Scatr Series One Limit of Detection (LOD) Study

The Scatr Series One has scanned approximately 9000 street drug samples across multiple cities in Canada. To further refine its capabilities, we investigated the device's limit of detection (LOD) for fentanyl at lower concentrations when mixed with caffeine and D-mannitol, two of the most commonly detected fillers in street fentanyl samples. The Scatr Series One algorithm was assessed in its ability to detect fentanyl at varying concentrations, ranging from 10% to as low as 0.1%, in solid mixtures. The Scatr Series One was evaluated using two methods: quick scans, which are lower in resolution with a scan time of approximately 3 minutes, and standard scans, offering higher resolution with a scan time of about 8 minutes. Given the prevalence of caffeine and mannitol as cutting agents in illicit drug markets, this study closely mirrors the composition of typical street samples, making it a highly representative analysis for real-world applications. The results provide insight into the sensitivity and detection capabilities of the Series One device in identifying trace amounts of fentanyl in complex mixtures.

Methods

Sample Preparation

The preparation of the samples involved a systematic process to ensure accurate and homogeneous mixtures of fentanyl, caffeine, and mannitol. Six mixtures were created, each containing a different fentanyl concentration: 10%, 5%, 1%, 0.75%, 0.5%, and 0.1%. To maintain a total mass of 40 mg per sample, precise amounts of caffeine and mannitol were added to complement the fentanyl. For example, the 10% fentanyl mixture consisted of 4 mg of fentanyl, 18 mg of caffeine, and 18 mg of mannitol. For lower concentrations, sequential dilutions were performed by combining portions of higher concentration mixtures with additional caffeine and mannitol. The powders were thoroughly ground using a pestle and weighing paper, then mixed repeatedly by folding with a spatula until a uniform composition was achieved. Approximately 20 milligrams of each prepared mixture were then carefully transferred onto a 4 mm chip, which can hold up to 20 mg, ensuring proper sample coverage for analysis. Half of each batch was used for experimentation, while the remaining half was reserved for further dilutions or repeat analyses.

Table 1. Percentage of fentanyl and caffeine in two-component mixtures

Mixture	% Fentanyl	% Caffeine
A	10	90
B	5	95
C	1	99
D	0.75	99.25
E	0.5	99.5
F	0.1	99.9

Table 2. Percentage of fentanyl and caffeine in three-component mixtures

Mixture	% Fentanyl	% Caffeine	% D-Mannitol
A	10	45	45
B	5	45	50
C	1	45	54
D	0.75	45	54.25
E	0.5	45	54.5
F	0.1	45	54.9

Acquisition

Each sample was acquired first in quick-scan mode (total 147 pixels/map in three dimensions) and then standard mode (507 pixels/map in three dimensions).

Statistical Analysis

The Mann-Whitney U test was employed in this analysis to compare the Raman intensity distributions at the 1000 cm^{-1} peak between different fentanyl concentrations and the control sample of pure caffeine or mannitol. This non-parametric test is particularly suited for cases where the data does not follow a normal distribution, as was observed here. By ranking the intensity values, the Mann-Whitney U test assesses whether one sample distribution significantly differs from another, making it an ideal choice for comparing the intensity variations across multiple pixels without assuming equal variance or normality.

Results and Discussion

Two-component mixtures

The Scatr Series One machine learning model was assessed in its ability to detect both components of the fentanyl/caffeine mixtures on quick and standard three-dimensional scans. In the **quick** scans, which produced 147 spectra per map in three dimensions, the algorithm successfully detected fentanyl in the 10%, 5%, 0.5%, and 0.1% concentrations but failed to detect fentanyl in the 1% or 0.75% scans. Caffeine was detected in all quick scans. In the **standard** scans, which generated 507 spectra per map in three dimensions, the algorithm detected both fentanyl and caffeine in all cases (Table 3). There were no false positives in any scan. Since the peak at 1000 cm^{-1} is the most prominent peak in fentanyl, this peak was averaged in all pixels to generate an average peak intensity. When comparing the peak intensities of each map at the 1000 cm^{-1} peak, the average 1000 cm^{-1} peak was significantly different in each fentanyl-containing map compared to the averaged caffeine-only control (Figure 1). This was particularly notable since only a few pixels in the 0.1% to 1% maps would contribute to raising this average. In addition, the maximum peaks were substantially higher in fentanyl-containing maps than in the caffeine control map (colored dots in Figure 1). An enhanced view of the trace fentanyl maps (0.1% to 1%) is shown in Figure 2, demonstrating that the average 1000 cm^{-1} peak was significantly greater in these maps than in the caffeine control. There was no correlation between the average 1000 cm^{-1} peak intensity between the 0.1% and 1% maps, indicating that while detection was possible in these trace amounts, differentiating their quantification is unlikely to occur. However, there was a strong correlation between 1%, 5% and 10% fentanyl, indicating that the average 1000 cm^{-1} peak increases as the concentration of fentanyl increases when it is above 1%.

