B27 Portable Quadrupole-Based Gas Chromatography/Mass Spectrometer (GC/MS) Versus a GC/MS Benchtop System: An Analytical Comparison

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Learning Overview: After attending this presentation, attendees will understand the efficiency of a platform newly applied to the analysis of drugs of abuse and adulterants in seized material, the FLIR G510, a portable quadrupole-based gas chromatography/mass spectrometer, as compared to a regular benchtop gas chromatography/mass spectrometry (GC/MS) system.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by providing information about the accuracy and reliability of new methodologies used for on-site seized drug material screening.

Cutting agents, classified as diluents (pharmacologically inactive and readily available substances; e.g., sugars) and adulterants (pharmacologically active, more expensive and less available; e.g., phenacetin) are commonly used to increase profits and they are constantly changing over time, increasing the risks to the user's health caused by the compounds interactions. Knowledge about cutting agents is commonly neglected either because they are not detected or not reported. This leads to a lack of information that could be useful for management of acute intoxications in hospitals or criminal investigations, or in helping in the identification of routes of trafficking.

Seventy-five mock samples were prepared by an independent researcher at different concentrations and proportions of cocaine, heroin, methamphetamine, and adulterants. Samples were screened using FLIR G510 and confirmed by Agilent GCMS. FLIR G510 was operated on full scan acquisition ranged from 43 – 425 *m/z*. 1µL sample injection was introduced into the injection port at 250°C (splitless mode). Chromatographic separation was achieved using a low thermal mass DB-5 column bundle. The oven temperature ramped from 50°C to 300°C with a heating rate of 30°C/min and a final hold at 300°C for 4 min resulting in a 13.2 min chromatographic run. GCMS analysis were conducted using a Gas chromatograph model 6890N, coupled with a mass selective detector model 5975B operated in electron impact mode, using full scan acquisition in the range 40 – 550 *m/z*. Chromatographic separation was achieved using a DB-1 column. The chromatographic conditions were as follows: injection volume of 1 µL, splitless mode, injection and detection temperature of 265°C and 300°C, respectively. The oven program temperature was: 50°C to 340°C, heating rate of 30°C/min, and hold at 340°C for 2.33 min, resulting in a 12 min chromatographic run. FLIR G510 and GCMS qualitative results were compared to assess the reliability for detecting the presence of drugs. Analysis was performed using Receiver Operating Characteristic (ROC) analysis. True positive (TP) samples were screened and confirmed positive; true negative (TN) samples were negative in both screening and confirmatory assays; false positive (FP) samples were screened positive, but the target drug was not present at the confirmatory assay; and false negative (FN) samples screened negative but subsequently tested positive for the target drug by GCMS. Sensitivity, specificity, PPV (positive predictive value), NPV (negative predictive value) and accuracy, as well as the number of TP, TN, FP and FN samples analyzed by FLIR G510 and compared with GCMS results are shown in **Table 1** for all compounds.

Table1. Results in percentage of the FLIR G510 evaluation in comparison with GCMS for cocaine (COC), levamisole (LEV), benzocaine (BZC), theophylline (THP), phenacetin (PHN), hydroxyzine (HYDZ), diltiazem (DTZ), acetaminophen (ACT), caffeine (CAF), heroin (HER), fentanyl (FEN), strychnine (STYC), codeine (COD), morphine (MOR), thebaine (THB), methamphetamine (METH) and ephedrine (EPH).

FLIR G510 vs. GCMS (%)									
Drug	*TP*	*FN*	*FP*	*TN*	*Sensitivity*	*Specificity*	*Accuracy*	*PPV*	*NPV*
COC	25	-	-	50	100	100	100	100	100
LEV	-	2	-	73	-	100	97.3	-	97.3
BZC	9	-	-	66	100	100	100	100	100
THP	4	3	-	68	57.1	100	96	100	95.7
PHN	5	-	-	70	100	100	100	100	100
HYDZ	2	3	-	70	100	100	96	100	95.8
DTZ	1	3	-	71	25	100	96	100	95.9
ACT	10	1	-	64	90.9	100	98.6	100	98.4
CAF	19	-	-	56	100	100	100	100	100

HER	21	4	-	50	84	100	94.6	100	92.5
FEN	5	-	-	70	100	100	100	100	100
STYC	3	-	-	72	100	100	100	100	100
COD	8	3	-	64	72.7	100	96	100	95.5
MOR	3	-	3	69	100	95.8	96	50	100
THB	1	1	-	73	50	100	98.6	100	98.6
METH	24	1	-	50	96	100	98.6	100	98
EPH	6	-	-	69	100	100	100	100	100

The accuracy of a test refers to the degree of agreement between the screening test results and confirmatory test results. Accuracy values close to 100% are ideal, but in some situations a higher sensitivity or specificity are preferable. Sensitivity is directly affected by the number of FN as we can see on **Table 1**. THP, DTZ and THB sensitivities are low due to the proportion of FN detected for these substances. The PPV (which evaluate the confirmability of positive value) of MOR is low in comparison with the rest of the substances due to the FP cases detected for this specific substance. In general, accuracy values were at or close to 100% classifying the FLIR G510 as a suitable tool for field-based screening in seized material analysis.

Portable GC/MS, GC/MS, Seized Drugs