

TBI-FORENSIC SERVICES DIVISION PERFORMANCE VERIFICATION FORM

Instrument/Method to Verify:

Check the appropriate box: New Validation Modification Performance Check

Laboratory: NCL KCL MCL Unit: _____

Based on training and competency, the following analyst(s) are authorized by the Technical Leader to participate in this study:

Name _____ Title _____ Initials _____

Completed: Signature/Date _____

Name _____ Title _____ Initials _____

Completed: Signature/Date _____

Name _____ Title _____ Initials _____

Completed: Signature/Date _____

Verification of final review:

Unit Supervisor/Date _____

Unit Supervisor/Date _____

Unit Supervisor/Date _____

Crime Laboratory Regional Supervisor/Date _____

Crime Laboratory Regional Supervisor/Date _____

Crime Laboratory Regional Supervisor/Date _____

Quality Assurance Manager/Date _____

By signing below, I have verified this study meets all requirements and I deem this procedure/instrument fit for the intended use:

Technical Leader/Date _____

All information must be submitted to the Quality Assurance Manager prior to the implementation of the procedure/instrument. If applicable, include training plan and competency testing schedule.

Forensic Chemistry Performance Verification

**Nicolet iS20 FTIR with Smart iTX ATR attachment and Golden Gate ATR
attachment (SN: BEP2310112/ SN#Z100784)
TBI FCU ID- COCO**

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COCO

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Forensic Chemistry Performance Verification

Nicolet iS20 FTIR with Smart iTX ATR attachment and Golden Gate ATR attachment (SN: BEP2310112/ SN#Z100784) TBI FCU ID- COCO

1. Purpose:

Each Fourier-transform infrared (FTIR) spectrometer acquired by the TBI FCU must demonstrate that it will accurately reproduce spectra previously obtained within the laboratory. The TBI FCU currently uses Attenuated Total Reflectance (ATR) attachments since this technique is efficient and does not destroy the sample during analysis.

Although properly maintained instruments all adhere to the theories of FTIR, unique factors may exist within each system that can generate slightly different spectra between different instruments.

This instrument differs from the previous models of FTIR spectrometers (Nicolet iS10) used in the laboratory in that it uses a solid-state diode laser instead of the traditional Helium/Neon laser to track the position of the moving mirror in the interferometer.

The Smart iTX ATR attachment also differs from its predecessors (Golden Gate and Smart iTR) because it uses a monolithic diamond crystal that provides the benefits of traditional diamond crystal without the need for ZnSe lenses.

This performance verification will assess the following:

- The spectrometer's ability to generate accurate spectra of certified reference standards compared to previously run laboratory standard spectra using the Smart iTX accessory
- The ability to use the Golden Gate accessory as a primary ATR accessory for both future FTIR acquisitions and for serving as a potential back-up in the event of an attachment failure

Forensic Chemistry Performance Verification

Nicolet iS20 FTIR with Smart iTX ATR attachment and Golden Gate ATR attachment (SN: BEP2310112/ SN#Z100784) TBI FCU ID- COCO

2. Components and Experiment Setup:

<i>Instrument Components</i>	
iS20 FTIR	Smart iTX attachment
Source: Single point	Crystal plate type Monolithic Diamond
Beam splitter KBr/Ge coated	Verification Standard Polystyrene "lollipop"
Laser Type Solid-state Diode	
Detector DTGS KBr	
Internal Verification Polystyrene/NG Glass	
Standard Wheel	
Experiment parameters	
Scans	16
Resolution	4
Spectral Range	4000-600 (iTX) and Golden Gate
Gain	Auto
Optical Velocity	0.4747
Aperture	Medium Resolution

Golden Gate State of TN ID # K37255 was used since this attachment had been in service recently.

3. Procedure:

Ten certified reference standards were tested on this instrument using the Smart iTX attachment and Golden Gate attachment. Several of these standards were selected because they are frequently encountered in case work. Both salt forms of cocaine were tested to determine if salt forms could be determined. Non-controlled substances were also tested to determine if the spectrometer could detect possible adulterants. Out of these ten, five standards were tested using the Smart iTX attachment and five standards were tested using the Golden Gate attachment.

Prior to running these standards, the routine monthly maintenance as outlined in TBI SOP was performed to ensure the instrument was operating according to acceptable standards. Additionally, laser alignment is recommended every two months by the manufacturer since a slight drift in output is possible. In this performance check, the laser verification was performed each time.

Forensic Chemistry Performance Verification

Nicolet iS20 FTIR with Smart iTX ATR attachment and Golden Gate ATR attachment (SN: BEP2310112/ SN#Z100784) TBI FCU ID- COCO

All standards were run in their pure form - no extractions, washes, or other alterations were performed. If available, the same chemical lots utilized to create the FCU ATR spectral library were used. Prior to each standard run, the instrument's sampling area was cleaned, and a background spectrum was collected to ensure no cross-contamination occurred.

4. Standards Used:

Standard	Source	Lot Number
Aspirin*	Cayman	0479934-17
Alprazolam	Sigma	117K4017
Caffeine	Acros Organics	A0237979
Carisoprodol	Cayman	0588428-4
Cocaine base*	Sigma	69H1240
Cocaine HCl*	Sigma	59H0640
Diazepam	Sigma	105F0451
Methamphetamine*	Sigma	071K1580
3,4-MDMA*	Sigma	016K4088
Oxycodone	Sigma	085K1833

*These standards were used for performance checking the Golden Gate attachment.

5. Results and Conclusions

Spectra for the ten standards generated by COCO were compared to library standard spectra. Results from COCO using both the iTX and Golden Gate attachments were consistent with and matched the library spectra satisfactorily for identification.

During the test, the sample gain for all the iTX data was at 4.0, and the Oxycodone standard with the Golden Gate was set at 4.0. For the rest of the Golden Gate data, the sample gain was 8.0. All the data was consistent with the library standards, and this difference did not affect the identification of the sample.

All data generated for the iS20 using the iTX attachment can be found in Appendix A. Golden Gate data can be found in Appendix B.

Forensic Chemistry Performance Verification

**Nicolet iS20 FTIR with Smart iTX ATR attachment and Golden Gate ATR
attachment (SN: BEP2310112/ SN#Z100784)
TBI FCU ID- COCO**

The ValPro Qualification reports outlined in the Procedure section as well as the current maintenance log are in Appendix C. The factory validation performed was also included within this appendix.

The laser monitoring requirement will be incorporated into the monthly maintenance to ensure the laser is verified regularly.

In summary, this instrument has demonstrated satisfactory results for use within the TBI FCU. The operation is the same as the unit's other ATRs. Therefore, no additional training requirements will be needed for currently trained scientists.

Training for monthly maintenance requirements will be conducted according the user manual for the iS10 and iS20 instruments located in ensur.

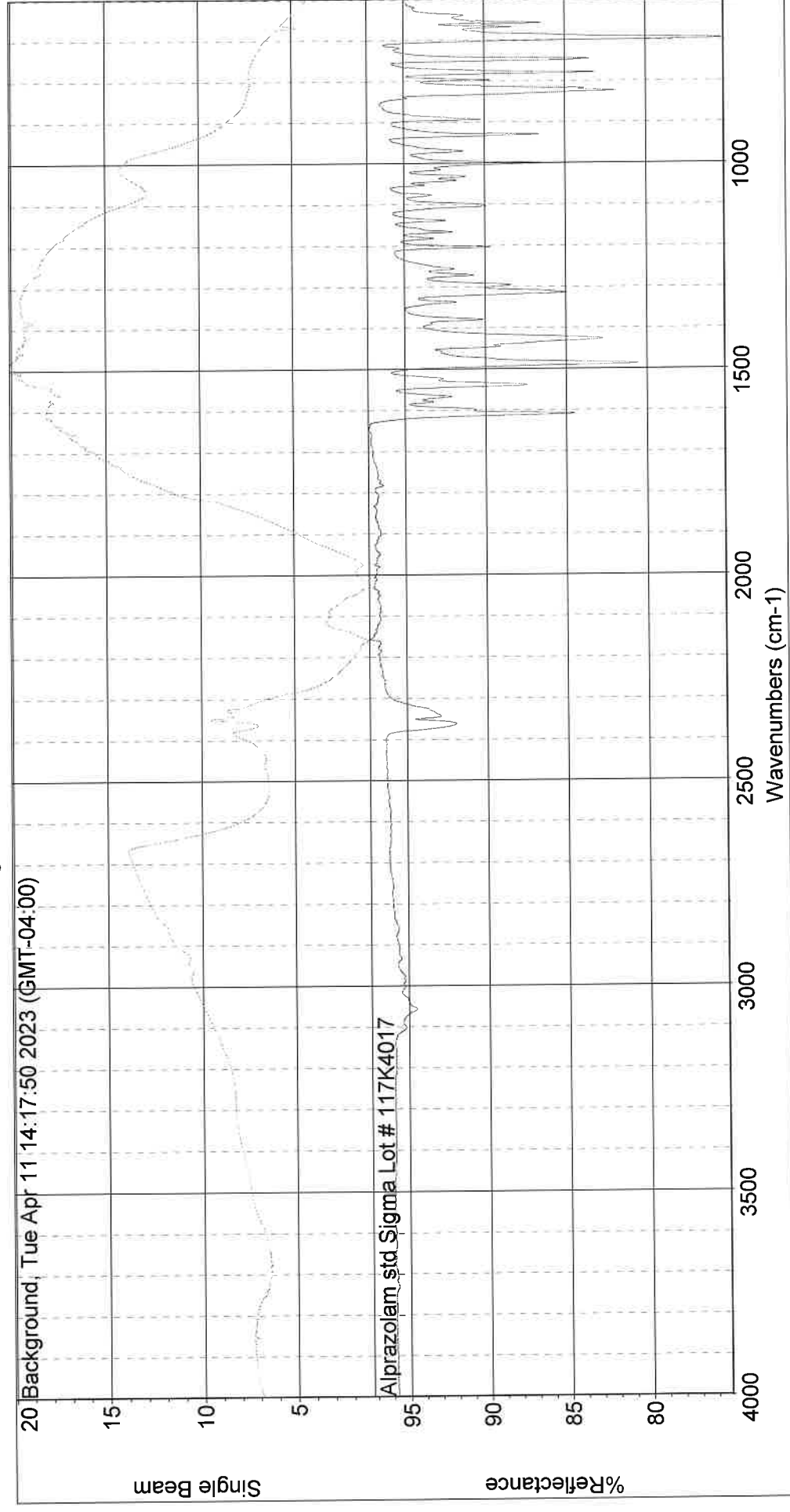
Forensic Chemistry Performance Verification

**Nicolet iS20 FTIR with Smart iTX ATR attachment and Golden Gate ATR
attachment (SN: BEP2310112/ SN#Z100784)
TBI FCU ID- COCO**

Appendix A-ATR data from Smart iTX

TBI Knoxville Crime Laboratory

Collection time: Tue Apr 11 14:19:48 2023 (GMT-04:00)



ATR - COCO

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 4.0
Optical velocity: 0.4747
Aperture: 80.00

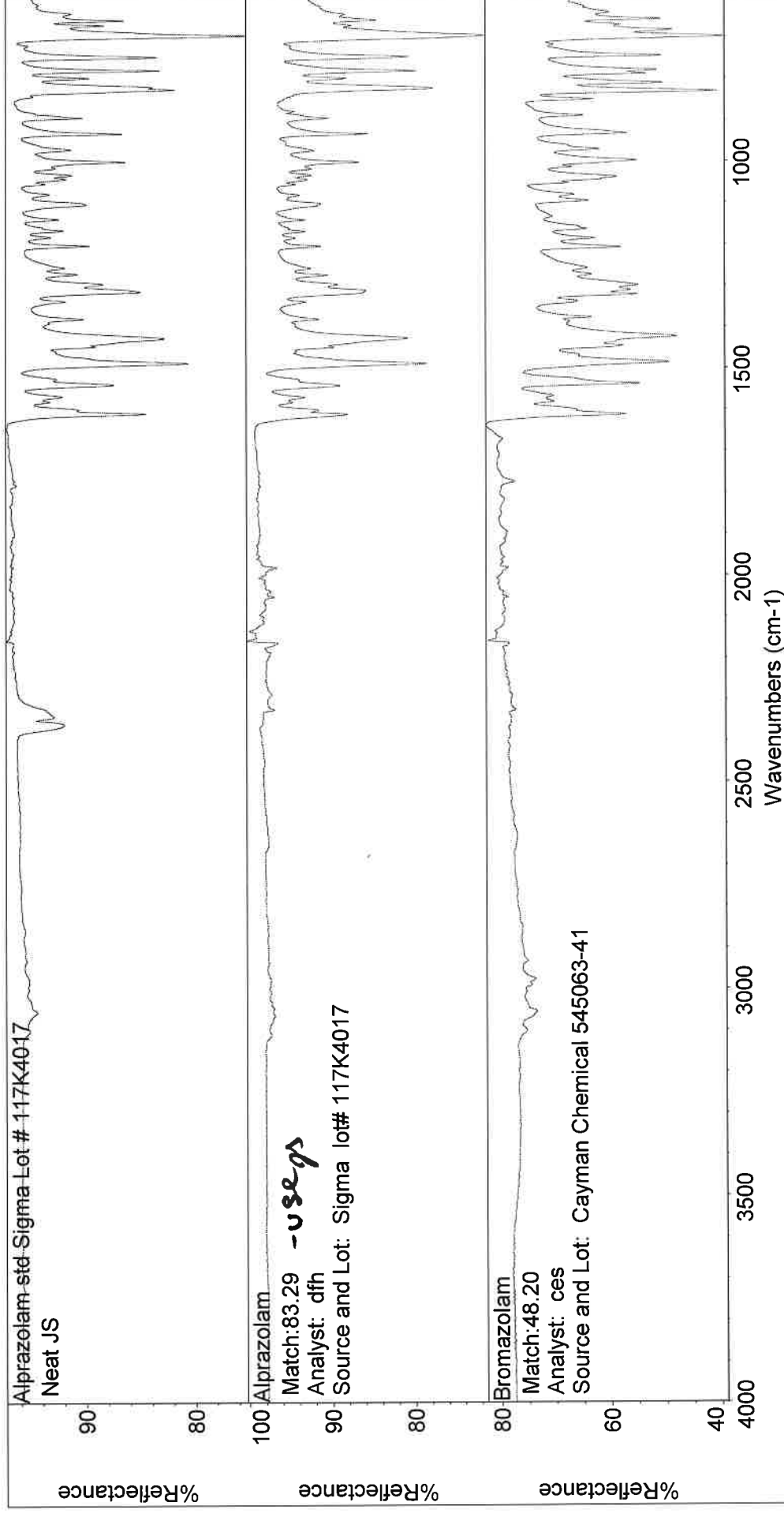


Alprazolam std Sigma Lot # 117K4017

Neat JS

TBI Knoxville Crime Laboratory

Collection time: Tue Apr 11 14:19:48 2023 (GMT-04:00)