Table 3. Comparing the machine learning model's classification performance between quick and standard 3D scans of two-component mixtures. The algorithm successfully detected fentanyl at concentrations as low as 0.1% in standard scans. In contrast, quick scans struggled with detection below 5%.

Scan Type	% Fentanyl in Sample	Component Detected?	
		Fentanyl	Caffeine
Quick	**10%**	Detected	Detected
Standard		Detected	Detected
Quick	**5%**	Detected	Detected
Standard		Detected	Detected
Quick	**1%**	Not Detected	Detected
Standard		Detected	Detected
Quick	**0.75%**	Not Detected	Detected
Standard		Detected	Detected
Quick	**0.5%**	Detected	Detected
Standard		Detected	Detected
Quick	**0.1%**	Detected	Detected
Standard		Detected	Detected
Quick	**0% (pure caffeine)**	Not Detected	Detected
Standard		Not Detected	Detected

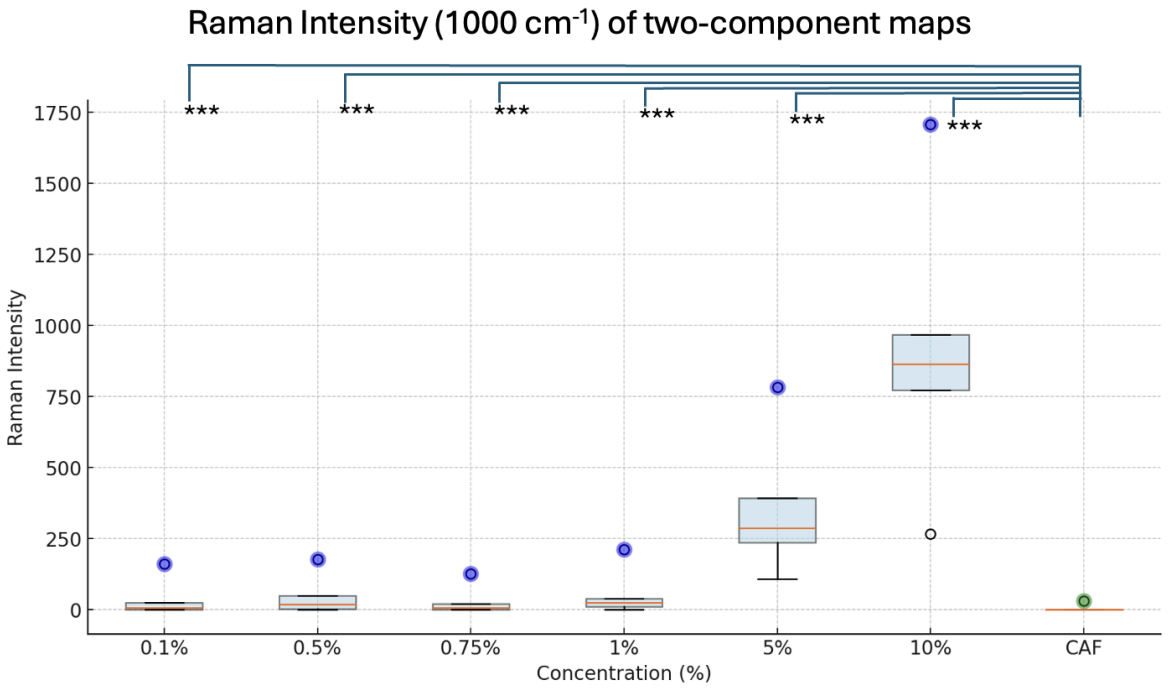

Figure 1. The mean intensity of the 1000 cm^{-1} peak, averaged across 507 spectra from each map of two-component mixtures, demonstrated that the maximum peak in fentanyl-containing mixtures (blue dots) was significantly higher than in pure caffeine (green dots). Additionally, the mean intensity of the 1000 cm^{-1} peak was consistently greater in all fentanyl-containing maps compared to pure caffeine. *** p<0.001

