

TBI-FORENSIC SERVICES DIVISION PERFORMANCE VERIFICATION FORM

Instrument/Method to Verify:

Nicolet is20 FTIR with Golden gate attachment (S/N BEP2110574) GADGET

Check the appropriate box: New Validation ☐ Modification ☐ Performance Check ☒

Laboratory: NCL ☒ KCL ☐ MCL ☐ Unit: Forensic Chemistry

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

Name Lela Jackson Title SA/FS Initials LJ

Completed: Signature/Date Lela Jackson
Digitally signed by Lela Jackson
DN: cn=Lela Jackson, o=Tennessee Bureau of Investigation,
ou, email=Lela.Jackson@tn.gov, c=US
Date: 2021.11.22 08:37:15 -06'00'

Name _____ Title _____ Initials _____

Completed: Signature/Date _____

Name _____ Title _____ Initials _____

Completed: Signature/Date _____

Verification of final review:

Unit Supervisor/Date Glenn Everett
Digitally signed by Glenn Everett
DN: cn=Glenn Everett, o=TBI, ou, email=glenn.everett@tn.gov, c=US
Date: 2021.11.22 13:26:10 -06'00'

Unit Supervisor/Date _____

Unit Supervisor/Date _____

Crime Laboratory Regional Supervisor/Date 
Digitally signed by Jennifer Hall
DN: cn=Jennifer Hall, o=Tennessee Bureau of Investigation, ou=Forensic Services Lab,
email=jennifer.hall@tn.gov, c=US
Date: 2021.11.22 12:41:06 -06'00'

Crime Laboratory Regional Supervisor/Date _____

Crime Laboratory Regional Supervisor/Date _____

Quality Assurance Manager/Date CDJ
Digitally signed by Chad D Johnson
Date: 2021.11.23 10:55:39 -06'00'

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 Glenn Everett
Digitally signed by Glenn Everett
DN: cn=Glenn Everett, o=TBI, ou, email=glenn.everett@tn.gov,
c=US
Date: 2021.11.22 13:26:29 -06'00'

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 Golden Gate #3 attachment (SN: BEP2110574)

TBI FCU ID – GADGET

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Forensic Chemistry Performance Verification

Nicolet iS20 FTIR with Golden gate ATR attachment (SN: BEP2110574)
TBI FCU ID – GADGET

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 Avatar 380, 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.

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
- The ability to use the Golden Gate accessory as a primary ATR accessory for 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 Golden gate ATR attachment (SN: BEP2110574)

TBI FCU ID – GADGET

2. Components and Experiment Setup:

Instrument Components

iS20 FTIR	
Source	Single point
Beam splitter	KBr/Ge coated
Laser Type	Solid-state Diode
Detector	DTGS KBr
Internal Verification Standard	Polystyrene/NG Glass wheel

Experiment parameters

Scans	16
Resolution	4
Spectral Range	4000 – 600 (Golden Gate)
Gain	Auto
Optical Velocity	0.4747
Aperture	Medium resolution

Golden Gate #3 S/N 0703009 was used since this attachment had been in service recently.

3. Procedure:

Ten certified reference standards were tested on this instrument using the 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.

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.

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.

Forensic Chemistry Performance Verification

Nicolet iS20 FTIR with Golden gate ATR attachment (SN: BEP2110574)

TBI FCU ID – GADGET

4. Standards Used:

Standard	Source	Lot Number
Acetaminophen	Sigma-Aldrich	088K0040
Alprazolam	Upjohn	487RA
Caffeine	Eastman Kodak	355
Carisoprodol	Alltech	311 (label A)
Cocaine base	Merck	U7472
Cocaine HCl	Sigma-Aldrich	SLCF4870
Diazepam	Lipomed	107.1B0.2
Methamphetamine	K&K Labs	732A
3,4-MDMA	Cayman Chemical	0460656-7
Oxycodone	Sigma	128H1012

5. Results and Conclusions

Spectra for the ten standards generated by GADGET were compared to library standard spectra. Results from GADGET using the Golden Gate attachment was consistent with the library standard spectra and matched satisfactorily for identification.

