POLICE DEPARTMENT
CITY OF NEW YORK

May 6, 2021

From: Police Laboratory

To: District Attorney's Offices

Subject: **INFORMATION REGARDING REPEATED RETENTION TIME OF THE INTERNAL STARDARD VALUE**

The purpose of this memorandum is to provide clarifying information regarding a repeated value displayed on printed gas chromatography/mass spectrometry (GC/MS) data printouts. Included for reference to this memorandum are Figures 1 and 2, which are two styles of mass spectral data printouts that the Laboratory generated. For a period of time, a value was incorrectly repeated, but it has been determined that the incorrectly displayed values did not change the already reported results on the Controlled Substance Analysis Section reports.

The Laboratory identified that the numerical value displayed in the area labeled RtIs (retention time of the internal standard) under the SAMPLE DATA section of GC/MS mass spectral data printouts [See letter "A" in Figures 1 and 2] was displaying the same value from the RtIs of the STD DATA (standard data) section [See letter "B" in Figures 1 and 2]. After review, the Laboratory determined that this repeated value was a result of an incorrect line of code in the GC/MS software that regulated the printing of the mass spectral data printouts. This incorrect line of code was introduced into the software in the late fall of 2016. The amended line of code was put into effect on March 10, 2021. As such, this memorandum is relevant to mass spectral data printouts generated between late Fall 2016 through March 9, 2021.

The software is designed to obtain the retention time of the internal standard in both the standard data and sample data and compare both numbers to ensure that this information is within the laboratory's criteria. If the retention time criterion is fulfilled, the data will then be printed. If the retention time criterion is unsatisfactory, the printout will not be generated or printed. The coding for the retention time comparisons were reviewed and found to be working correctly during the time of the incorrect coding for printing.

The repeated RtIs value under the SAMPLE DATA section on the mass spectral data printout does not affect either the identification of the controlled substance depicted on each mass spectral data printout, nor the testing work results. The purpose of using an internal standard and monitoring its retention time is to ensure that a sample was introduced correctly into the GC/MS and as one of a variety of quality controls used to determine instrument maintenance needs. The misprinting did not impact the purposes of the internal standard. The internal standard is also not used to make conclusions or identifications about the controlled substances themselves. Controlled substances are identified by comparing both the mass spectral and retention time data of a sample to a known

standard of the controlled substance and that information was not affected. Therefore, the reported results on the laboratory reports are unaffected.

Although the use of an internal standard is not necessary to make identifications of controlled substances, there is a laboratory criterion associated with the retention time of the internal standard. The criterion is that the retention time of the internal standard in the sample must fall within +/- 0.1 minutes (6 seconds) of the retention time of the internal standard in the standard mixture run that day. While the numerical value for RtIs is included on mass spectral data printouts to conveniently evaluate the criterion, it is possible to evaluate and state that the criterion was met despite the misprint because:

- There are preventative measures in the software that prevents mass spectral data printouts from printing if certain criteria are not met including the criterion for the retention time of the internal standard. The coding for the preventative measures were reviewed and found to be working correctly during the time of the incorrect coding for printing. Therefore, if the retention time of the internal standard in the sample did not meet the criterion, the mass spectral data sheet would not have been printed.

- Analysts review the data using computer software and evaluate retention time on the screen; this is typically done as an overlay of chromatograms in which a +/- 0.1 minute shift (6 seconds) would be apparent. The analyst then generates a printed hardcopy representation of the electronic data (Figures 1 and 2).

In addition, the numerical listing of RtIs described above is only one area that depicts the retention time. All mass spectral data printouts include a graphical representation, shown as peaks plotted along a time axis, called a chromatogram [See the two boxes labeled "D" in Figures 1 and 2]. Some chromatograms also have a numerical labeling on the peak for retention time [See letters "C" in Figure 2].

The mass spectral data printouts are representations of the analytical data and are not electronically stored in that format. They are generated through processing of the analytical data which must be done each time a printout is needed. Therefore, mass spectral data printouts cannot be reprinted in the same manner that a text document could be reprinted. Reprocessing of the data to update the RtIs value of the sample will not guarantee that each reprocessing would produce the same values in all other areas of the mass spectral data printout due to analysts' selections and variations in software settings. The RtIs of the sample data falls within +/- 0.1 minutes of the value of the RtIs of the standard data [See letter "B" in Figures 1 and 2].