ATR - COCO

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 4.0
Optical velocity: 0.4747
Aperture: 80.00

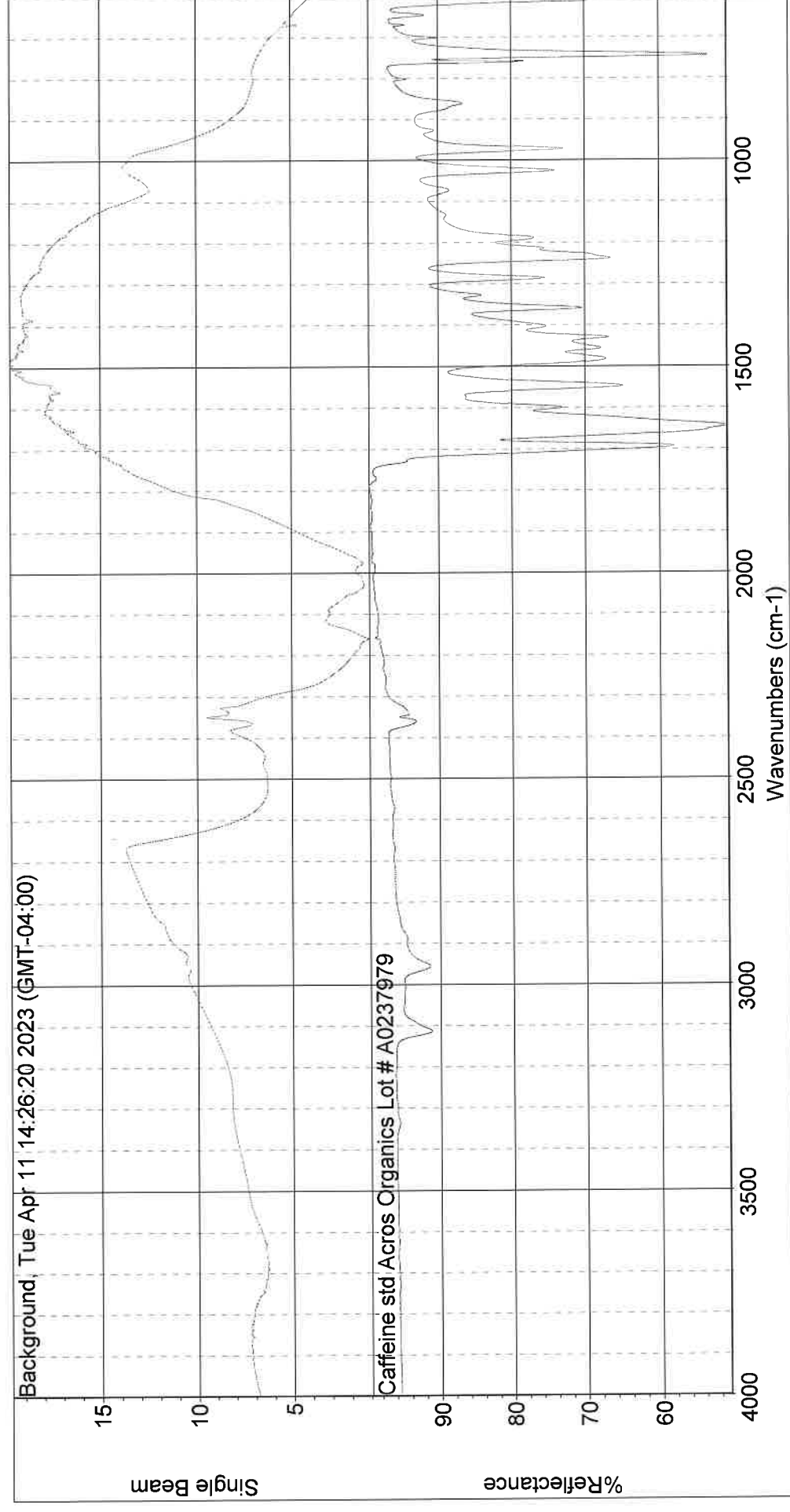


Alprazolam std Sigma Lot # 117K4017

Neat JS

TBI Knoxville Crime Laboratory

Collection time: Tue Apr 11 14:28:33 2023 (GMT-04:00)



ATR - COCO

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 4.0
Optical velocity: 0.4747
Aperture: 80.00

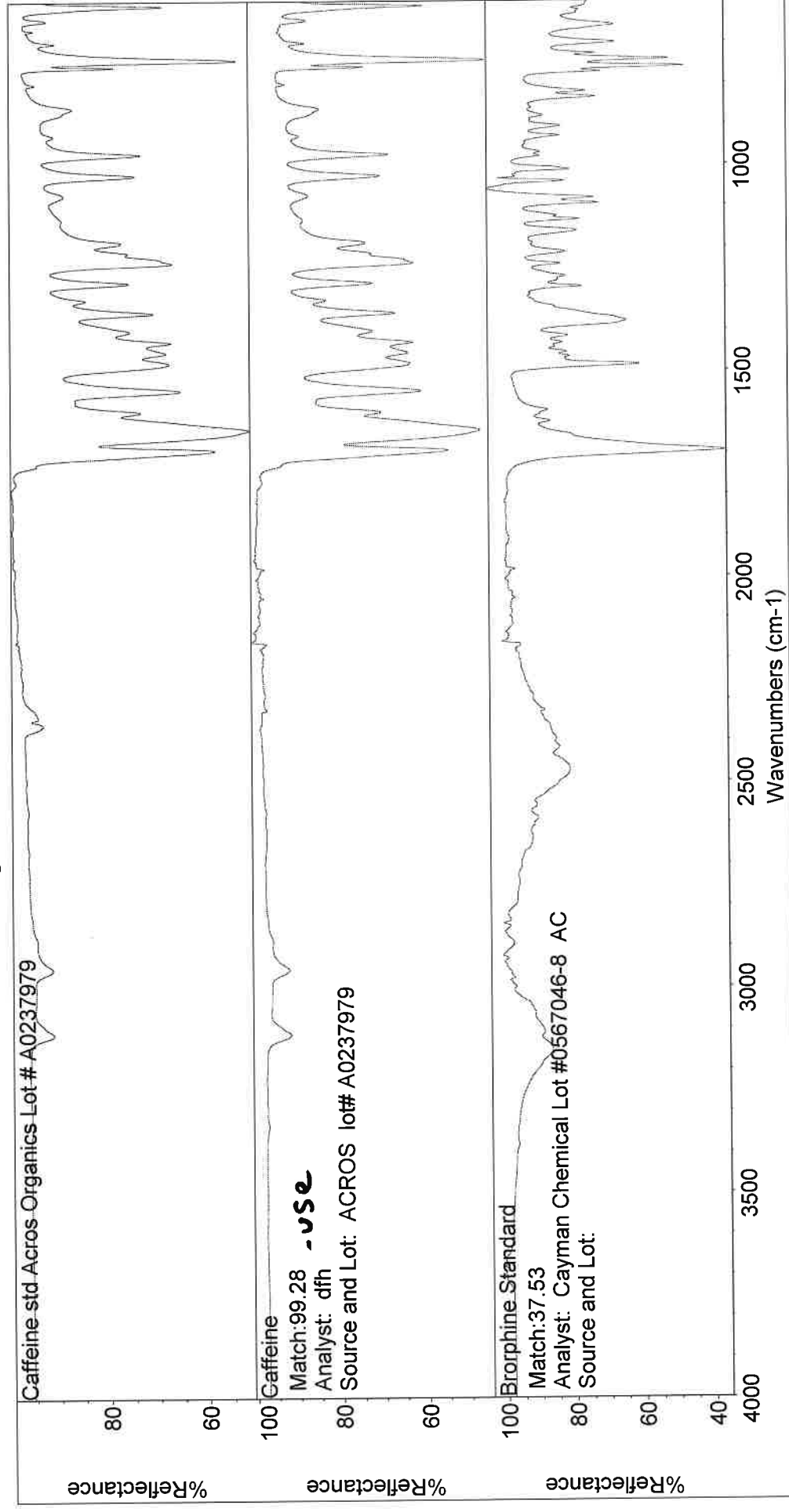


Caffeine std Across Organics Lot # A0237979

Neat JS

TBI Knoxville Crime Laboratory

Collection time: Tue Apr 11 14:28:33 2023 (GMT-04:00)



ATR - COCO

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 4.0
Optical velocity: 0.4747
Aperture: 80.00

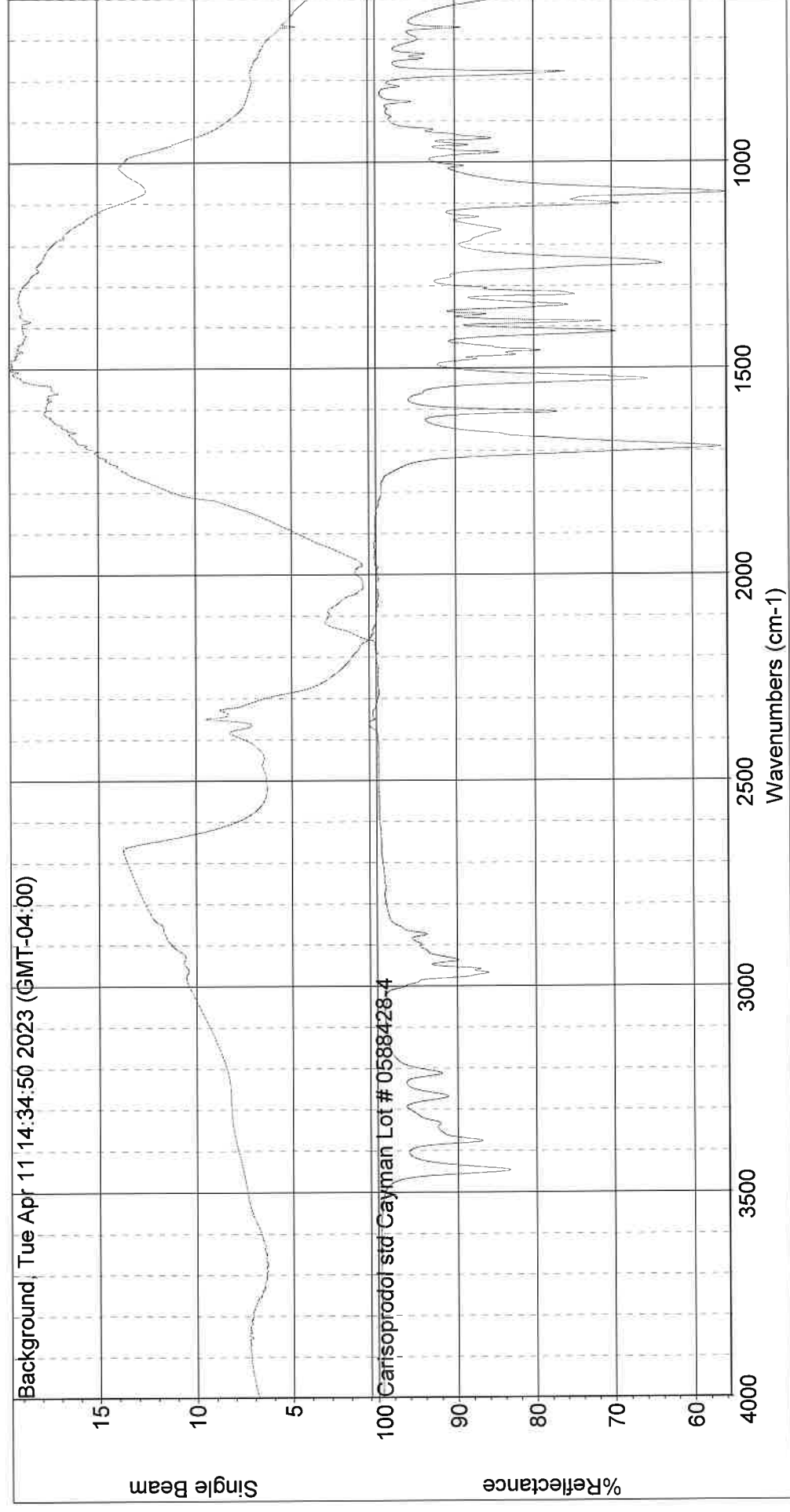


Caffeine std Acros Organics Lot # A0237979

next ps

TBI Knoxville Crime Laboratory

Collection time: Tue Apr 11 14:37:17 2023 (GMT-04:00)



ATR - COCO

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 4.0
Optical velocity: 0.4747
Aperture: 80.00

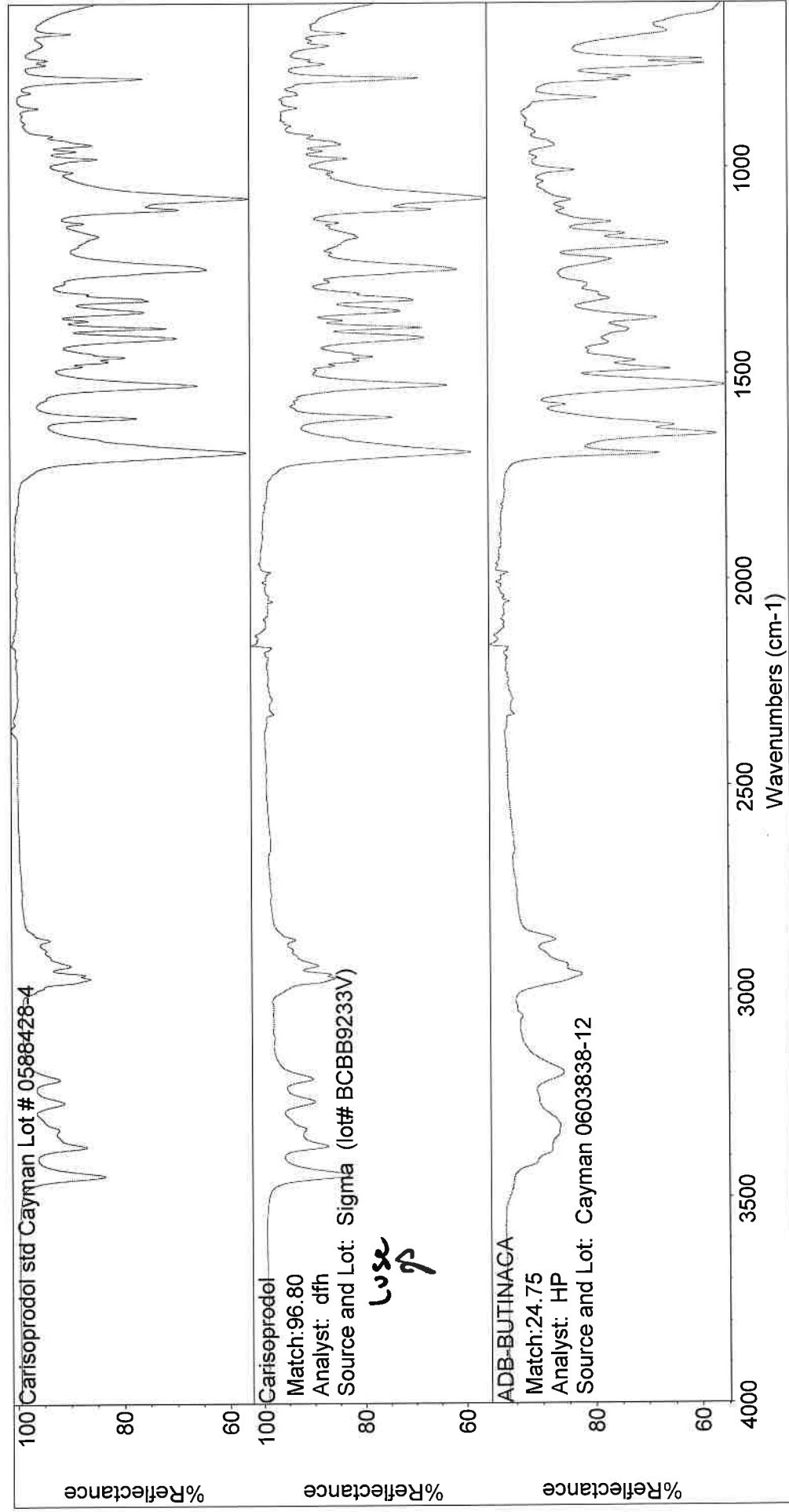


Carisoprodol std Cayman Lot # 0588428-4

Neat JS

TBI Knoxville Crime Laboratory

Collection time: Tue Apr 11 14:37:17 2023 (GMT-04:00)



