HIGH EXPLOSIVES DETECTION IN INTERNATIONAL MAIL USING SEE-THROUGH RAMAN SPECTROSCOPY ASSISTED BY MULTIVARIATE ANALYSIS

ALERT — AWARENESS AND LOCALIZATION OF EXPLOSIVES-RELATED THREATS

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Abstract

See-Through Raman Spectroscopy (ST-RS) was used for the non-invasive, non-destructive sample analysis of high explosives (HEs) in mail envelopes or flats. The method resulted in a safe and rapid analysis of HEs: AN, UN, and PETN. The ST-RS system is a portable, rapid, high throughput technology that enables the characterization of chemical and biological threats by exciting their vibrational modes. Multivariate analysis was applied due to the vast amount of data generated in the experiments, and the spectral interferences presented by the envelopes. Exploratory Data Analysis (EDA) was applied to separate HE signals from mail flats spectral data. Principal Component Analysis (PCA)-based models were efficient in classifying HEs' vibrational markers even when contained within several flats layers and classifying HEs into different clusters. PC loadings were used to determine each variable's contribution to the PCA models, which resulted in correlation coefficients (R^2 values).

Motivation/Introduction

Chemical and biological threats (CBTs) are of significant concern for the safety of the population. These threats are usually present in high populational density sites, government installations, airports, and International Mail Facilities (IMFs). To counter the threats posed by CBTs used in terrorist acts, early detection is critical. High explosives (HEs) and homemade explosives (HMEs) are commonly used as chemical threats affecting civilians and the environment's security. See-Through Raman Spectroscopy (ST-RS) enables identifying and characterizing chemical and biological compounds in a non-invasive manner, even when confined in opaque containers. Therefore, it is ideal for detecting HEs in international mail since suspect packages can be analyzed for rapid and non-invasive identification of CBTs.

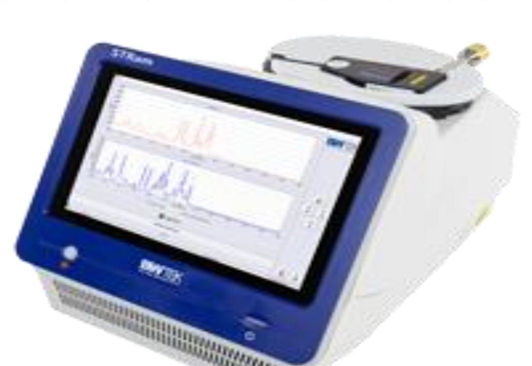
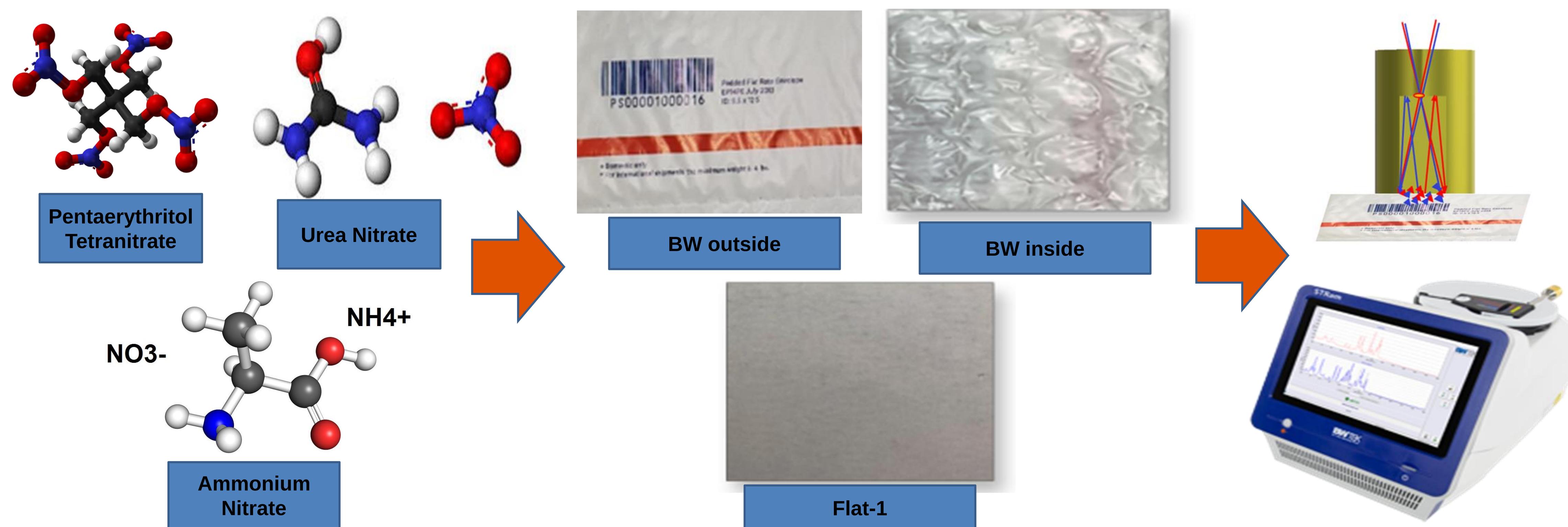