In summary, the incorrectly displayed RtIs of the sample data did not impact the reported results on laboratory reports or the purpose of the internal standard. It can be concluded that the criterion for the retention time of the internal standard was met based on the preventative measures and the evaluation of electronic data. The retention time is also presented in other ways on the mass spectral data printouts. Other than issuing this memorandum, no other action is deemed necessary at this time.
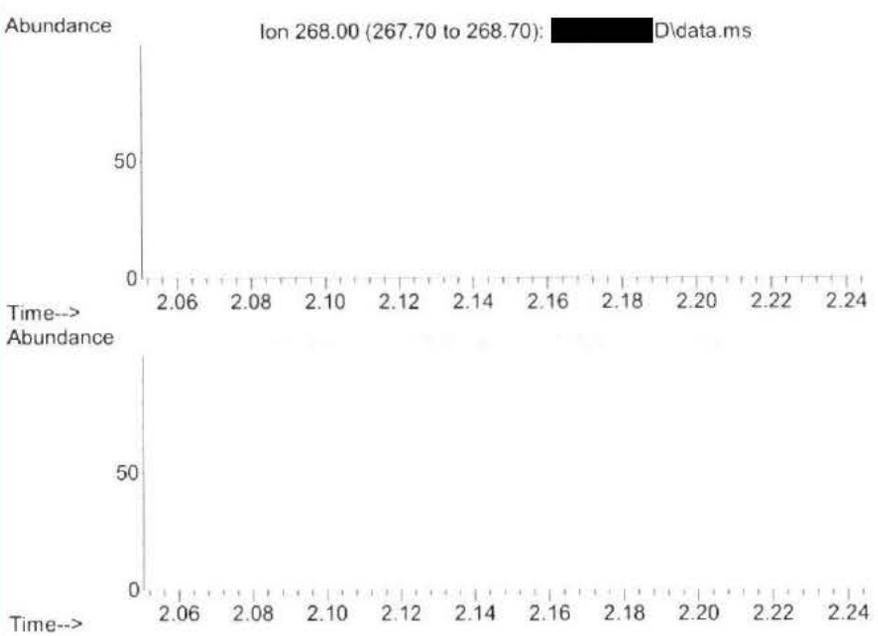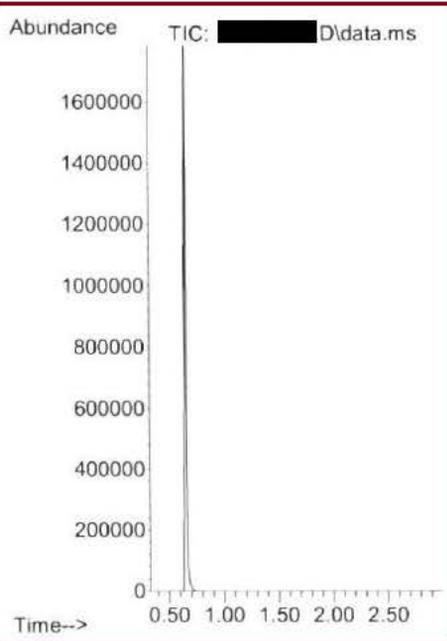
FIGURE 1

*********MASS SPECTRAL DATA*********
*****BLANK DATA*****
======================

Data File:C:\MassHunter\GCMS\1\data\032921\▬▬▬.D
Acquired:29 Mar 2021 18:58
Sample:▬▬▬
MiscInfo:▬▬▬

Analyst:▬▬▬
Instr:▬
Method:METHODA.M
Vial:▬

RtIs:0.655

*****STD DATA*****
====================

DataFile:C:\MassHunter\GCMS\1\data\032921\▬▬▬.D
RtStd:2.149   Name:CHECK MIXTURE   RtIs:0.654 **B**

Acquired:29 Mar 2021 05:24
LotStd:USPJ1G200

*****SAMPLE DATA*****
====================

Data File:C:\MassHunter\GCMS\1\data\032921\▬▬▬.D
Acquired:29 Mar 2021 19:03
Sample:▬▬▬
MiscInfo: N/A