ATR - COCO

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 4.0
Optical velocity: 0.4747
Aperture: 80.00

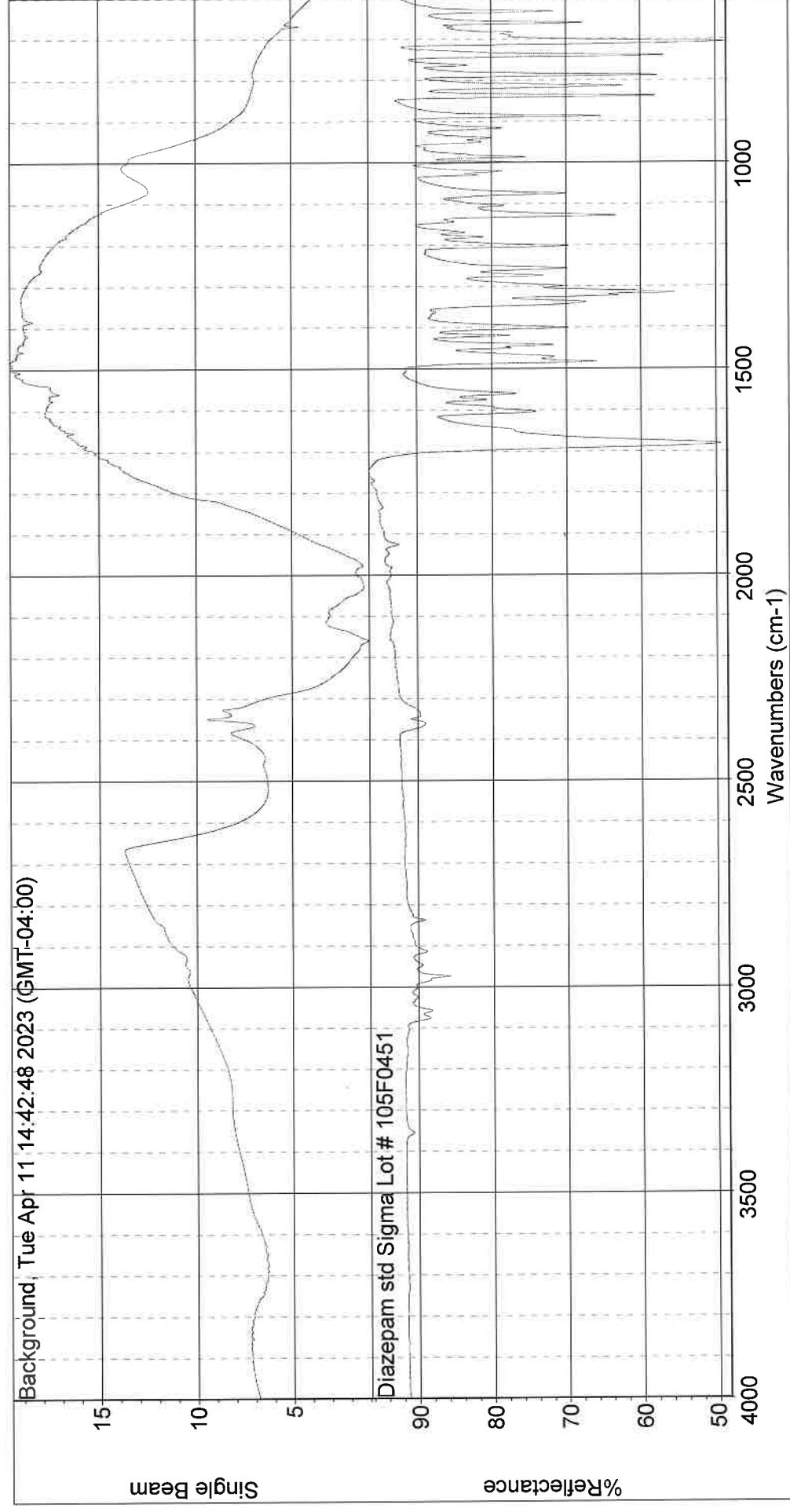
Carisoprodol std Cayman Lot # 0588428-4



gs
dfh
Next
gs

TBI Knoxville Crime Laboratory

Collection time: Tue Apr 11 14:44:45 2023 (GMT-04:00)



ATR - COCO

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 4.0
Optical velocity: 0.4747
Aperture: 80.00

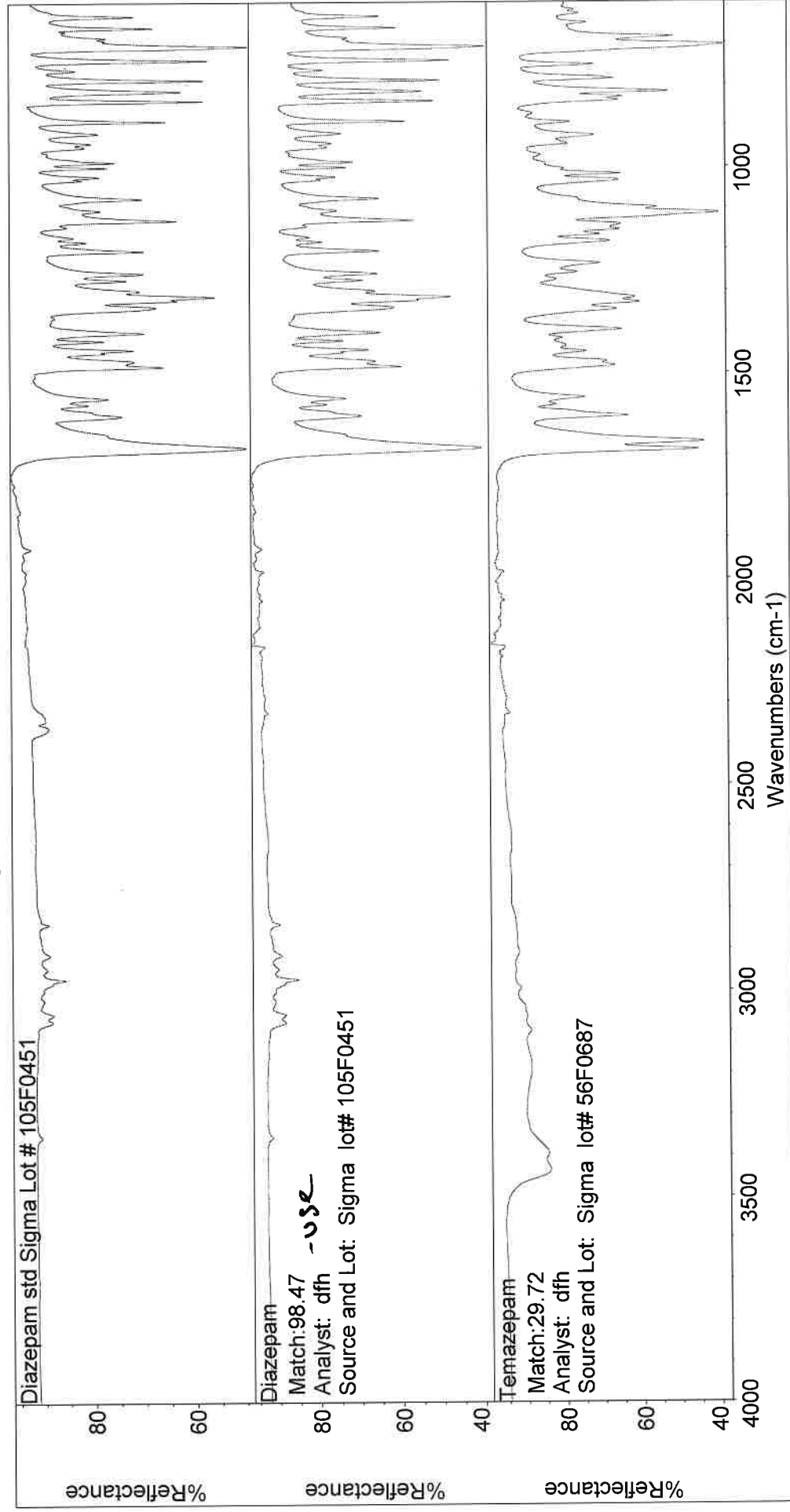


Diazepam std Sigma Lot # 105F0451

Neat JS

TBI Knoxville Crime Laboratory

Collection time: Tue Apr 11 14:44:45 2023 (GMT-04:00)



ATR - COCO

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 4.0
Optical velocity: 0.4747
Aperture: 80.00



Diazepam std Sigma Lot # 105F0451

Neat JS

Forensic Chemistry Performance Verification

**Nicolet iS20 FTIR with Smart iTX ATR attachment and Golden Gate ATR
attachment (SN: BEP2310112/ SN#Z100784)
TBI FCU ID- COCO**

Appendix B -ATR data from Golden Gate TN ID # K37255 attachment used on COCO

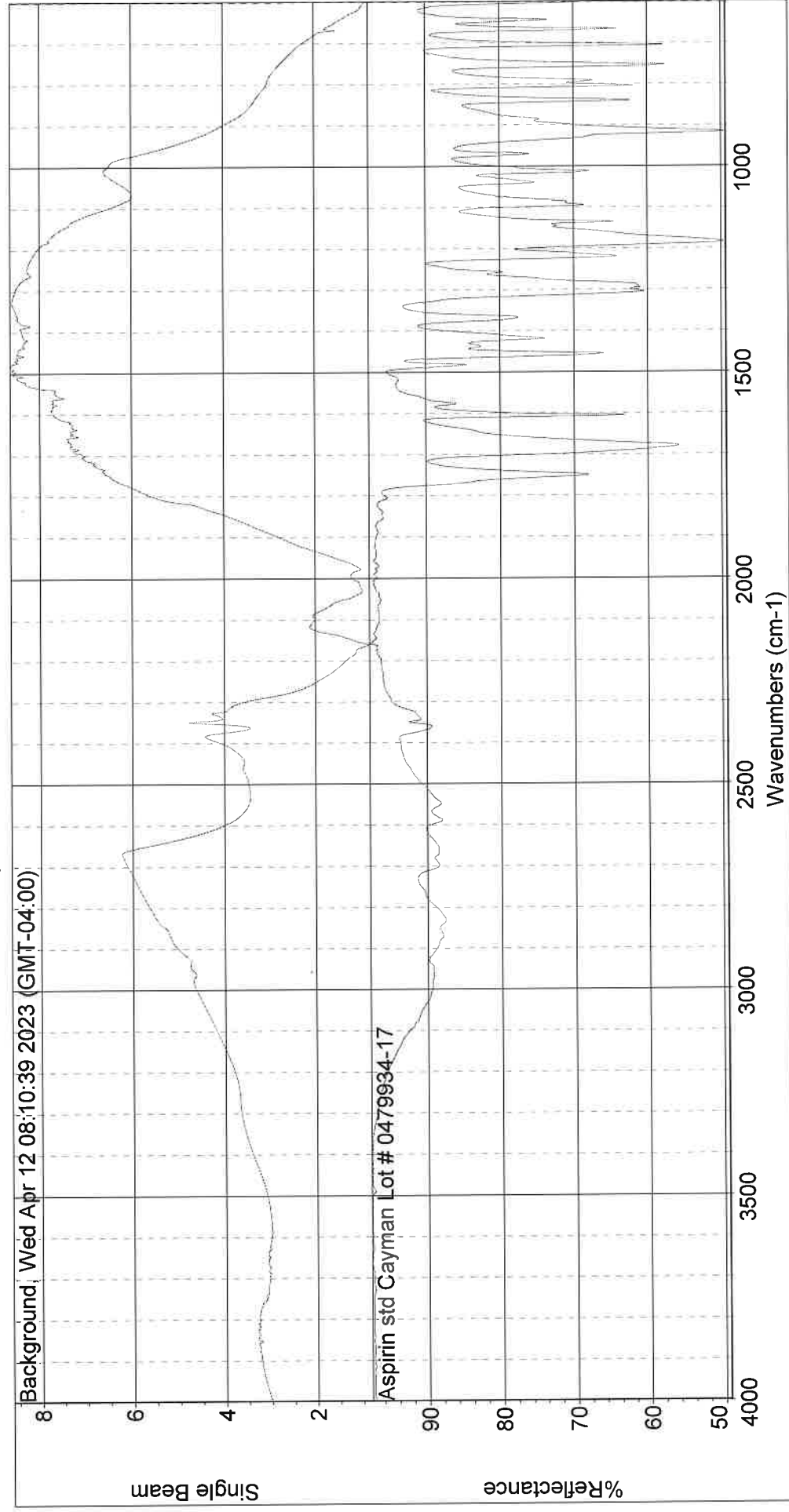
Forensic Chemistry Performance Verification

**Nicolet iS20 FTIR with Smart iTX ATR attachment and Golden Gate ATR
attachment (SN: BEP2310112/ SN#Z100784)
TBI FCU ID- COCO**

Appendix B -ATR data from Golden Gate# 3 attachment used on COCO

TBI Knoxville Crime Laboratory

Collection time: Wed Apr 12 08:12:37 2023 (GMT-04:00)



ATR - COCO

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 8.0
Optical velocity: 0.4747
Aperture: 80.00