Figure 1: Portable 765 nm ST-RS (STRam® **BW Tek)**

Methodology

Sample Preparation



Spectral Characterization

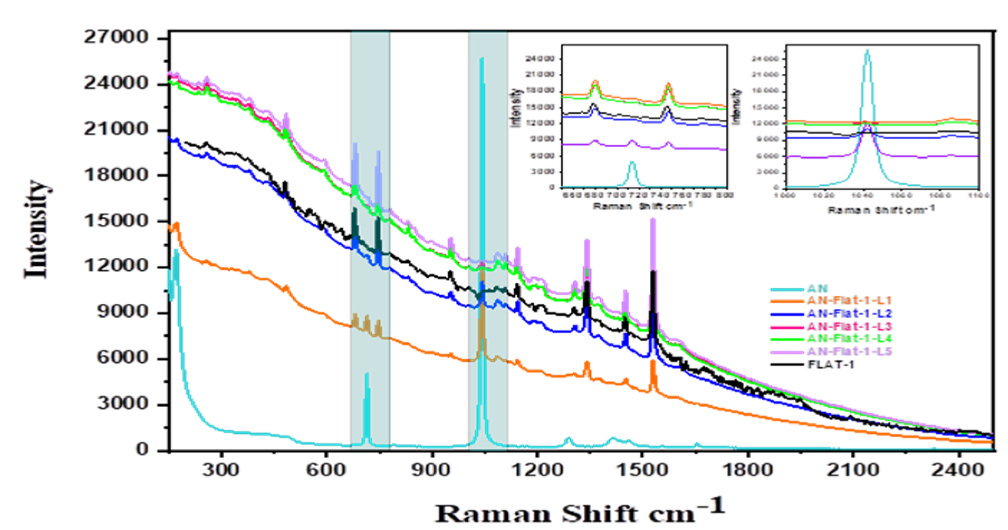


Figure 3: NH_4NO_3 (AN) with multiple layers of Flat-1 mail envelope.