RtIs:0.654 **A**

Analyst:▬▬▬
Instr:▬
Method:METHODA.M
Vial:▬

Scan 427 (2.149 min):▬▬▬D\data.ms (-422) (-)
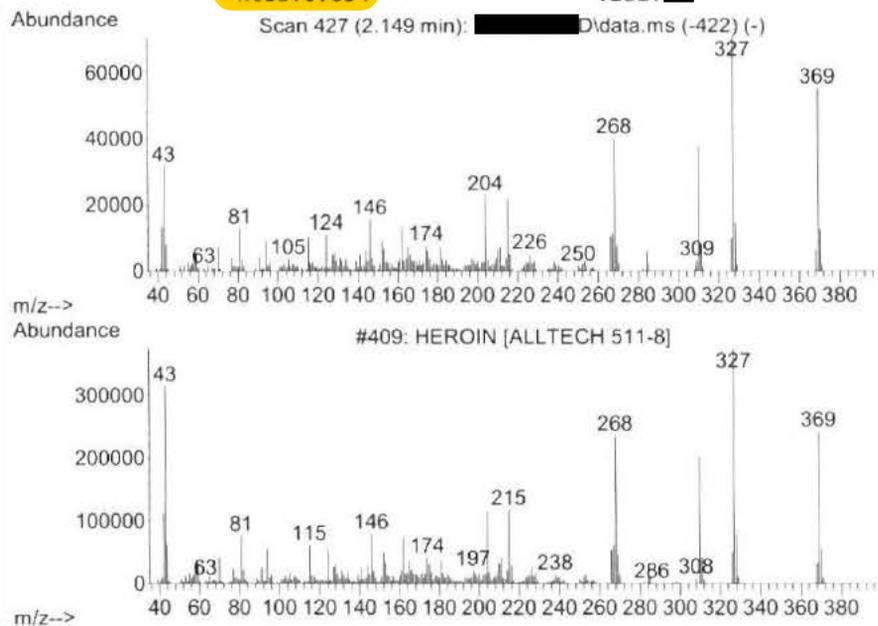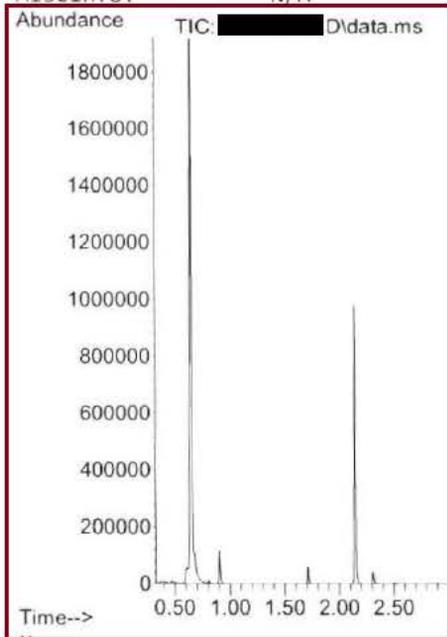
#409: HEROIN [ALLTECH 511-8]

Name
HEROIN
Library:C:\DATABASE\NYPD.L

M.W   Quality
369   99
LotRefSpec:ALLTECH 511-8

A: RT of Internal Standard in Sample
B: RT of Internal Standard in Check Mixture
D: Chromatograms

Analyst Initials:▬▬▬   Page ▬

GC-MS   Wed Mar 31 14:07:17 2021

FIGURE 2

**********MASS SPECTRAL DATA**********
*****BLANK DATA*****
=====================

Data File:C:\MassHunter\GCMS\1\data\040121 ███████.D   Analyst:███████
Acquired:01 Apr 2021 21:16   Instr:███
Sample ███████   Method:SCREENII.M
MiscInfo:███████   RtIs:7.239   Vial ███   **D**

Abundance   TIC:███████ D\data.ms   7.239 **C**
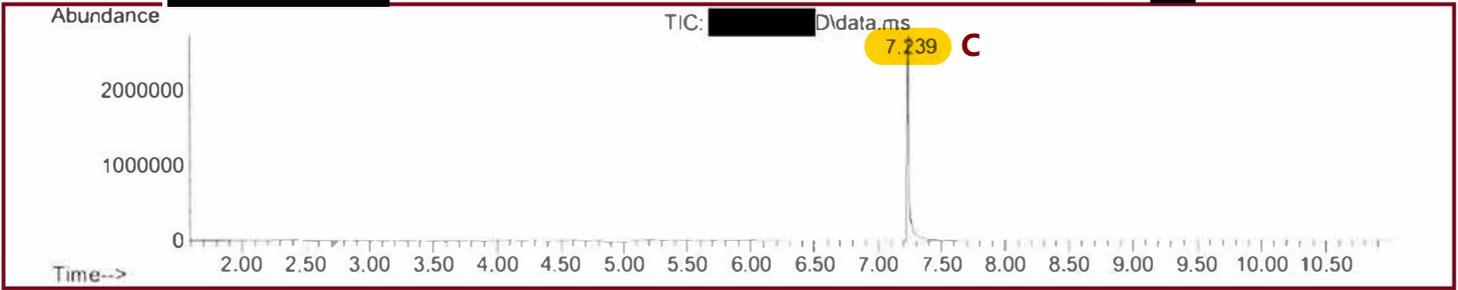
No Peaks Integrated

*****STD DATA*****
=====================

DataFile:C:\MassHunter\GCMS\1\data\040121 ███████.D   Acquired:01 Apr 2021 03:44
RtStd:3.142   Name:COCKTAIL II   RtIs:7.239 **B**   LotStd:031021A286IVS

*****SAMPLE DATA*****
=====================

Data File:C:\MassHunter\GCMS\1\data\040121 ███████.D   Analyst:███████
Acquired:01 Apr 2021 21:31   Instr:███
Sample ███████   Method:SCREENII.M
MiscInfo:10MG/10ML CHCL3 BE   RtIs:7.239 **A**   Vial:███   **D**