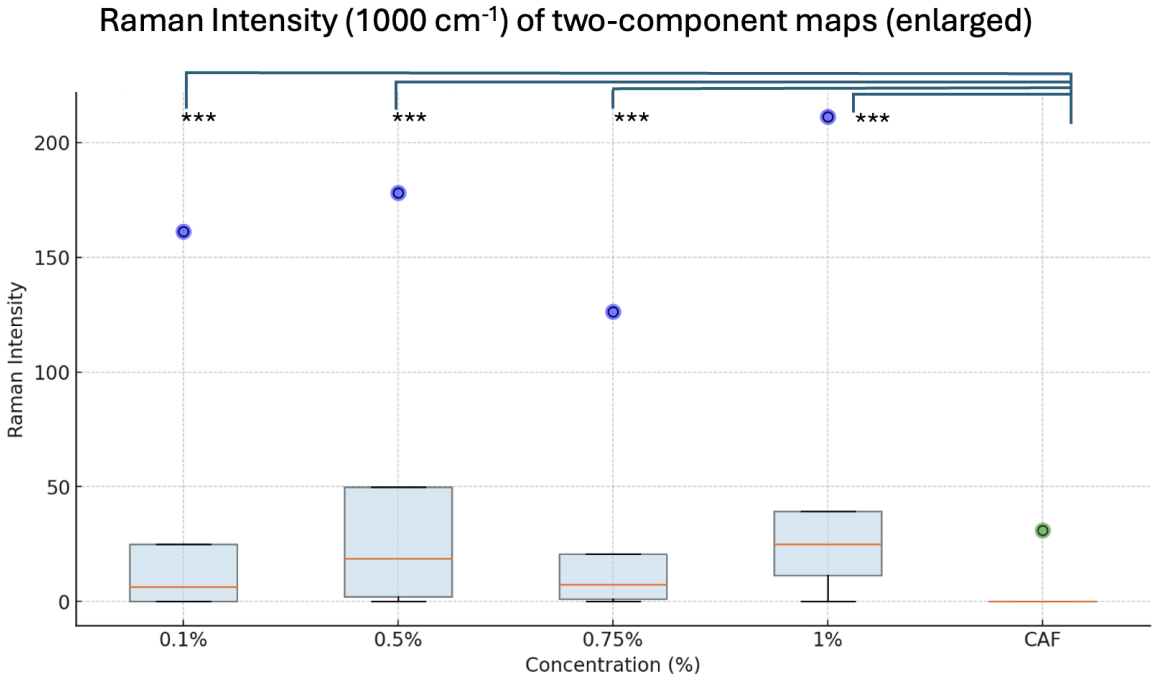

Figure 2. The mean intensity of the 1000 cm^{-1} peak, averaged over 507 spectra from each map for two-component mixtures, was analyzed, excluding the 5% and 10% mixtures to focus more closely on the lower concentration maps. The average intensity of the 1000 cm^{-1} peak was significantly higher in all maps containing fentanyl compared to those with pure caffeine. *** p<0.001

Three-component mixtures

The Scatr Series One machine learning model was assessed in its ability to detect three-component mixtures containing fentanyl, caffeine and D-mannitol on quick and standard three-dimensional scans. In the quick scans, which produced 147 spectra per map in three dimensions, the algorithm successfully detected fentanyl in the 10%, 5%, and 1% concentrations but failed to detect fentanyl in the 0.75%, 0.5%, or 0.1% scans. Caffeine was detected in all quick scans. In the standard scans, which generated 507 spectra per map in three dimensions, the algorithm detected both fentanyl and caffeine in all cases (Table 4). There were no false positives in any scan. Similar to the two-component mixtures, the 1000 cm^{-1} peak was averaged in all pixels to generate an average peak intensity. When comparing the peak intensities of each map at the 1000 cm^{-1} peak, the averaged 1000 cm^{-1} peak was significantly different in the 1%, 5%, and 10% maps, but not the 0.75%, 0.5%, or 0.1% maps (Figure 3). This was consistent with expectations since only a few pixels are not likely to contribute to the overall average, which contained 99% or more caffeine. In addition, the maximum peaks were substantially higher in all fentanyl-containing maps than in the caffeine control maps (colored dots in Figure 3). An enhanced view of the trace fentanyl maps (0.1% to 1%) is shown in Figure 2, which demonstrates that while the average peak intensity was not different between trace fentanyl-containing maps and controls, the maximum 1000 cm^{-1} peak was substantially greater in these maps than in any of the control maps.