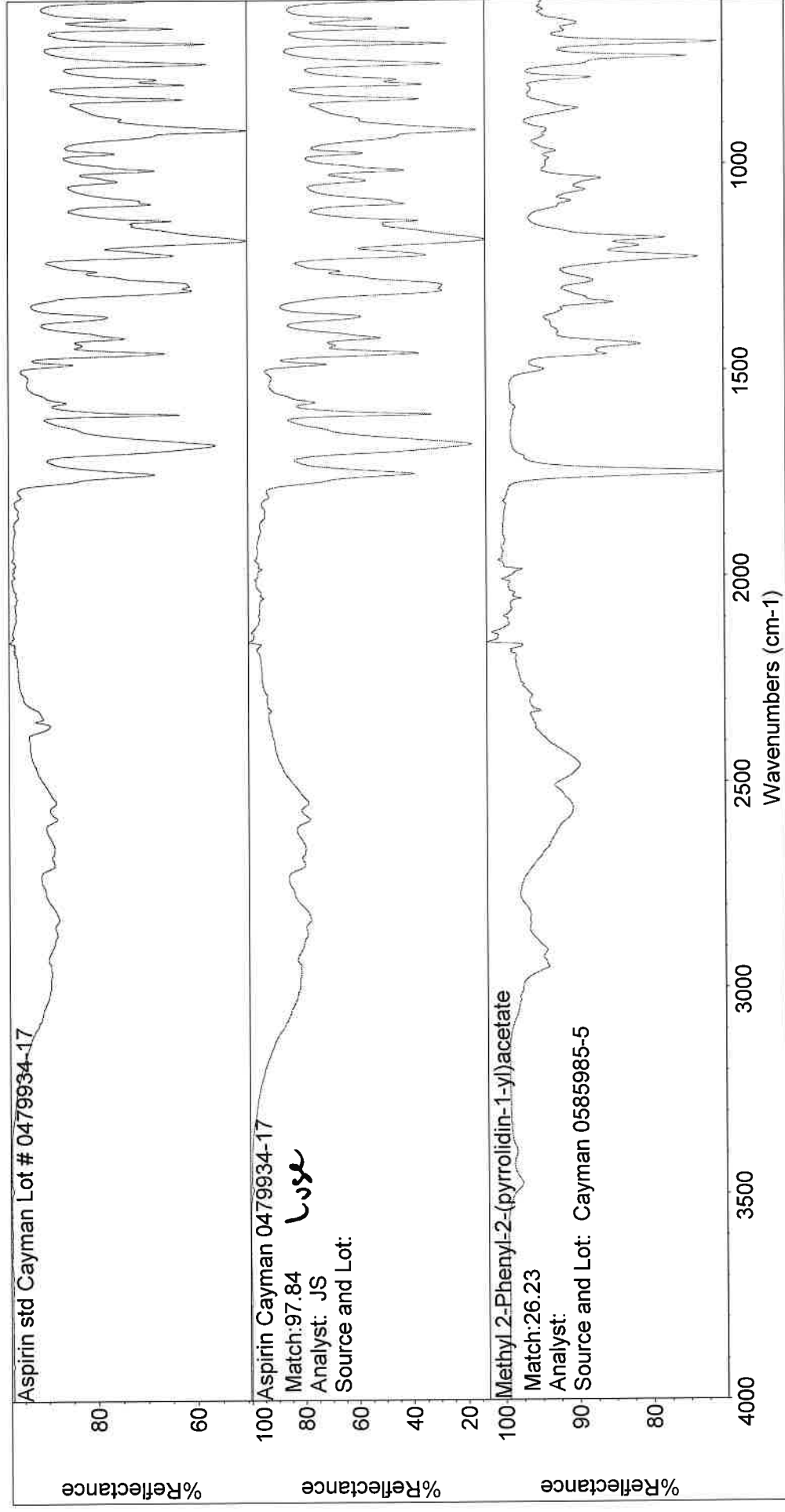


Aspirin std Cayman Lot # 0479934-17

Neat JS

TBI Knoxville Crime Laboratory

Collection time: Wed Apr 12 08:12:37 2023 (GMT-04:00)



ATR - COCO

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 8.0
Optical velocity: 0.4747
Aperture: 80.00

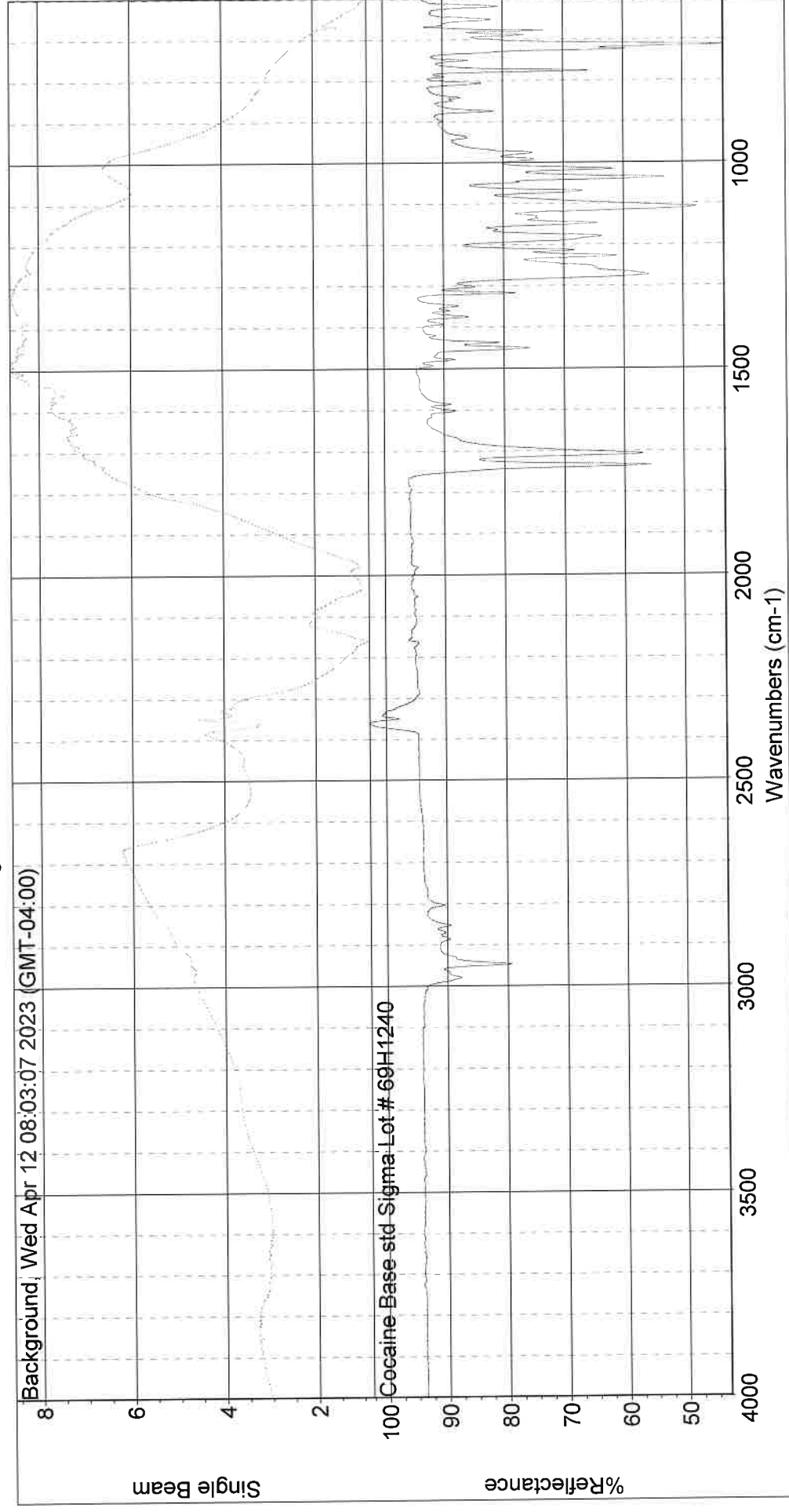


Aspirin std Cayman Lot # 0479934-17

Next JS

TBI Knoxville Crime Laboratory

Collection time: Wed Apr 12 08:05:05 2023 (GMT-04:00)



ATR - COCO

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 8.0
Optical velocity: 0.4747
Aperture: 80.00

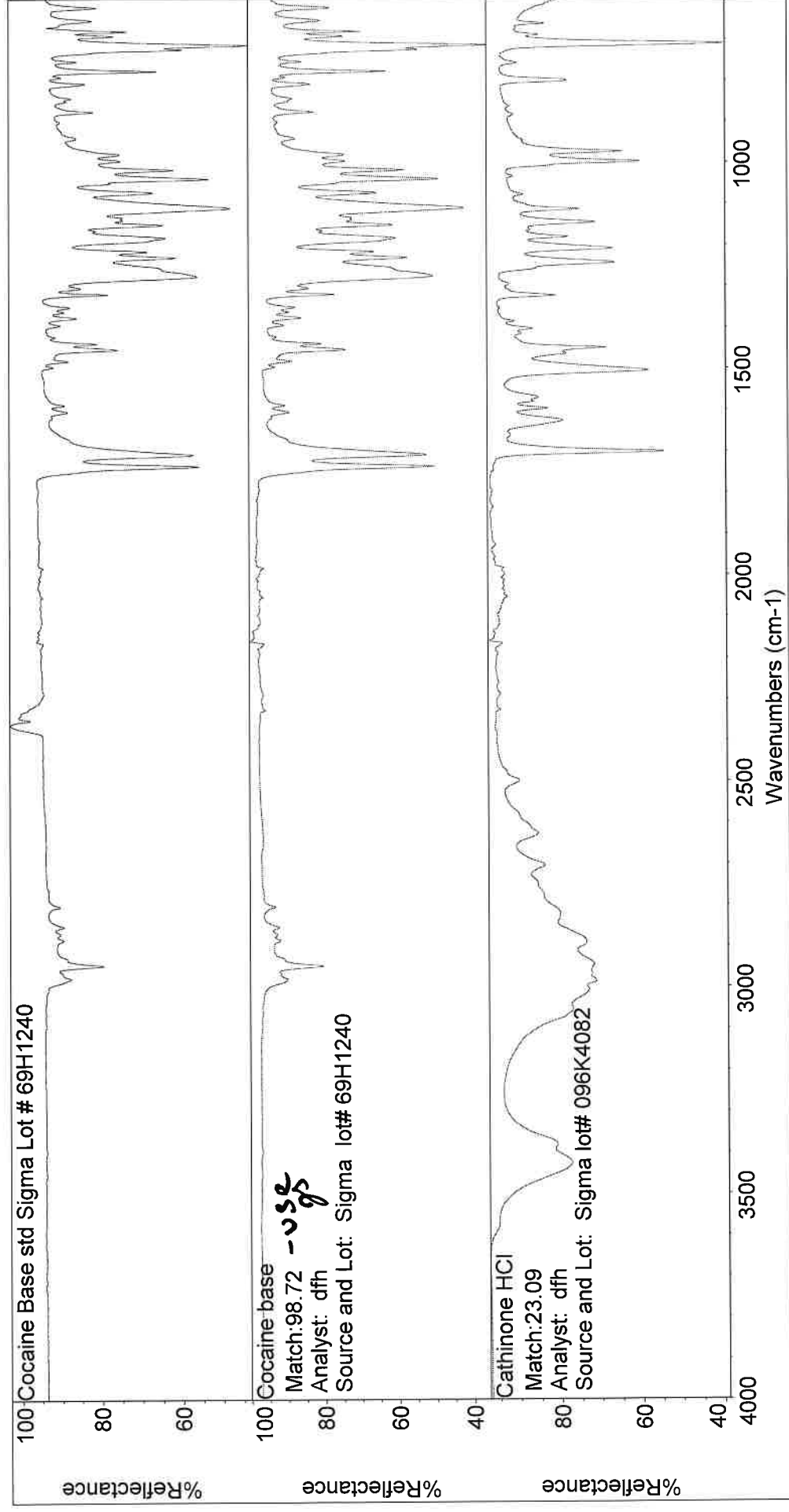


Cocaine Base std Sigma Lot # 69H1240

Neat JS

TBI Knoxville Crime Laboratory

Collection time: Wed Apr 12 08:05:05 2023 (GMT-04:00)



ATR - COCO

Cocaine Base std Sigma Lot # 69H1240

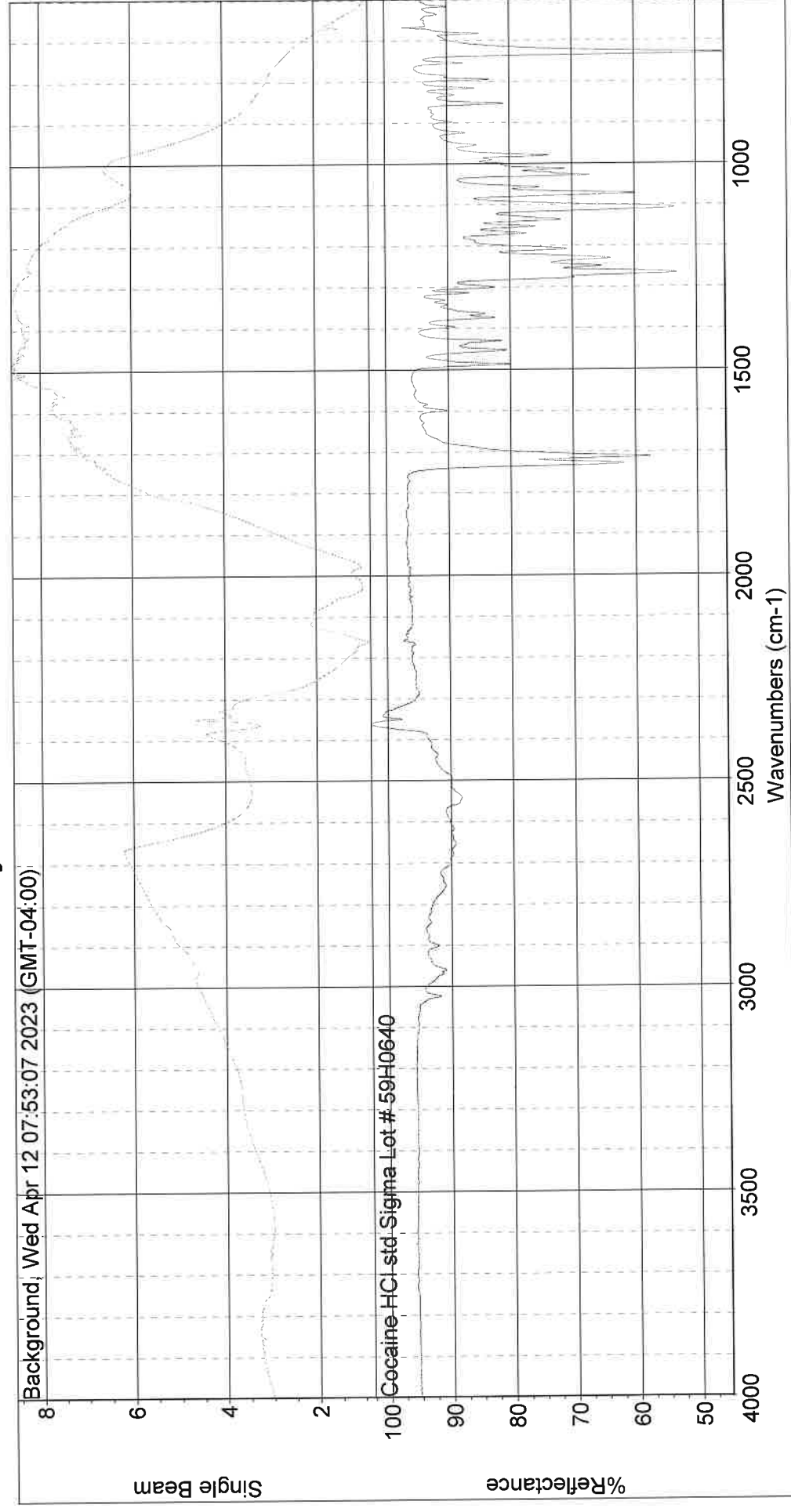


Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 8.0
Optical velocity: 0.4747
Aperture: 80.00