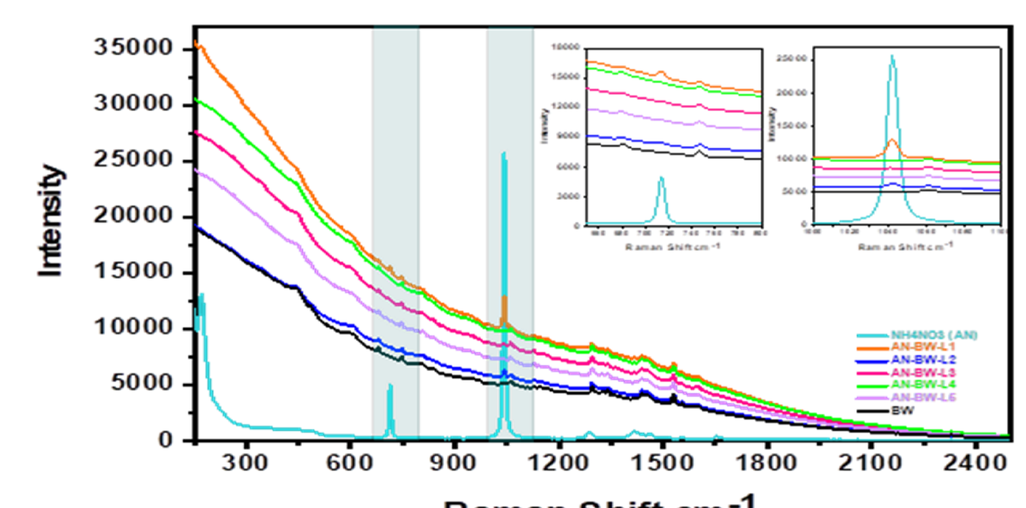


Figure 4: NH_4NO_3 with multiple layers of the BW mail envelope

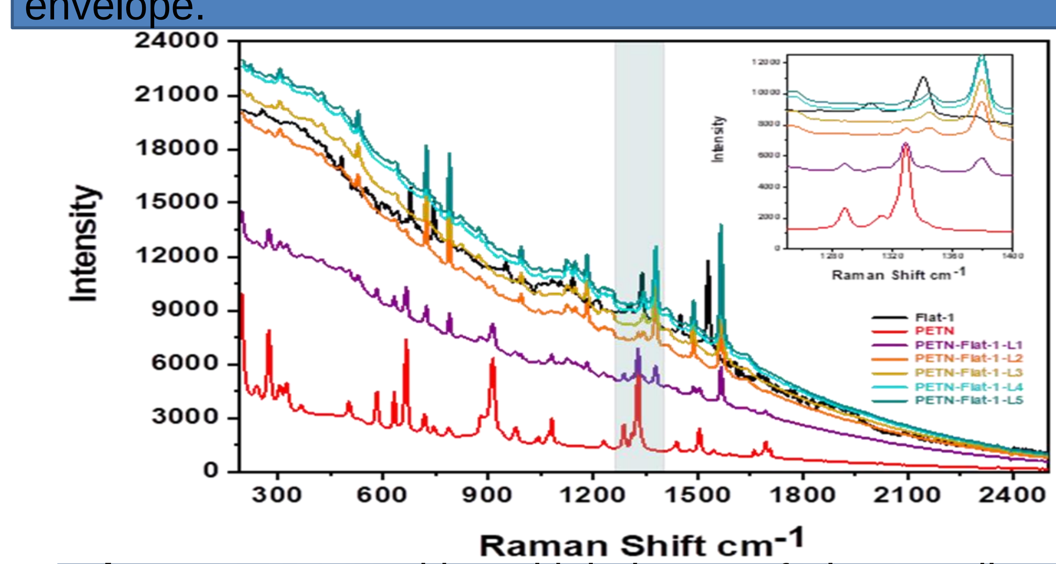


Figure 5: PETN with multiple layers of Flat-1 mail envelope.