Table 4. Comparing the machine learning model's classification performance between quick and standard 3D scans of three-component mixtures. The algorithm successfully detected fentanyl at concentrations as low as 0.1% in standard scans. In contrast, quick scans struggled with detection below 1%.

Scan Type	% Fentanyl in Sample	Component Detected?		
		Fentanyl	Caffeine	D-mannitol
Quick	10%	Detected	Detected	Detected
Standard		Detected	Detected	Detected
Quick	5%	Detected	Detected	Detected
Standard		Detected	Detected	Detected
Quick	1%	Detected	Detected	Detected
Standard		Detected	Detected	Detected
Quick	0.75%	Not Detected	Detected	Detected
Standard		Detected	Detected	Detected
Quick	0.5%	Not Detected	Detected	Detected
Standard		Detected	Detected	Detected
Quick	0.1%	Not Detected	Detected	Detected
Standard		Detected	Detected	Detected
Quick	0% (pure caffeine)	Not Detected	Detected	Not Detected
Standard		Not Detected	Detected	Not Detected
Quick	0% (pure D-mannitol)	Not Detected	Not Detected	Detected
Standard		Not Detected	Not Detected	Detected
Quick	0% (50/50 mixture, caffeine/ D-mannitol)	Not Detected	Detected	Detected
Standard		Not Detected	Detected	Detected

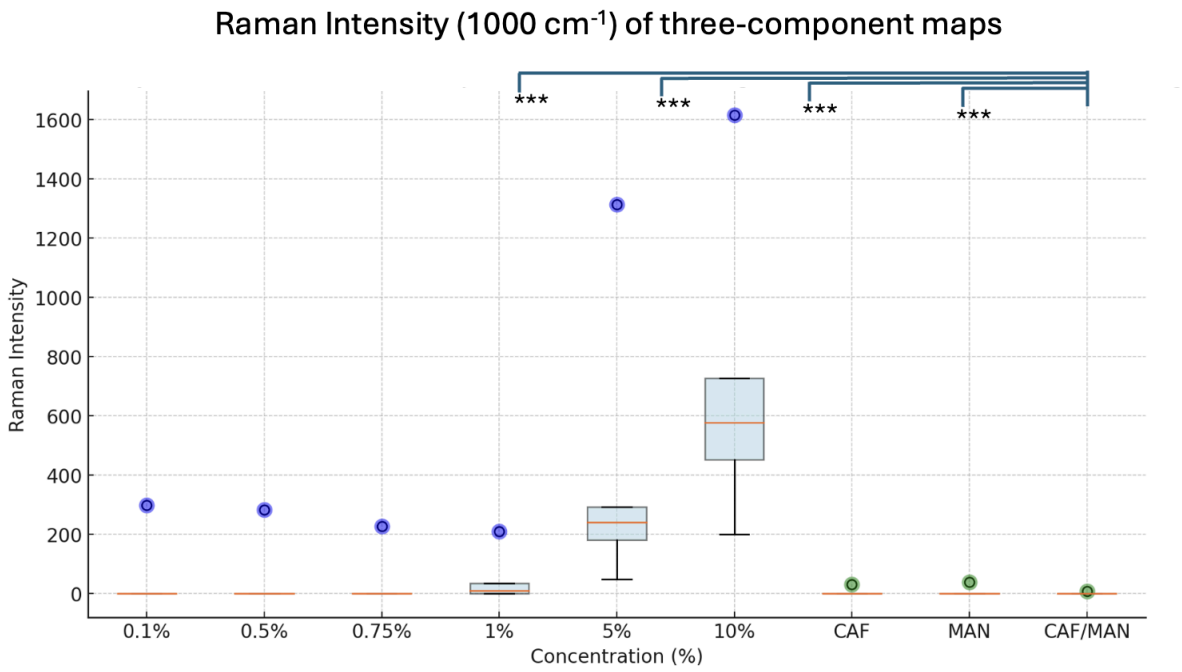

Figure 3. The mean intensity of the 1000 cm^{-1} peak, averaged across 507 spectra from each map of three-component mixtures, demonstrated that the maximum peak in fentanyl-containing mixtures (blue dots) was significantly higher than in pure caffeine, pure D-mannitol, or a 50/50 mixture of D-mannitol and caffeine (green dots). *** p<0.001