Weak JS

TBI Knoxville Crime Laboratory

Collection time: Wed Apr 12 07:54:50 2023 (GMT-04:00)



Cocaine HCl std Sigma Lot # 59H0640

Neat JS

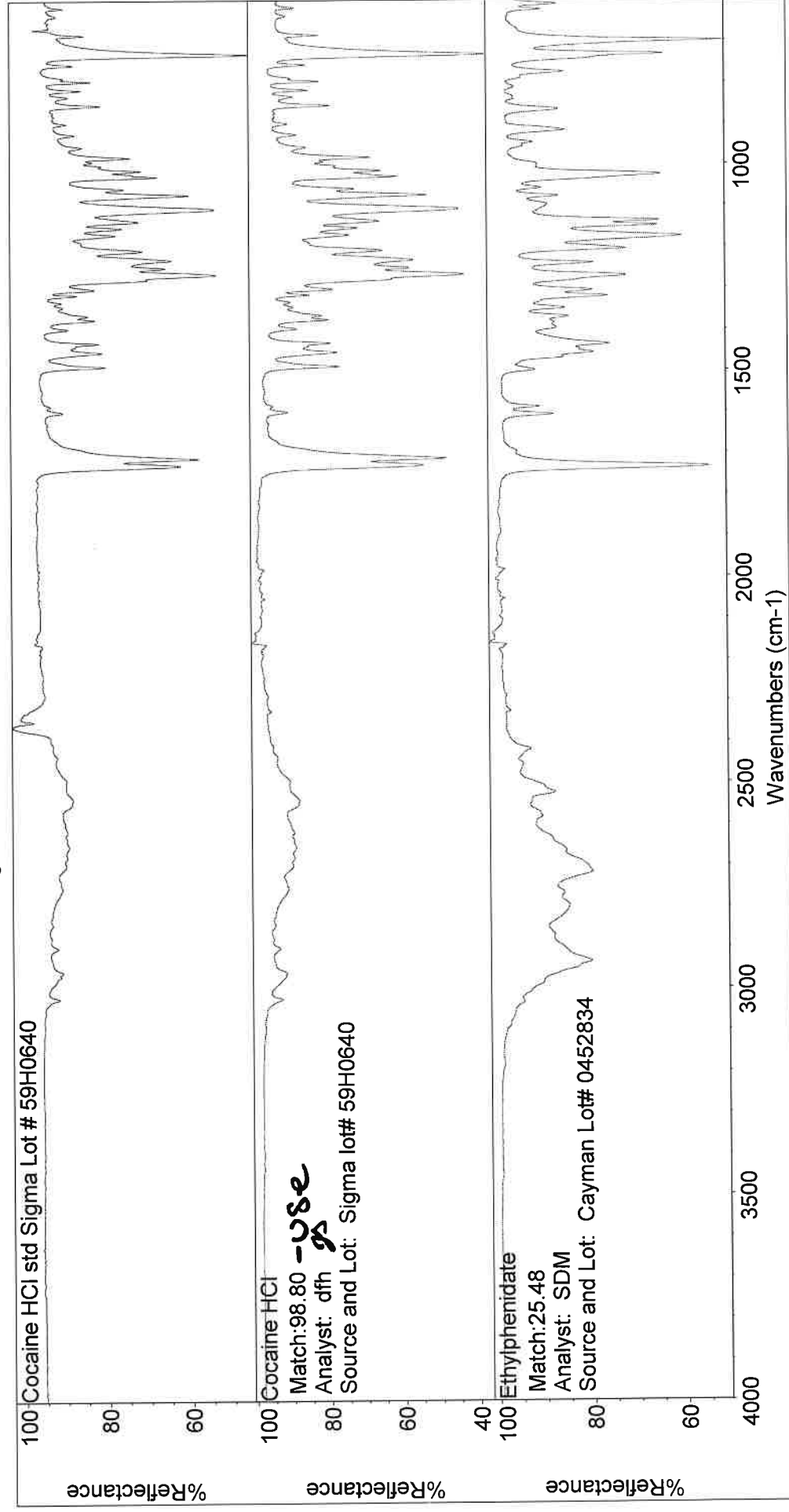


ATR - COCO

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 8.0
Optical velocity: 0.4747
Aperture: 80.00

TBI Knoxville Crime Laboratory

Collection time: Wed Apr 12 07:54:50 2023 (GMT-04:00)



ATR - COCO

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 8.0
Optical velocity: 0.4747
Aperture: 80.00

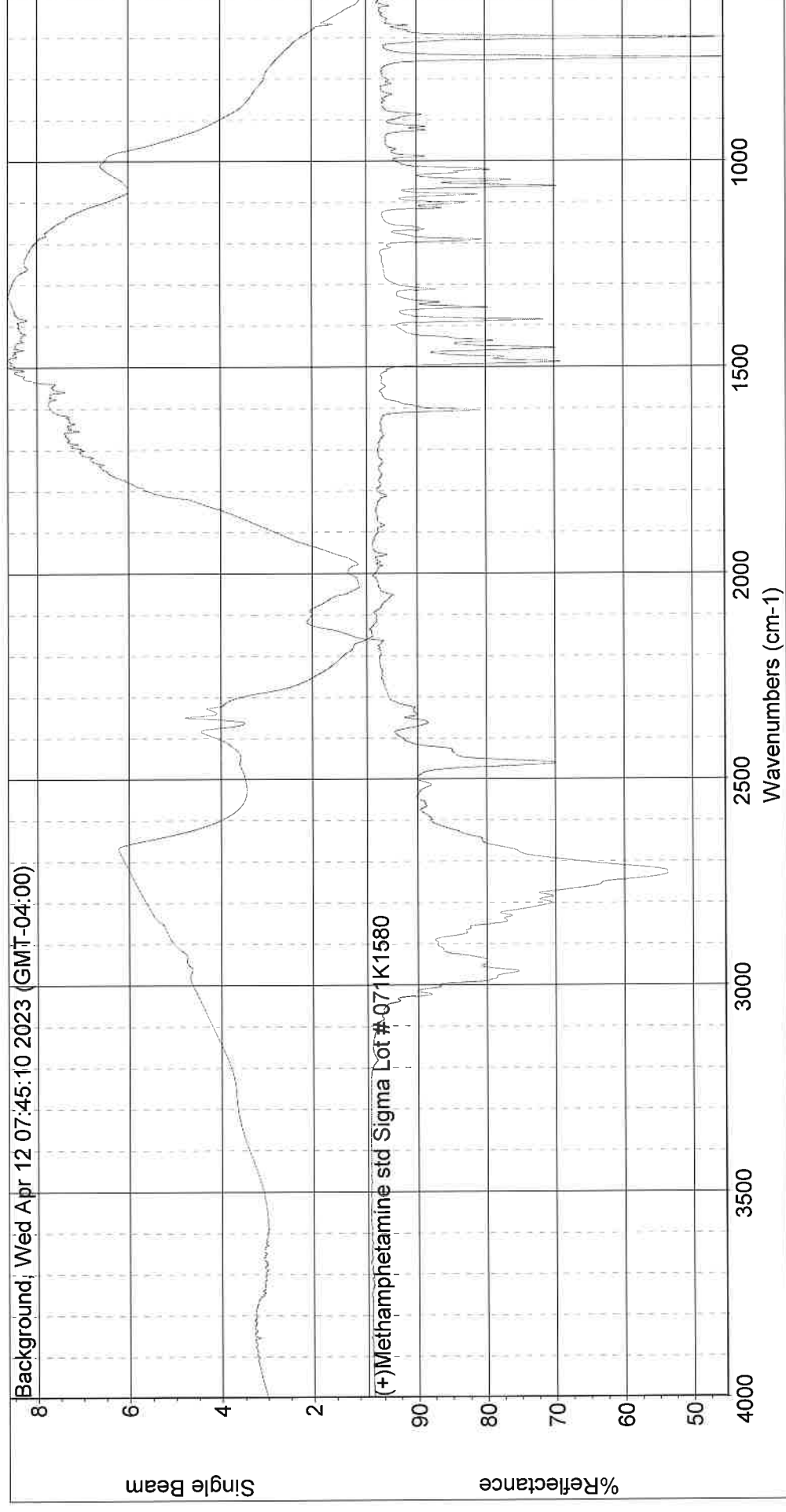
Cocaine HCl std Sigma Lot # 59H0640



Neat SS

TBI Knoxville Crime Laboratory

Collection time: Wed Apr 12 07:47:29 2023 (GMT-04:00)



ATR - COCO

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 8.0
Optical velocity: 0.4747
Aperture: 80.00

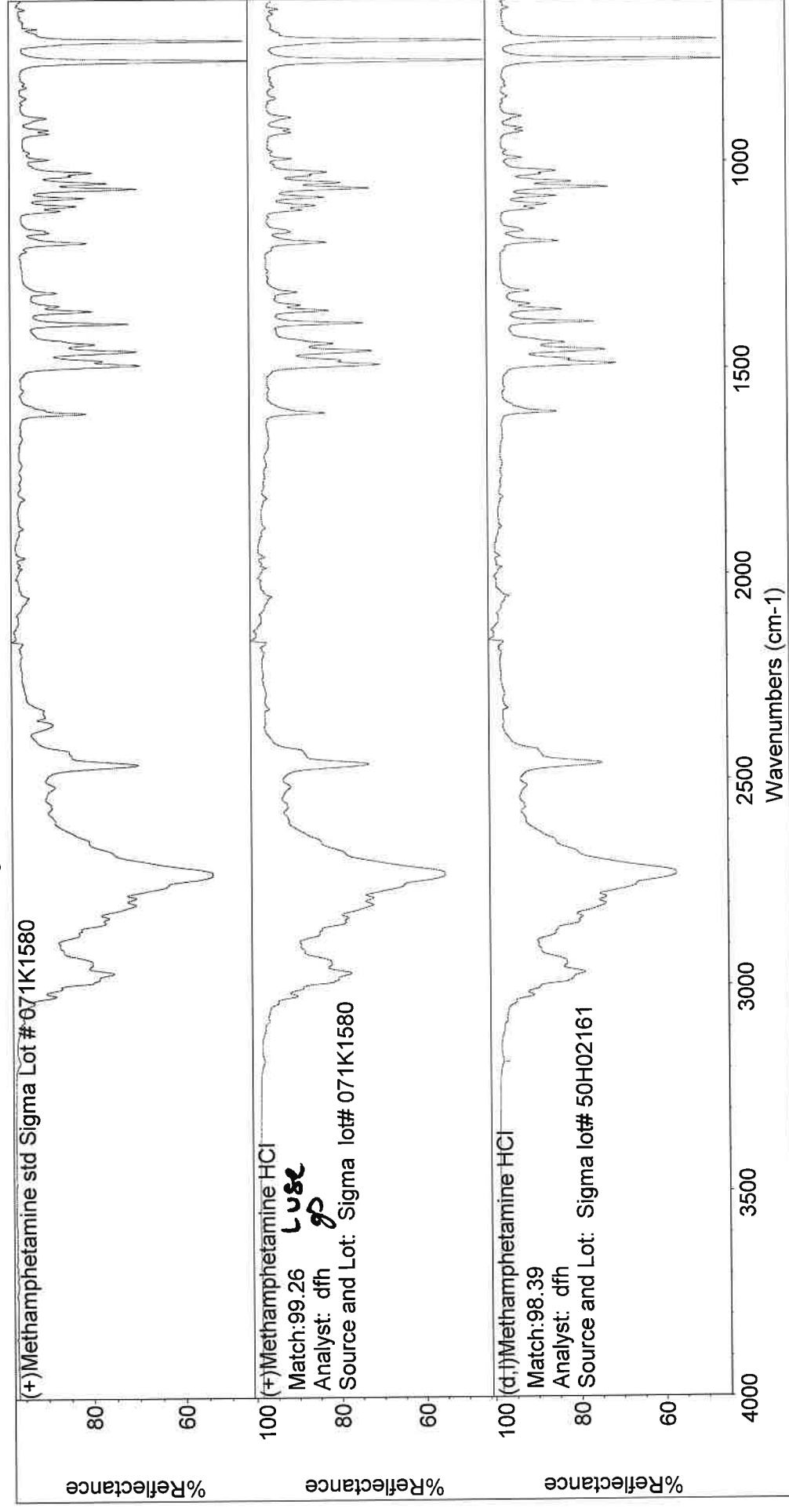


(+)Methamphetamine std Sigma Lot # 071K1580

Neat JS

TBI Knoxville Crime Laboratory

Collection time: Wed Apr 12 07:47:29 2023 (GMT-04:00)



ATR - COCO

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 8.0
Optical velocity: 0.4747
Aperture: 80.00