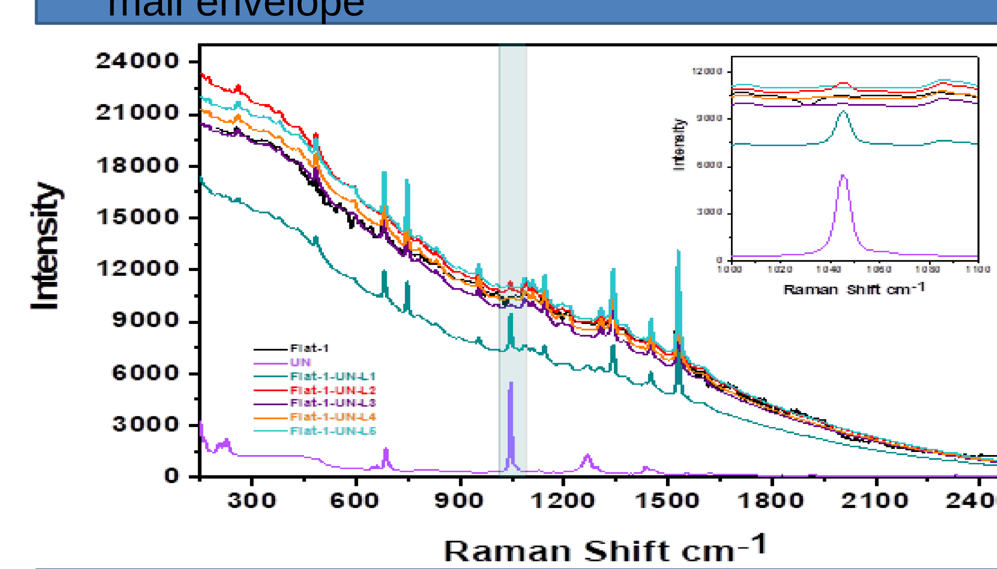


Figure 7: Urea Nitrate (UN) with multiple layers of Flat-1 mail envelope.

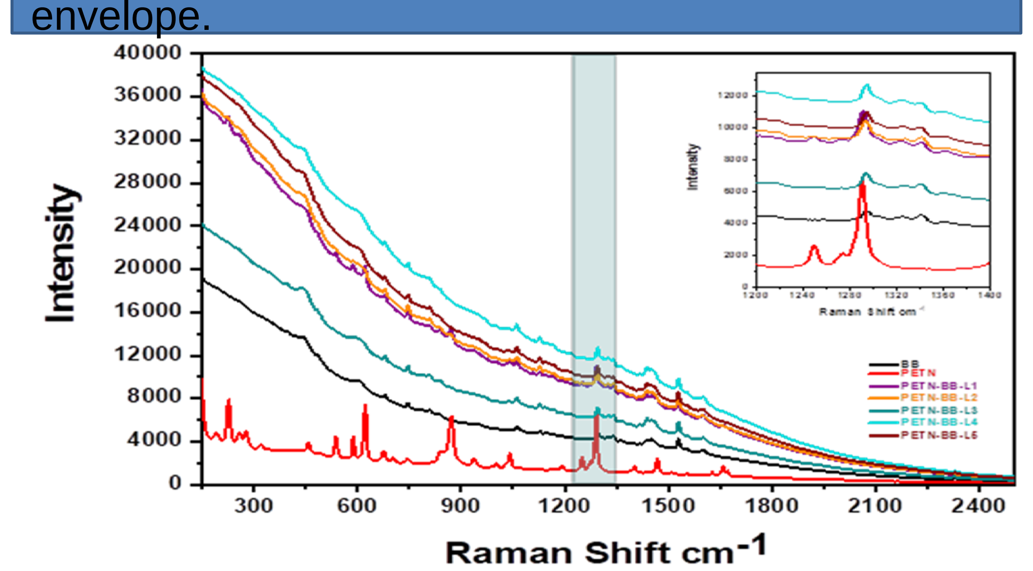


Figure 6: PETN with multiple layers of the BW mail envelope.

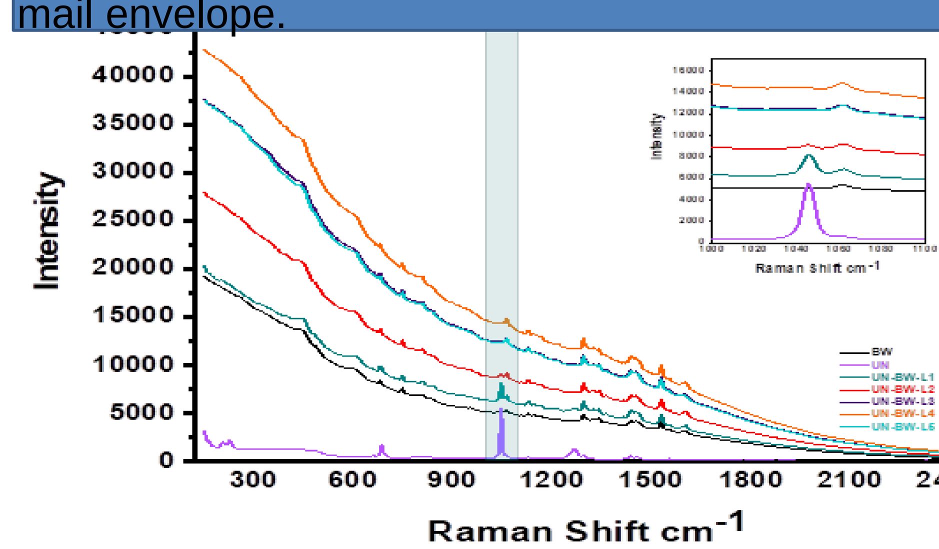


Figure 8: Urea Nitrate with multiple layers of the BW mail envelope.