Abundance   TIC:███████ D\data.ms   7.241 **C**   3.133 **C**

Scan 361 (3.133 min):███████ D\data.ms (-352) (-)
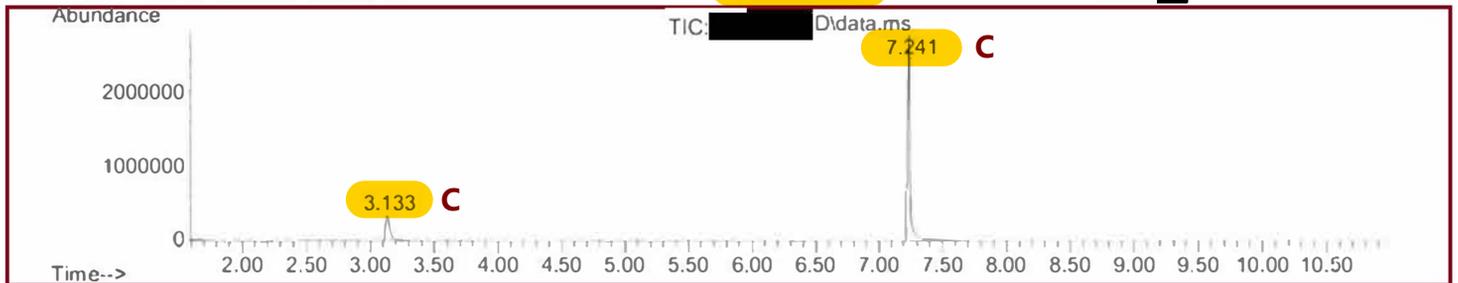
#16: Methamphetamine[SIGMA 127H0320-1]
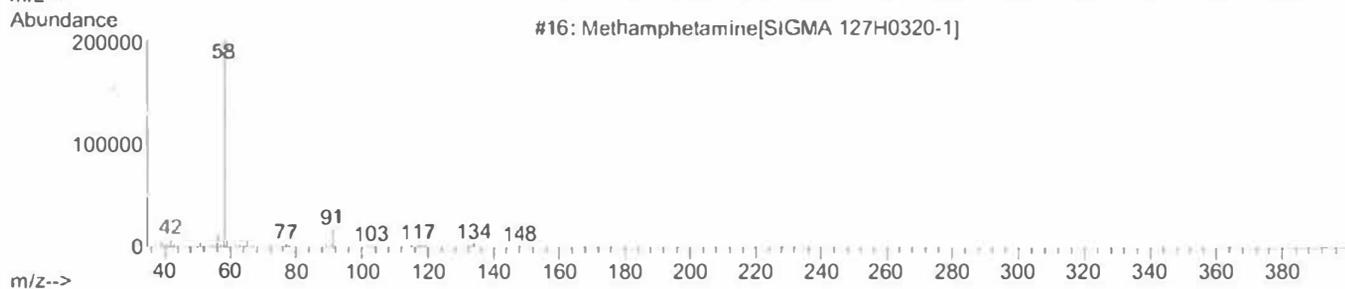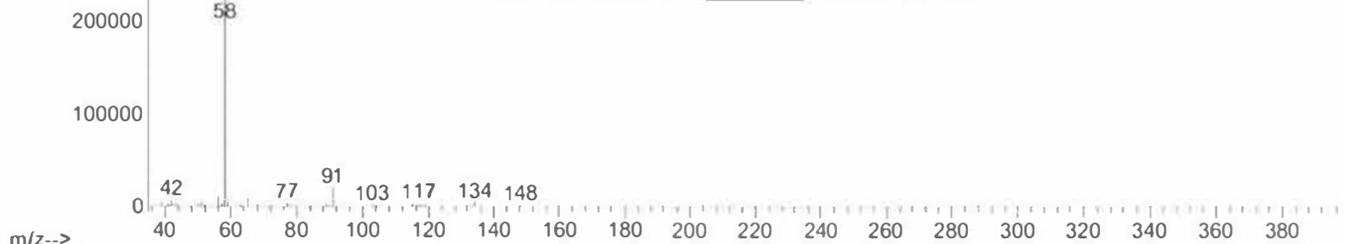
Name	M.W	Quality
Methamphetamine	149	90
Library:C:\DATABASE\NYPD.L	LotRefSpec:SIGMA 127H0320-1	

A: RT of Internal Standard in Sample
B: RT of Internal Standard in Standard
C: RT Label on Integrated Peak
D: Chromatograms

Inst Monitor Initials:███████   Analyst Initials:███████   Page 16

GC-MS   Fri Apr 02 07:19:21 2021