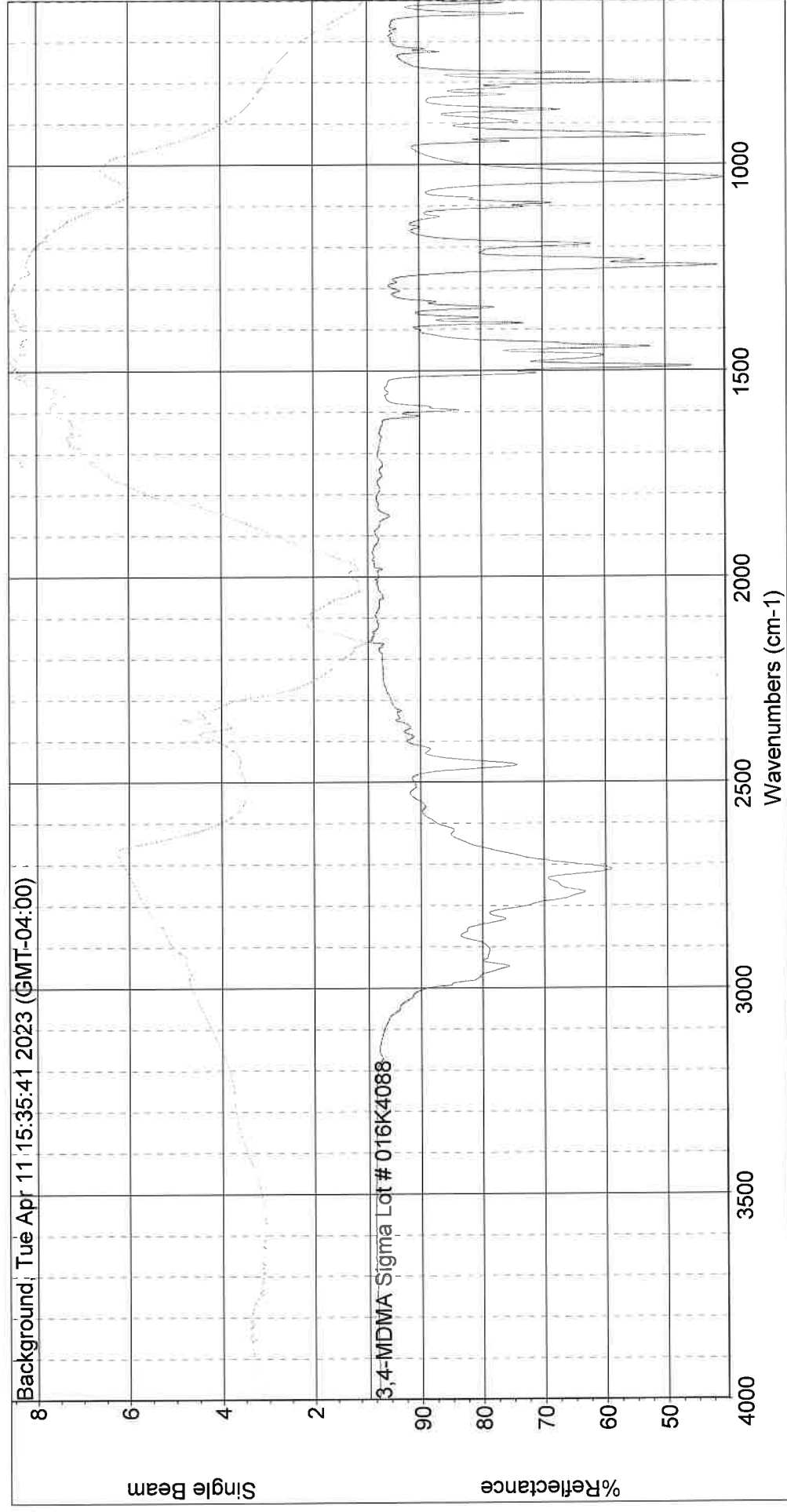


(+)Methamphetamine std Sigma Lot # 071K1580

Neat JS

TBI Knoxville Crime Laboratory

Collection time: Tue Apr 11 15:37:40 2023 (GMT-04:00)



ATR - COCO

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 8.0
Optical velocity: 0.4747
Aperture: 80.00

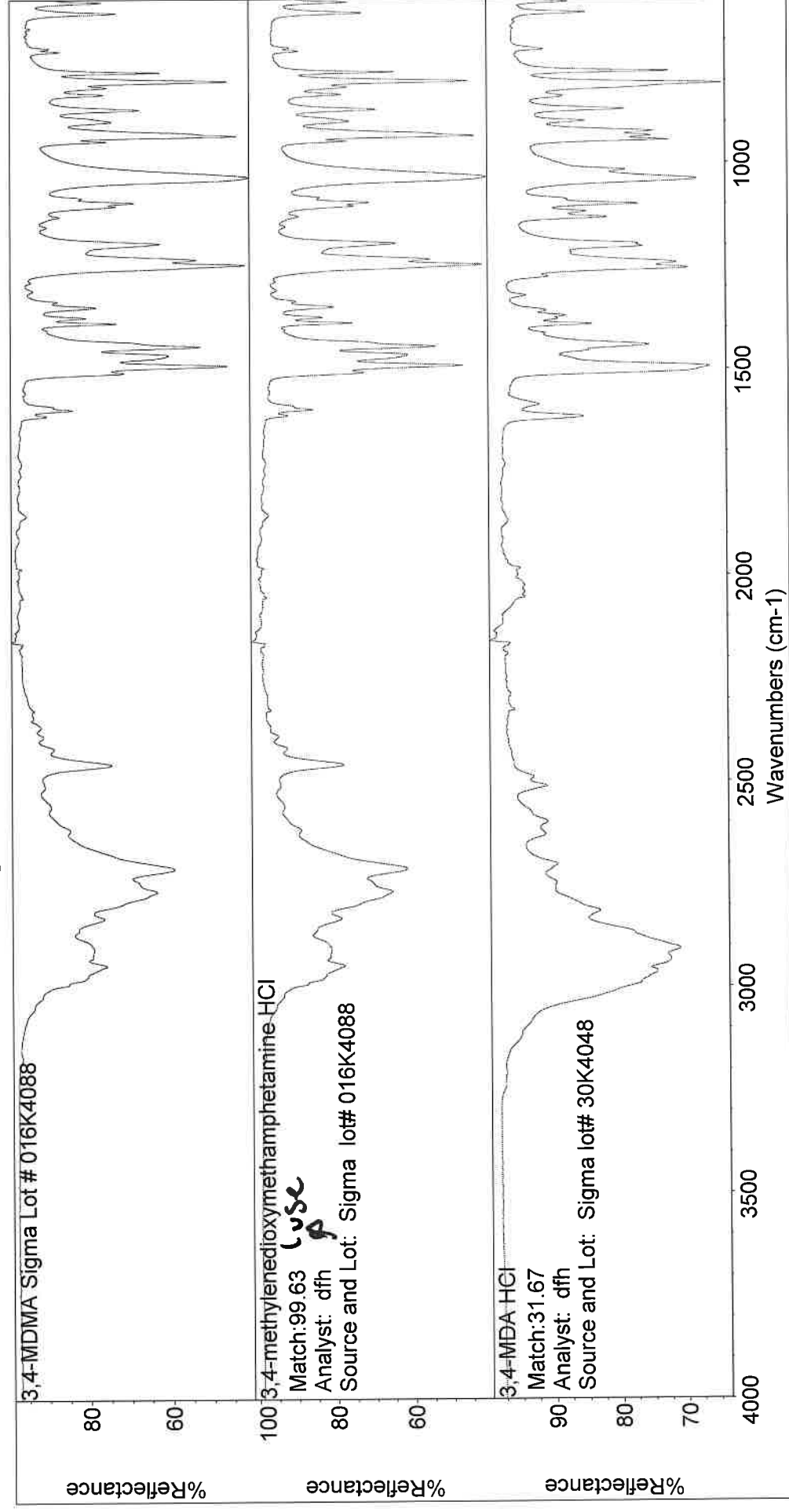


3,4-MDMA Sigma Lot # 016K4088

Neat JS

TBI Knoxville Crime Laboratory

Collection time: Tue Apr 11 15:37:40 2023 (GMT-04:00)



ATR - COCO

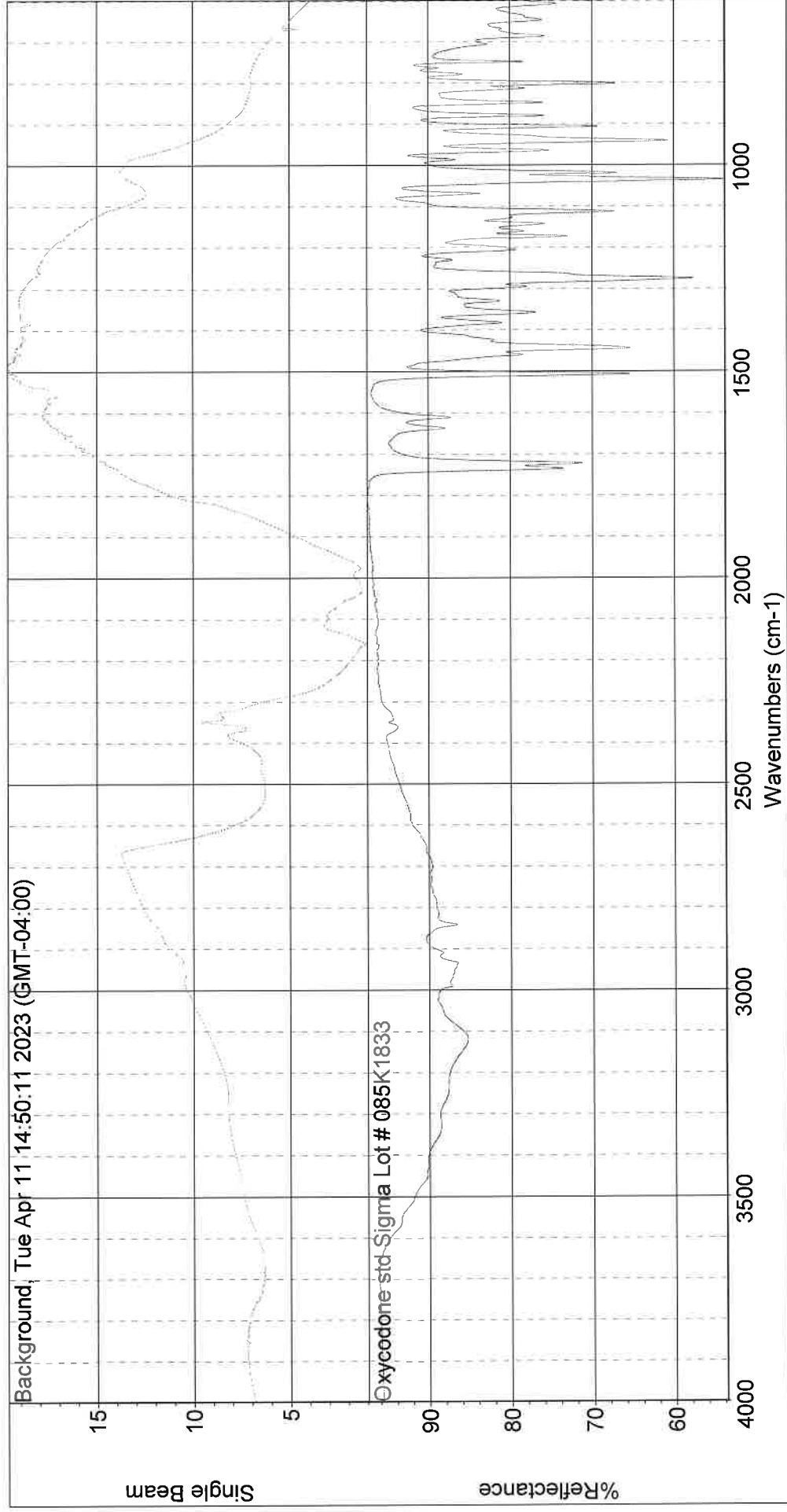
Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 8.0
Optical velocity: 0.4747
Aperture: 80.00

3,4-MDMA Sigma Lot # 016K4088

Next 9's

TBI Knoxville Crime Laboratory

Collection time: Tue Apr 11 14:52:35 2023 (GMT-04:00)



ATR - COCO

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 4.0
Optical velocity: 0.4747
Aperture: 80.00

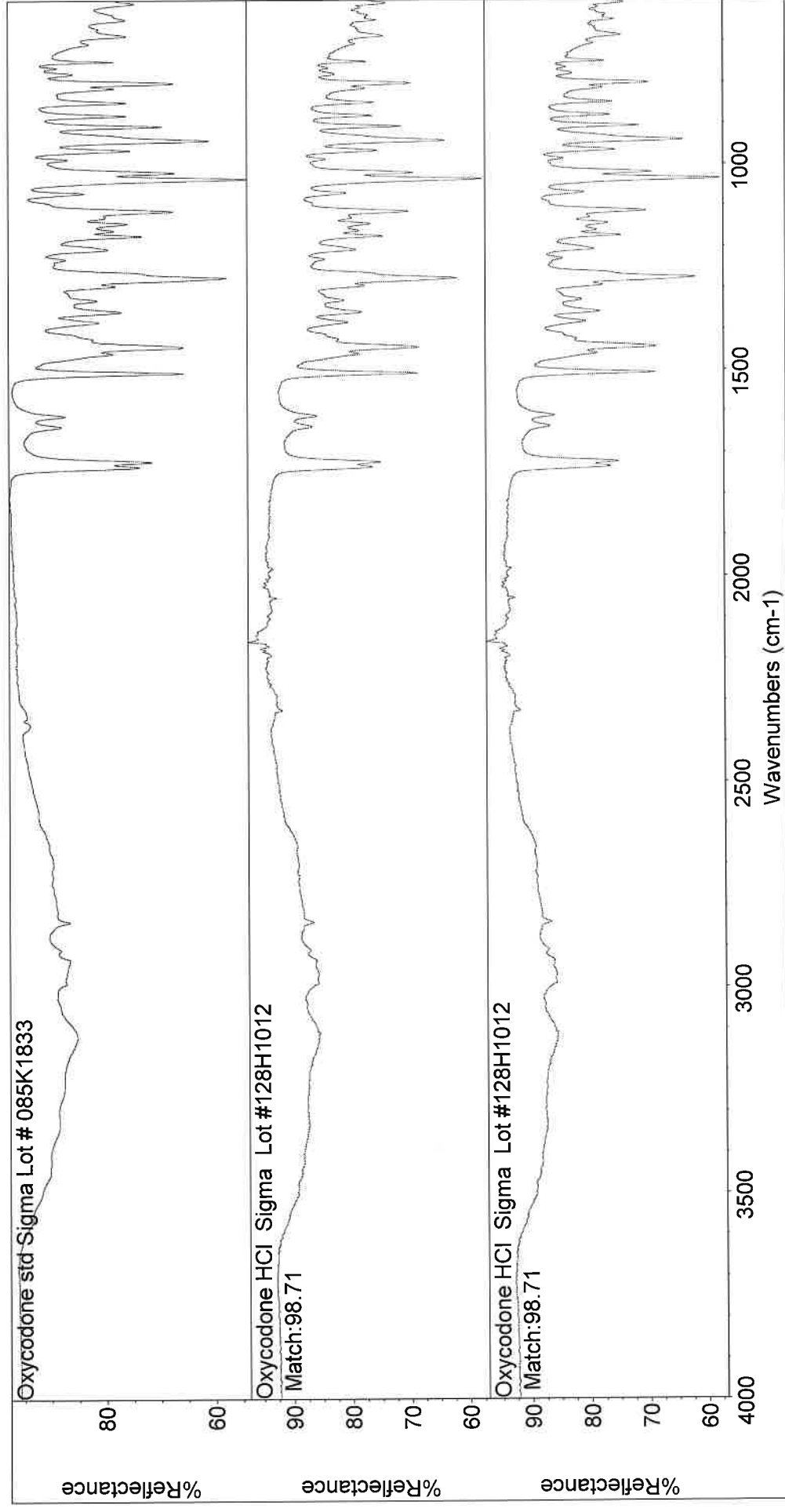


Oxycodone std Sigma Lot # 085K1833

Neat JS

TBI Knoxville Crime Laboratory

Collection time: Tue Apr 11 14:52:35 2023 (GMT-04:00)



Oxycodone std Sigma Lot # 085K1833



ATR - COCO

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 4.0
Optical velocity: 0.4747
Aperture: 80.00

Next 95

Forensic Chemistry Performance Verification

**Nicolet iS20 FTIR with Smart iTX ATR attachment and Golden Gate ATR
attachment (SN: BEP2310112/ SN#Z100784)
TBI FCU ID- COCO**

Appendix C- ValPro Qualification Data and Maintenance Log

ATR Maintenance Log

Instrument ID

Colo

[illegible]

Other Maintenance

[illegible]

ValPro Qualification Report**Qualification test: Nicolet iS20 system KBr - PV****Operator: OMNICAdmin****Date: Tuesday, April 11, 2023 1:30:47 PM (GMT-04:00)****Instrument: Nicolet iS20 Serial number: BEP2310112****Filename: Nicolet iS20 system KBr - PV_20230411_133047.spg**

Test description	High limit	Low limit	Measured	Result
Energy ratio				
Energy ratio 4000 / 2000	1.00	0.20	0.34	Pass
Energy ratio 2000 / 1000	4.00	0.80	1.29	Pass
Noise level				
P-P noise 4050 - 3950 (%T)	0.25	0.00	0.01	Pass
P-P noise 2050 - 1950 (%T)	0.221	0.00	0.007	Pass
P-P noise 1050 - 950 (%T)	0.10	0.00	0.04	Pass
P-P noise 550 - 450 (%T)	1.50	0.00	0.18	Pass
RMS noise 4050 - 3950	0.05	0.00	0.00	Pass
RMS noise 2050 - 1950	0.039	0.00	0.002	Pass
RMS noise 1050 - 950	0.014	0.00	0.010	Pass
RMS noise 550 - 450	0.30	0.00	0.05	Pass
Detector linearity				
Slope	1.10	0.90	1.03	Pass
Intercept (%T)	1.00	-1.00	0.08	Pass

Performed by: Title: SA / FS IIDate: 4/11/23

Approved by: _____

Title: _____

Date: _____

Comments: _____

Digital comment(s):

No digital comments found.