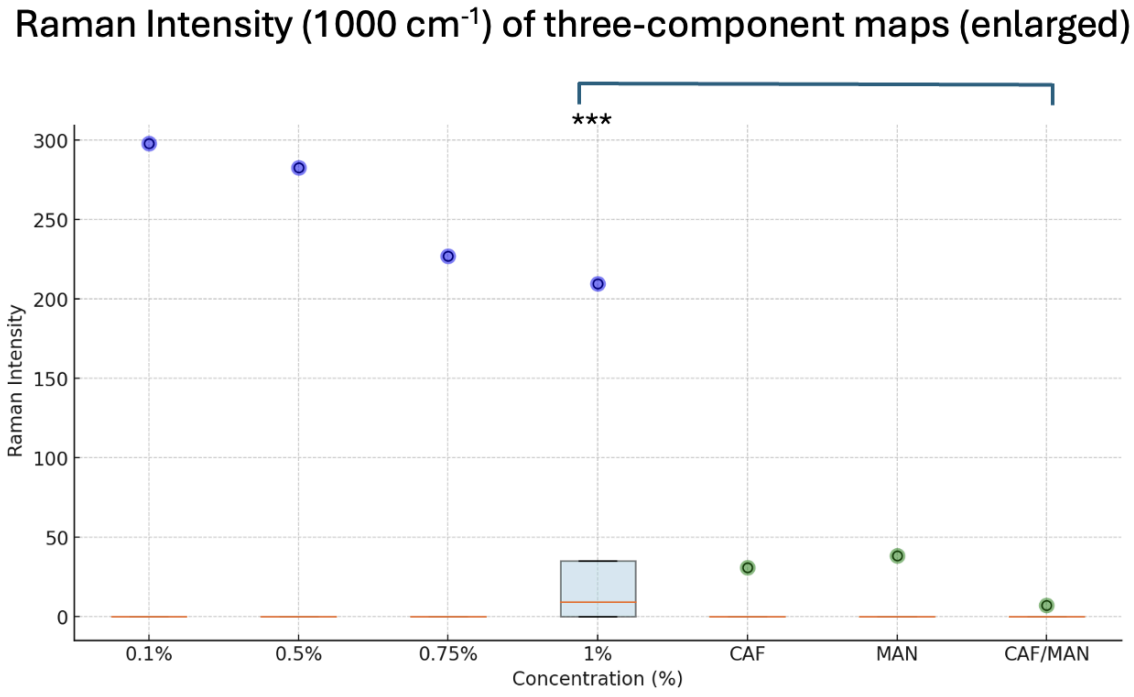

Figure 4. The mean intensity of the 1000 cm^{-1} peak, averaged over 507 spectra from each map for two-component mixtures, was analyzed, excluding the 5% and 10% mixtures to focus more closely on the lower concentration maps. The average intensity of the 1000 cm^{-1} peak was significantly higher in 1% fentanyl, 5% fentanyl, and 10% fentanyl compared to those with pure caffeine, pure D-mannitol, or a 50/50 mixture of D-mannitol and Caffeine. In addition, the maximum peak intensity was notably greater in all fentanyl-containing maps (blue dots) compared to any of the controls (green dots). *** p<0.001

Conclusion

This study aimed to identify the limits of detection of the Scatr Series One, both based on the algorithm alone and on the peak intensities of the most prominent fentanyl Raman peak.

Quick Scans

In two-component mixtures of fentanyl and caffeine, the limit of detection of fentanyl appears to be 5%. In three-component mixtures of fentanyl, caffeine and D-mannitol, the limit of detection appears to be 1%. Therefore, we can conclude that the limit of detection of fentanyl in mixtures of caffeine and fentanyl for quick scans is at least 5%.

Standard Scans

In two-component mixtures of fentanyl and caffeine, the limit of detection of fentanyl appears to be between 0.1% and 1%. In three-component mixtures of fentanyl, caffeine and D-mannitol, the limit of detection appears to be 0.1 and 1%. The algorithm detected fentanyl in all scans, including 0.1%, 0.5%, and 0.75%. However, a map's average 1000 cm^{-1} peak is a more replicable assessment of the detection limit. Since the average 1000 cm^{-1} peak only increased in 1%, 5% and 10% scans, we can conclude that the limit of detection of fentanyl in a standard scan of caffeine and/or mannitol is at least 1%.