Multivariate Analysis

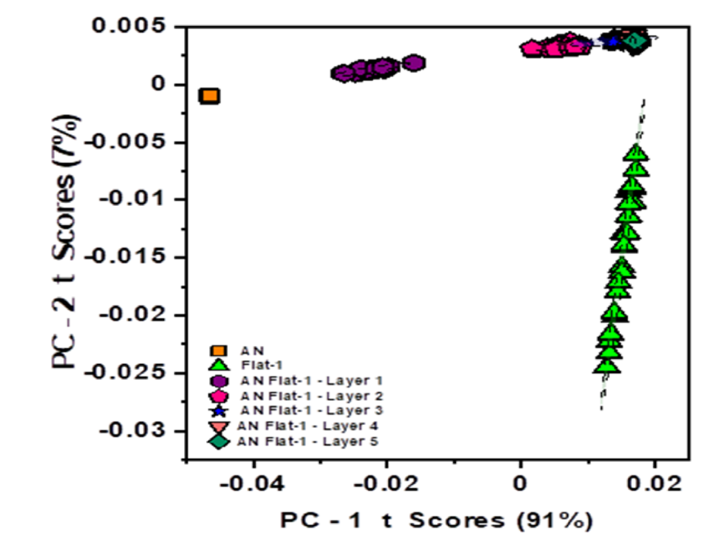


Figure 9: PCA score plot for AN in Flat-1 mail envelope for up to 5 layers.

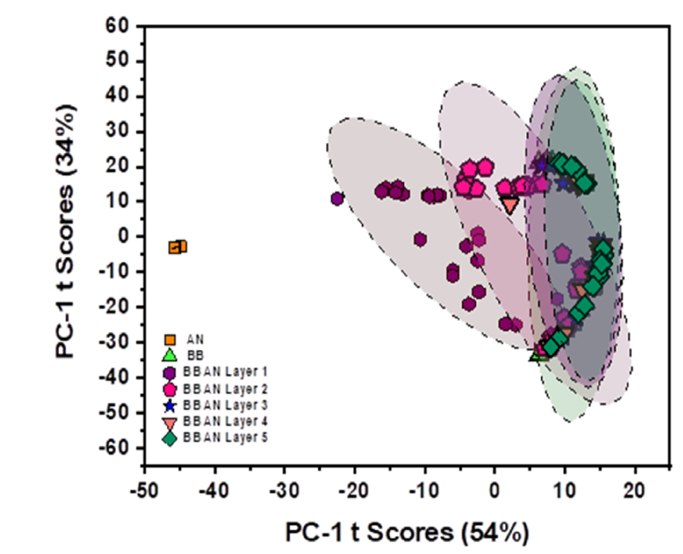


Figure 10: PCA score7 plot for AN in BW flat for one to 5 layers.

Table 1: Correlation of HEs with its corresponding loading PC

HEs	Substrate	PC-1 R^2	PC-2 R^2
AN	BW	0.55	$1.1x10^{-5}$
	Flat-1	0.61	$5.7x10^{-4}$
UN	BW	0.99	$5.5x10^{-4}$
	Flat-1	0.48	0.034
PETN	BW	$7.8x10^{-2}$	0.27
	Flat-1	0.92	0.037

Conclusions

- Results demonstrate the effectiveness of ST-RS in detecting HEs in mail flats.
- ST-RS enables detection with high penetration through opaque substrates, removes the need for sample preparation, is rapid and portable.

Future works

- Analysis of varying concentrations of HEs when mixed with other components and with one another to determine the limits of detection of the targets under these conditions.
- Analysis should also be done for several analytes (HEs) to build a library that facilitates the interpretation of results at the *in situ* analysis.

References