Signature verification was SUCCESSFUL

File: c:\omnic data\valproresults\NicoletiS20 KBr-PV.qrs

By: OMNICAdmin

Date: 04-11-2023 13:44:07 (GMT-04:00)

Reason: Authorship - signifies ownership

Signature verification was SUCCESSFUL

File: C:\Omnic Data\spectra\Nicolet iS20 system KBr - PV_20230411_133047.spg

By: OMNICAdmin

Date: Apr/11/2023 13:44:06 (GMT-04:00)

Reason: Authorship - signifies ownership

ValPro Qualification Report**Qualification test: Nicolet iS20 system KBr - USP****Operator: OMNICAdmin****Date: Tuesday, April 11, 2023 1:44:57 PM (GMT-04:00)****Instrument: Nicolet iS20 Serial number: BEP2310112****Filename: Nicolet iS20 system KBr - USP_20230411_134457.spg**

Test description	High limit	Low limit	Measured	Result
Wavenumber accuracy				
Peak at 3060.0 (cm-1)	3061.0	3059.0	3059.5	Pass
Peak at 2849.5 (cm-1)	2850.5	2848.5	2849.2	Pass
Peak at 1942.9 (cm-1)	1943.9	1941.9	1942.5	Pass
Peak at 1601.2 (cm-1)	1602.2	1600.2	1601.0	Pass
Peak at 1583.0 (cm-1)	1584.0	1582.0	1582.9	Pass
Peak at 1154.5 (cm-1)	1155.5	1153.5	1154.4	Pass
Peak at 1028.3 (cm-1)	1029.3	1027.3	1028.3	Pass

Performed by: <u>JS</u>	Title: <u>SA/FS II</u>	Date: <u>4/11/23</u>
Approved by: _____	Title: _____	Date: _____
Comments: _____		

Digital comment(s):

No digital comments found.

Signature verification was SUCCESSFUL

File: c:\omnic data\valproresults\NicoletiS20 KBr-USP.qrs

By: OMNICAdmin

Date: 04-11-2023 13:53:04 (GMT-04:00)

Reason: Authorship - signifies ownership

Signature verification was SUCCESSFUL

File: C:\Omnic Data\spectra\Nicolet iS20 system KBr - USP_20230411_134457.spg

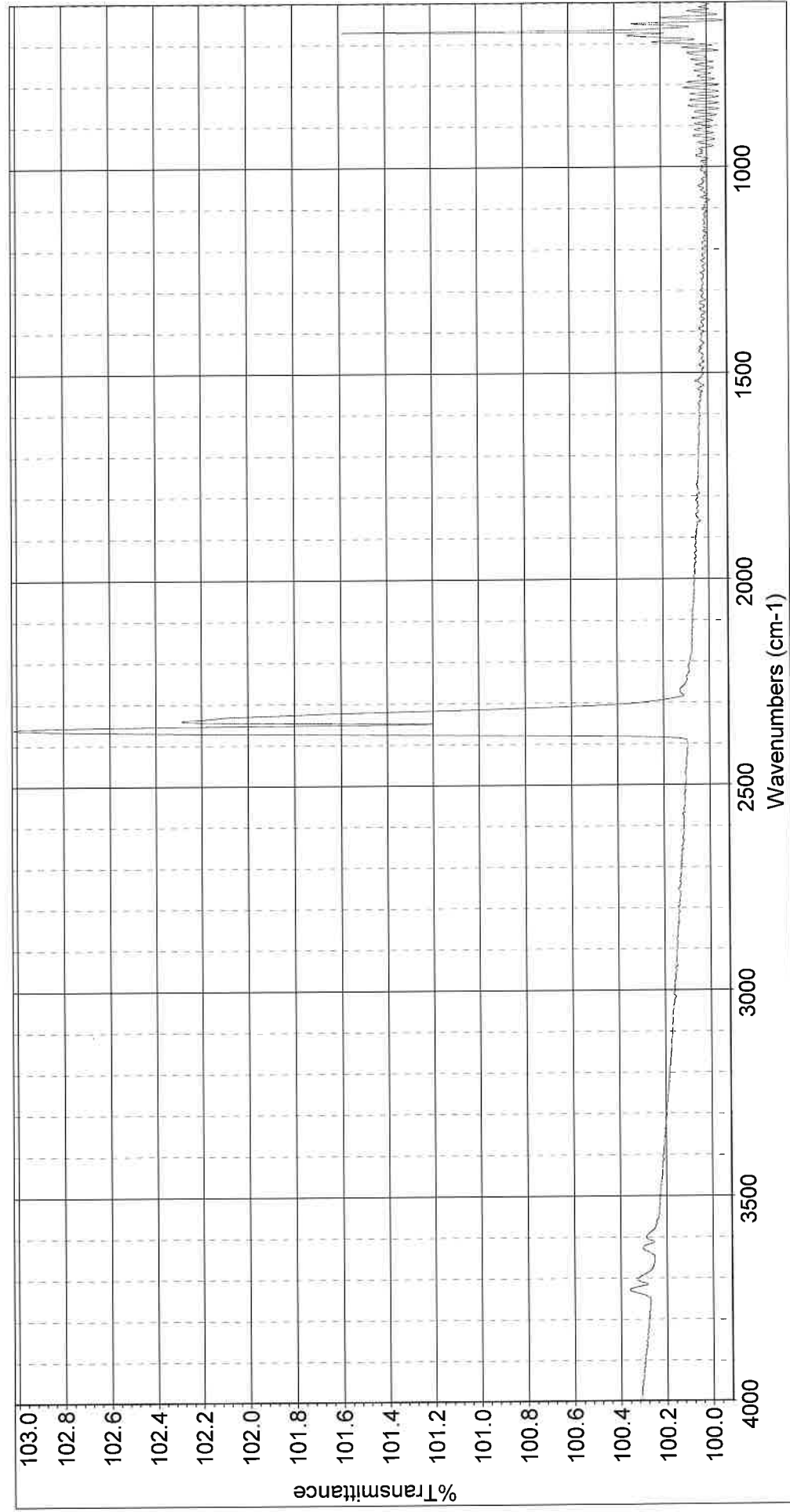
By: OMNICAdmin

Date: Apr/11/2023 13:53:04 (GMT-04:00)

Reason: Authorship - signifies ownership

TBI Knoxville Crime Laboratory

Collection time: Tue Apr 11 13:56:11 2023 (GMT-04:00)



ATR - COCO

Number of sample scans: 36
Number of background scans: 36
Resolution: 4.000
Sample gain: 1.0
Optical velocity: 0.6329
Aperture: 80.00

Tue Apr 11 13:55:28 2023 (GMT-04:00)



2200.0-2100.0 = 0.008 PERFORMANCE TEST
PASS JS

Power Supply	Status	Current	Acceptable Range
+ 5 Volt	Pass	4.89V	4.50V to 5.50V
+ 12 Volt	Pass	11.92V	10.80V to 13.20V
- 12 Volt	Pass	-11.92V	-13.20V to -10.80V
+3.3 Volt	Pass	3.31V	3.00V to 3.60V

[Print](#)[View More](#)[Return](#)*P*

Item	Status	Current	Acceptable Range
Laser Current	Pass	0.20A	0.10A to 1.30A
Source Voltage	Pass	9.54V	4.00V to 13.00V
Source Current	Pass	1.88A	0.10A to 10.00A
Source Power		17.89W	
Temperature	Pass	46.50C	0.50C to 70.00C

P

Print

Return

ValPro Qualification Report

Qualification test: Smart iTX accessory - PV

Operator: OMNICAdmin

Date: Tuesday, April 11, 2023 2:02:55 PM (GMT-04:00)

Instrument: Nicolet iS20 Serial number: BEP2310112

Accessory serial number: Z100784

Filename: Smart iTX accessory - PV_20230411_140255.spg

Test description	High limit	Low limit	Measured	Result
Wavenumber accuracy				
Peak at 2849.5 (cm-1)	2850.5	2848.5	2849.2	Pass
Peak at 1601.2 (cm-1)	1602.2	1600.2	1600.8	Pass
Peak at 1583.0 (cm-1)	1584.0	1582.0	1582.9	Pass
Peak at 1154.5 (cm-1)	1155.5	1153.5	1154.3	Pass
Peak at 1028.3 (cm-1)	1029.3	1027.3	1027.7	Pass
Optical Resolution				
FWHH at 1154 (cm-1)	10.00	5.00	8.37	Pass
FWHH at 907 (cm-1)	14.00	5.00	13.06	Pass

Performed by: 	Title: SA/FS II	Date: 4/11/23
Approved by: _____	Title: _____	Date: _____
Comments: _____		

Digital comment(s):

No digital comments found.

Signature verification was SUCCESSFUL

File: c:\omnic data\valproresults\Smart iTX-PV.qrs

By: OMNICAdmin

Date: 04-11-2023 14:06:18 (GMT-04:00)

Reason: Authorship - signifies ownership

Signature verification was SUCCESSFUL

File: C:\Omnic Data\spectra\Smart iTX accessory - PV_20230411_140255.spg

By: OMNICAdmin

Date: Apr/11/2023 14:06:18 (GMT-04:00)

Reason: Authorship - signifies ownership



Qualification test: Quantification & Algorithms 2019 - ALL
 Date: Monday, April 3, 2023 12:14:13 PM (GMT-05:00)
 Operator: OMNICAdmin

Beer's Law

Test description	Expected	Measured	Result
Polystyrene - large peak	2.927	2.927	Pass
Polystyrene - small peak	2.974	2.974	Pass

Measures the thickness of a polystyrene sample by Beer's Law using a peak in the spectrum.

CLS

Test description	Expected	Measured	Result
Polystyrene - range	0.964	0.964	Pass

Measures the thickness of a polystyrene sample using the Classical Least Squares (CLS) algorithm using a spectrum region.

CLS-C

Test description	Expected	Measured	Result
CLS-C Polystyrene - error	0.0006	0.0006	Pass

Measures the standard error of the thickness of a polystyrene sample using the Classical Least Squares (CLS) algorithm using a spectrum region.

SMLR

Test description	Expected	Measured	Result
SMLR0 Polystyrene	2.953	2.953	Pass
SMLR1 Polystyrene first derivative	2.980	2.980	Pass
SMLR2 Polystyrene second derivative	2.988	2.988	Pass

Measures the thickness of a polystyrene sample by SMLR performing the analysis on the specified spectral data.

PLS

Test description	Expected	Measured	Result
PLS0 value	2.924	2.924	Pass
PLS0-C uncertainty in the thickness	0.0810	0.0810	Pass
PLS-S Polystyrene Savitsky-Golay smoothed - value	2.967	2.967	Pass
PLS-N1 Polystyrene Norris first derivative - value	2.965	2.965	Pass

PLS-N2 Polystyrene Norris second derivative - value	2.960	2.960	Pass
PLS with data missing in the calibration	2.965	2.965	Pass
PLS after reference standard subtraction	2.924	2.924	Pass

Measures the thickness of a polystyrene sample by PLS performing the analysis on the specified spectral data.

PCR

Test description	Expected	Measured	Result
value	0.9988	0.9988	Pass

Measures the thickness of a polystyrene sample by PCR.

PCR-C

Test description	Expected	Measured	Result
uncertainty of the thickness	0.0477	0.0477	Pass

Evaluates the uncertainty of the thickness of a polystyrene sample by PCR.

PCR-F

Test description	Expected	Measured	Result
full spectrum	99.991	99.991	Pass

Evaluates the full spectrum check value that is computed when measuring the thickness of a polystyrene sample by PCR.

PCR-R

Test description	Expected	Measured	Result
region check value	100.000	100.000	Pass

Evaluates the region check value that is computed when measuring the thickness of a polystyrene sample by PCR.

Similarity Match

Test description	Expected	Measured	Result
Similarity Match - Index	93.808	93.808	Pass

Measures the similarity index for a polystyrene sample using the Similarity Match algorithm.

Distance Match

Test description	Expected	Measured	Result
Similarity	1.3468	1.3468	Pass
Best Class or Category	0.000	0.000	Pass

Measures the class similarity for a polystyrene sample using the Distance Match algorithm; the spectrum is preprocessed with a Norris second derivative.

Distance Match-D

Test description	Expected	Measured	Result
Maximum Deviation	14.44	14.44	Pass

Measures the maximum deviation (in unit of standard deviations) between any standard and a polystyrene sample using the Distance Match algorithm; the spectrum is preprocessed with a Norris second derivative.

Discriminant Analysis

Test description	Expected	Measured	Result
Similarity	1.626	1.626	Pass

Measures the class similarity for a polystyrene sample using the Discriminant Analysis algorithm; the spectrum is smoothed using a Savitzky-Golay smooth.

Discriminant-M Analysis

Test description	Expected	Measured	Result
Best Class	2.0000	2.0000	Pass

Measures the best class or category for a polystyrene sample using the Discriminant Analysis algorithm; the spectrum is smoothed using a Savitzky-Golay smooth.

QC Compare

Test description	Expected	Measured	Result
Search metric	99.9789	99.9789	Pass
Best Class	1.000	1.000	Pass

Determines a search metric or best class assigned for a polystyrene sample using the QC Compare Search algorithm.

