional hit-score for TNP. In contrast, ***First* Defender's** DecisionEngine algorithms have a very sharp eye for spectroscopic inconsistencies between the measured data and the library spectra.



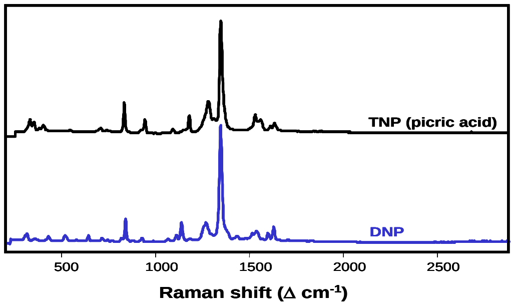


Figure 1. Molecular structures and Raman spectra for 2,4,6-trinitrophenol (picric acid), and 2,4-dinitrophenol.

The ability to accurately discern differences in library spectra is illustrated in **Figure 2** with two results screens, one from a measurement of DNP, and one from a measurement of TNP.

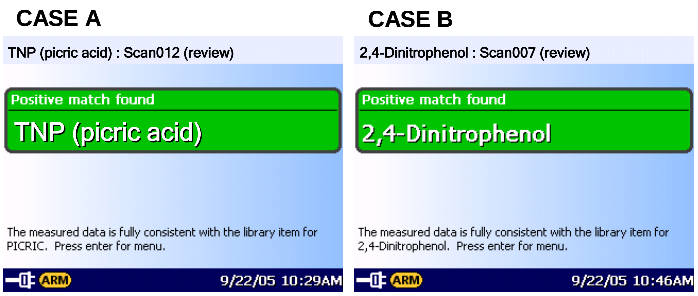


Figure 2. Screen shots from two cases. Case A was a measurement of TNP (picric acid), and Case B was a measurement of DNP.

From the results screen it is apparent that the DecisionEngine™ has no difficulty distinguishing TNP from DNP. Only a single match is reported in both cases, which means that there were inconsistencies with other library records causing them to be highly unlikely. In fact in **Case A** (a measurement of TNP), the DecisionEngine estimated that odds of the material being DNP was about 1 in 10^{16} – far lower odds than winning a Powerball lottery jackpot – versus over 99 in 100 for TNP. In **Case B** (a measurement of DNP), the odds of the material being picric acid were also miniscule – 1 in 10^{15}.

Summary

The similarity measures used by traditional spectral library search systems are prone to imprecise search results and have much higher false-positive rates than one would like for field decisions. Since ***First* Defender's** DecisionEngine scrutinizes the data for inconsistencies, it has much greater discrimination power for field material ID, keeping the risk of false-positives low and the information provided to the end-user of high and extremely reliable quality.