Search

Test description	Expected	Measured	Result
Search metric	99.9981	99.9981	Pass

Determines a search metric for a polystyrene sample using the Search algorithm.

Search-C

Test description	Expected	Measured	Result
Best Match Index	3.000	3.000	Pass

Determines the most similar spectral library entry for a polystyrene sample using the Search algorithm.

Search-F

Test description	Expected	Measured	Result
Full Spectrum	92.616	92.616	Pass

Determines the full spectrum check result that is calculated when analyzing a polystyrene sample using the Search

algorithm.

Fixed Location Height

Test description	Expected	Measured	Result
Height ratio	0.283	0.283	Pass

Measures the ratio of the heights of two peaks at fixed locations in a polystyrene spectrum.

Average Height in Range

Test description	Expected	Measured	Result
Average height	1.893	1.893	Pass

Measures the average height of a peak over a spectrum range in a polystyrene spectrum.

Maximum Height in Range

Test description	Expected	Measured	Result
Maximum height	0.389	0.389	Pass

Measures the maximum height of a peak over a spectrum range in a polystyrene spectrum.

Minimum Height in Range

Test description	Expected	Measured	Result
Minimum height	0.189	0.189	Pass

Measures the minimum height of a peak over a spectrum range in a polystyrene spectrum.

Absolute Maximum Height in Range

Test description	Expected	Measured	Result
Absolute height	0.699	0.699	Pass

Measures the absolute maximum height of a peak over a spectrum range in a polystyrene spectrum.

Area

Test description	Expected	Measured	Result
Area	29.8170	29.8170	Pass

Measures the area of a peak in a polystyrene spectrum.

Computed Area

Test description	Expected	Measured	Result
Area	67.7205	67.7205	Pass

Measures the computed area of a peak in a polystyrene spectrum.

RMS Noise

Test description	Expected	Measured	Result
RMS Noise	0.695	0.695	Pass

Measures the RMS noise over a spectrum range in a polystyrene spectrum.

Peak-to-Peak Noise

Test description	Expected	Measured	Result
P-P Noise	2.346	2.346	Pass

Measures the peak-to-peak noise over a spectrum range in a polystyrene spectrum.

Height at Exact Location

Test description	Expected	Measured	Result
Exact Location Height	0.166	0.166	Pass

Measures the interpolated height at an exact spectral location in a polystyrene spectrum.

Peak Height

Test description	Expected	Measured	Result
Interpolated Height	0.430	0.430	Pass

Measures the interpolated peak height for a peak in a polystyrene spectrum.

Peak Location

Test description	Expected	Measured	Result
Interpolated Location	5948.24	5948.24	Pass

Measures the interpolated peak location for a peak in a polystyrene spectrum.

Peak Width

Test description	Expected	Measured	Result
FWHM	116.54	116.54	Pass

Measures the peak width at half maximum for a peak in a polystyrene spectrum.

Single Beam % of Maximum

Test description	Expected	Measured	Result
Location at 1%	5622.46	5622.46	Pass
Location at 2%	5676.67	5676.67	Pass
Location at 5%	5742.05	5742.05	Pass
Location at 10%	5794.29	5794.29	Pass

Measures the location at which the intensity is a percentage of the peak maximum in a single beam spectrum.

CLS Interference

Test description	Expected	Measured	Result
CO	676.96	676.96	Pass
Interference	908.40	908.40	Pass

Measures the concentration of CO in the presence of an interference using Classical Least Squares (CLS) algorithm. The interference is measured in one region, but interferes in the CO analytical region.

Area Reference Subtract

Test description	Expected	Measured	Result
Area	0.828	0.828	Pass

Measures the area of a peak in a polystyrene spectrum after a reference spectrum has been subtracted.

Peak Measurement at Percent of Maximum

Test description	Expected	Measured	Result
Width at 40%	132.449	132.449	Pass
Area at 40%	43.368	43.368	Pass

Measures the peak width or area at 40% of the peak maximum for a peak in a polystyrene spectrum.

Peak Width Location Referenced

Test description	Expected	Measured	Result
Width - Low Location Referenced	95.89	95.89	Pass
Width - High Location Referenced	105.13	105.13	Pass

Measures the peak width at the "Location Referenced" for a peak in a polystyrene spectrum.

Height from Interferogram and Single Beam

Test description	Expected	Measured	Result
Sample IFG Height	4.073	4.073	Pass
Background IFG Height	7.756	7.756	Pass
Sample SB Height	25.908	25.908	Pass
Background SB Height	-0.995	-0.995	Pass

Computes a height from the sample interferogram, the background interferogram, the sample single beam and the background single beam.

Center of Gravity Peak Location

Test description	Expected	Measured	Result
COG Location	5944.875	5944.875	Pass

Measures the center of gravity peak location for a peak in a polystyrene spectrum.

Composite Components Test - A

Test description	Expected	Measured	Result
Component A	0.09361	0.09361	Pass
Component B	0.48897	0.48897	Pass
Component C	0.46627	0.46627	Pass
Component D	0.68433	0.68433	Pass
Average1=AVG	0.43330	0.43330	Pass
Average2=AVG(A,C,D)	0.41474	0.41474	Pass
Sum=SUM(A,B,C,D)	1.73319	1.73319	Pass
Std Dev 1=STD(C)	0.00000	0.00000	Pass
Std Dev 2=STD(A,B,C)	0.22200	0.22200	Pass
Abs Max=AMAX(A,B,C,D)	0.68433	0.68433	Pass
Abs Min=AMIN(A,B,C,D)	0.09361	0.09361	Pass
Abs Min(1)=AMIN(A)	0.09361	0.09361	Pass
Max=MAX	0.68433	0.68433	Pass
Min=MIN	0.09361	0.09361	Pass
File(1)=ZR+YS	-28.90445	-28.90445	Pass
File(2)=YR+ZS	17.28373	17.28373	Pass

Calculates a set of measurements using the predicted concentrations from four components.

Composite Components Test - B

Test description	Expected	Measured	Result
Component A	0.09361	0.09361	Pass
Component B	0.48897	0.48897	Pass
Component C	0.46627	0.46627	Pass
Component D	0.68433	0.68433	Pass
Simple=B	0.48897	0.48897	Pass
Sum=(A+C+D)	1.24422	1.24422	Pass
Diff=(C-D-A)	-0.31168	-0.31168	Pass
Prod=(B*C)	0.22799	0.22799	Pass
Quot=(D/C)	1.46767	1.46767	Pass
SumCon=A+1.23	1.32361	1.32361	Pass
DifCon=D-3.44	-2.75567	-2.75567	Pass
ProdCon=D*12	8.21200	8.21200	Pass
QuotCon=B/0.26	1.88066	1.88066	Pass
Par(1)=2.5*(A+B+-3.14)	-6.39354	-6.39354	Pass
Par(2)=1/(A+B+C)	8.59746	8.59746	Pass
Par(3)=(B+13)/(C+(B/5))	23.91388	23.91388	Pass
Par(4)=A+B/D*C/B+2/17	3.25162	3.25162	Pass
Par(5)=43.1628	43.16280	43.16280	Pass
Par(6)=(A+B)*(C+D)/(17+(B/C))	0.03714	0.03714	Pass
Zero=B-B	0.00000	0.00000	Pass
Negate=0-C	-0.46627	-0.46627	Pass

Calculates a set of measurements using the predicted concentrations from four components.

Composite Components Test - C

Test description	Expected	Measured	Result
Component A	0.09361	0.09361	Pass
Component B	0.48897	0.48897	Pass
Component C	0.46627	0.46627	Pass
Component D	0.68433	0.68433	Pass
AbsA=ABS(A)	0.09361	0.09361	Pass
AbsB=ABS(B)	0.48897	0.48897	Pass
ExpA=EXP(A)	1.09813	1.09813	Pass
ExpC=EXP(C)	1.59404	1.59404	Pass
ExpNegA=EXPNEG(A)	0.91064	0.91064	Pass
ExpNegC=EXPNEG(C)	0.62734	0.62734	Pass
TenA=TEN(A)	1.24055	1.24055	Pass
TenD=TEN(D)	4.83429	4.83429	Pass
TenNegA=TENNEG(A)	0.80610	0.80610	Pass
TenNegD=TENNEG(D)	0.20686	0.20686	Pass
LnA=LN(A)	-2.36859	-2.36859	Pass
LnB=LN(B)	-0.71545	-0.71545	Pass
NegLnA=NEGLN(A)	2.36859	2.36859	Pass
NegLnB=NEGLN(B)	0.71545	0.71545	Pass
LogA=LOG(A)	-1.02866	-1.02866	Pass
LogB=LOG(B)	-0.31072	-0.31072	Pass
NegLogA=NEGLOG(A)	1.02866	1.02866	Pass
NegLogB=NEGLOG(B)	0.31072	0.31072	Pass
SqrtA=SQRT(A)	0.30596	0.30596	Pass
SqrtC=SQRT(C)	0.68284	0.68284	Pass
InvSqrtA=INVSQRT(A)	3.26838	3.26838	Pass
InvSqrtC=IVNSQRT(C)	1.46447	1.46447	Pass

Calculates a set of measurements using the predicted concentrations from four components.

Report Options

Test description	Expected	Measured	Result
Compute	-0.0303	-0.0303	Pass
Less than zero	0.0000	0.0000	Pass
Less than error	0.0000	0.0000	Pass
Threshold high	-0.1000	-0.1000	Pass
Threshold low	0.1000	0.1000	Pass
C Report	-0.0303	-0.0303	Pass
C Threshold high	-0.1000	-0.1000	Pass
C Threshold low	0.1000	0.1000	Pass

Calculates a set of measurements using the predicted concentration of polystyrene, then checks reporting options.

Performed by: _____	Title: _____	Date: _____
Approved by: _____	Title: _____	Date: _____
Comments: _____		

Digital comment(s):

No digital comments found.

Signature verification was SUCCESSFUL

File: c:\omnic data\valproresults\Quantification & Algorithms 2019.qrs

By: OMNICAdmin

Date: 04-03-2023 12:15:10 (GMT-05:00)

Reason: Authorship - signifies ownership

PV Noise level

P-P noise 4050 -		0.0	0.0	Pas
P-P noise 2050 -		0.0	0.05	Pas
P-P noise 1050 -		0.0	0.0	Pas
P-P noise 550 -		0.0	0.2	Pas
RMS noise 4050	0.	0.0	0.0	Pas
RMS noise 2050	0.	0.0	0.01	Pas
RMS noise 105	0.0	0.0	0.00	Pas
RMS noise 55	0.3	0.0	0.0	Pas

PV Detector linearity

Slop	1.1	0.9	1.0	Pas
Intercept	1.0	-1.0	0.0	Pas

USP Wavenumber accuracy

Peak at 3060.	3	3059	3059	Pas
Peak at 2849.	2	2848	2849	Pas
Peak at 1942.	1	1941	1942	Pas
Peak at 1601.	1	1600	1601	Pas
Peak at 1583.	1	1582	1582	Pas
Peak at 1154.	1	1153	1154	Pas
Peak at 1028.	1	1027	1028	Pas

Performed by: Ken Wusmm Title: Field Service Engineer

Approved by: _____ Title: _____

Comments: _____

Digital comment(s):

No digital comments found.

Signature verification was SUCCESSFUL

File: c:\omnic data\valproresults\NicoletiS20 KBr-Factory.qrs

By: OMNICAdmin

Date: 04-03-2023 12:13:28 (GMT-05:00)

Reason: Authorship - signifies ownership

Signature verification was SUCCESSFUL

File: C:\Omnic Data\spectra\Nicolet iS20 KBr - Factory (CP,JP,PHEUR,PV,USP)

By: OMNICAdmin

Date: Apr/03/2023 12:13:28 (GMT-05:00)

Reason: Authorship - signifies ownership

ValPro Qualification Report**Qualification test: Smart iTX accessory - PV****Operator: OMNICAdmin****Date: Monday, April 3, 2023 12:16:36 PM (GMT-05:00)****Instrument: Nicolet iS20 Serial number: BEP2310112****Accessory serial number: Z100784****Filename: Smart iTX accessory - PV_20230403_121636.spg**

Test description	High limit	Low limit	Measured	Result
Wavenumber accuracy				
Peak at 2849.5 (cm-1)	2850.5	2848.5	2850.2	Pass
Peak at 1601.2 (cm-1)	1602.2	1600.2	1600.8	Pass
Peak at 1583.0 (cm-1)	1584.0	1582.0	1582.9	Pass
Peak at 1154.5 (cm-1)	1155.5	1153.5	1154.4	Pass
Peak at 1028.3 (cm-1)	1029.3	1027.3	1027.8	Pass
Optical Resolution				
FWHH at 1154 (cm-1)	10.00	5.00	8.27	Pass
FWHH at 907 (cm-1)	14.00	5.00	13.00	Pass

Performed by: _____ Title: _____ Date: _____

Approved by: _____ Title: _____ Date: _____

Comments: _____

Digital comment(s):

No digital comments found.

Signature verification was SUCCESSFUL

File: c:\omnic data\valproresults\Smart iTX-PV.qrs

By: OMNICAdmin

Date: 04-03-2023 12:19:39 (GMT-05:00)

Reason: Authorship - signifies ownership

Signature verification was SUCCESSFUL

File: C:\Omnic Data\spectra\Smart iTX accessory - PV_20230403_121636.spg

By: OMNICAdmin

Date: Apr/03/2023 13:19:39 (GMT-04:00)

Reason: Authorship - signifies ownership

ValPro Qualification Report

Qualification test: Smart iTX accessory - PV
Operator: OMNICAdmin
Date: Monday, April 3, 2023 12:16:36 PM (GMT-05:00)
Instrument: Nicolet iS20 Serial number: BEP2310112
Accessory serial number: Z100784
Filename: Smart iTX accessory - PV_20230403_121636.spg

	Test descr	High	Low	Meas	Resu
Wavenumber accuracy					
	Peak at 2849.	2	2848	2850	Pas
	Peak at 1601.	1	1600	1600	Pas
	Peak at 1583.	1	1582	1582	Pas
	Peak at 1154.	1	1153	1154	Pas
	Peak at 1028.	1	1027	1027	Pas
Optical Resolution					
	FWHH at 1154	10.0	5.0	8.2	Pas
	FWHH at 907 (	14.0	5.0	13.0	Pas

Performed by: Kai Wusmm Title: Field Service Engineer

Approved by: _____ Title: _____

Comments: _____

Digital comment(s):
No digital comments found.

Signature verification was SUCCESSFUL
File: c:\omnic data\valproresults\Smart iTX-PV.qrs
By: OMNICAdmin
Date: 04-03-2023 12:19:39 (GMT-05:00)
Reason: Authorship - signifies ownership

Signature verification was SUCCESSFUL
File: C:\Omnica Data\spectra\Smart iTX accessory - PV_20230403_121636.spg
By: OMNICAdmin
Date: Apr/03/2023 12:19:39 (GMT-05:00)
Reason: Authorship - signifies ownership