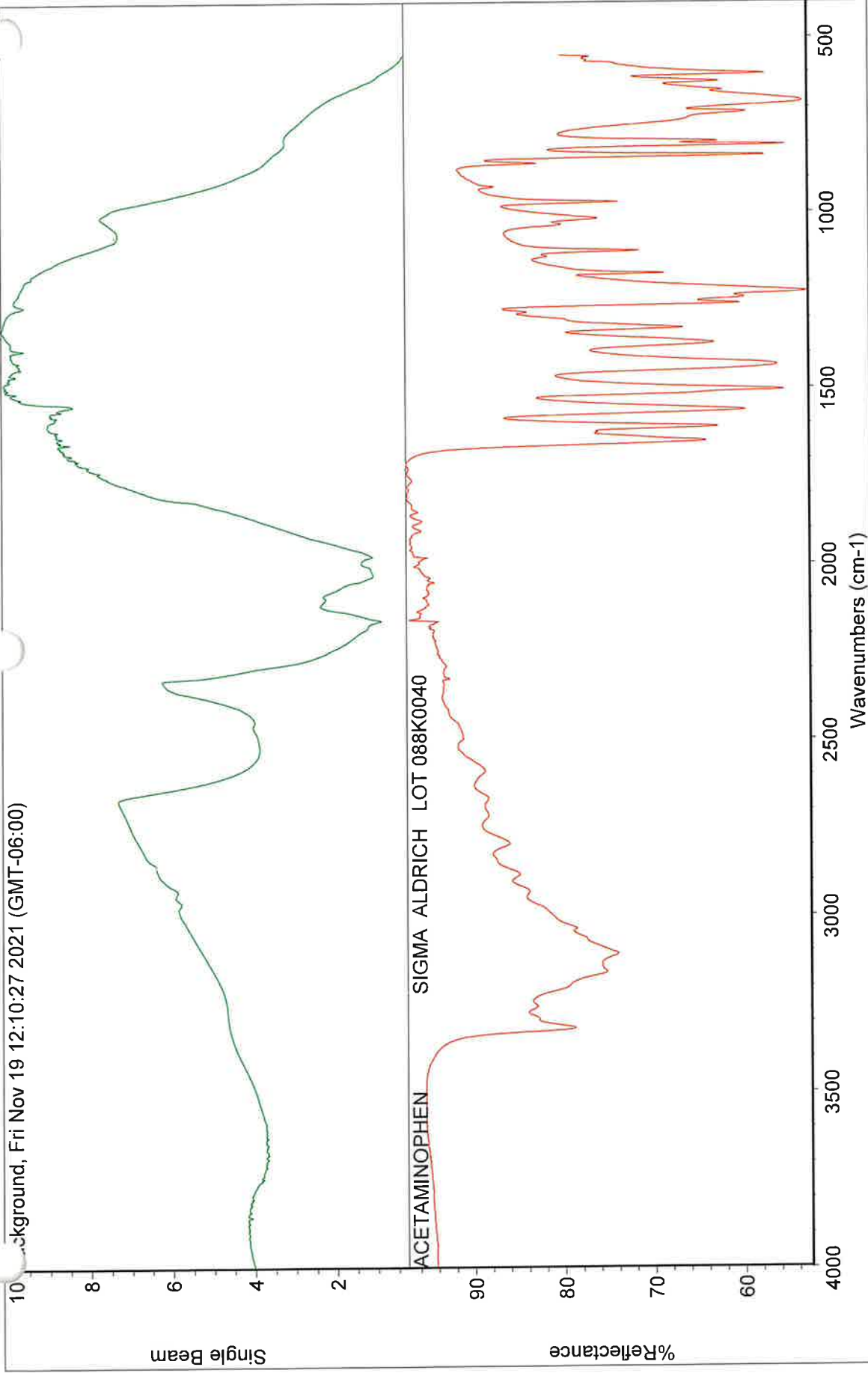
All data generated for the iS20 using the Golden gate attachment can be found in Appendix A.

The ValPro Qualification reports outlined in the Procedure section as well as the current maintenance log are in Appendix B. The full factory validation performed is also included in 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 with a few minor software differences for labeling spectra as documented in the validation for the HAL9000 iS20 in service. Therefore, no additional training requirements will be needed for currently trained scientists.

Background, Fri Nov 19 12:10:27 2021 (GMT-06:00)



ACETAMINOPHEN ~~NOT~~ SIGMA ALDRICH LOT 088K0040

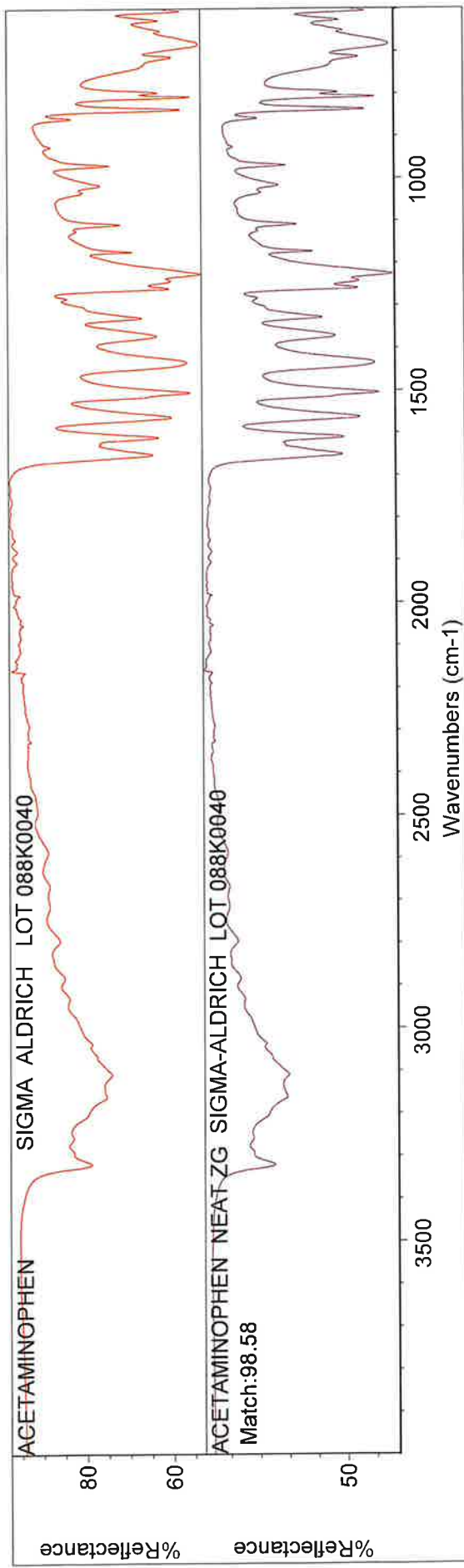
Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Detector: DTGS KBr
Sample gain: 8.0
Beamsplitter: KBr
Optical velocity: 0.4747
Source: IR
Aperture: 80.00

Collection time: Fri Nov 19 12:15:48 2021 (GMT-06:00)

GADGET

Search results for: ACETAMINOPHEN
 Date: Fri Nov 19 12:16:26 2021 (GMT-06:00)
 Search algorithm: Correlation
 Regions searched: 3998.72-599.78

SIGMA ALDRICH LOT 088K0040

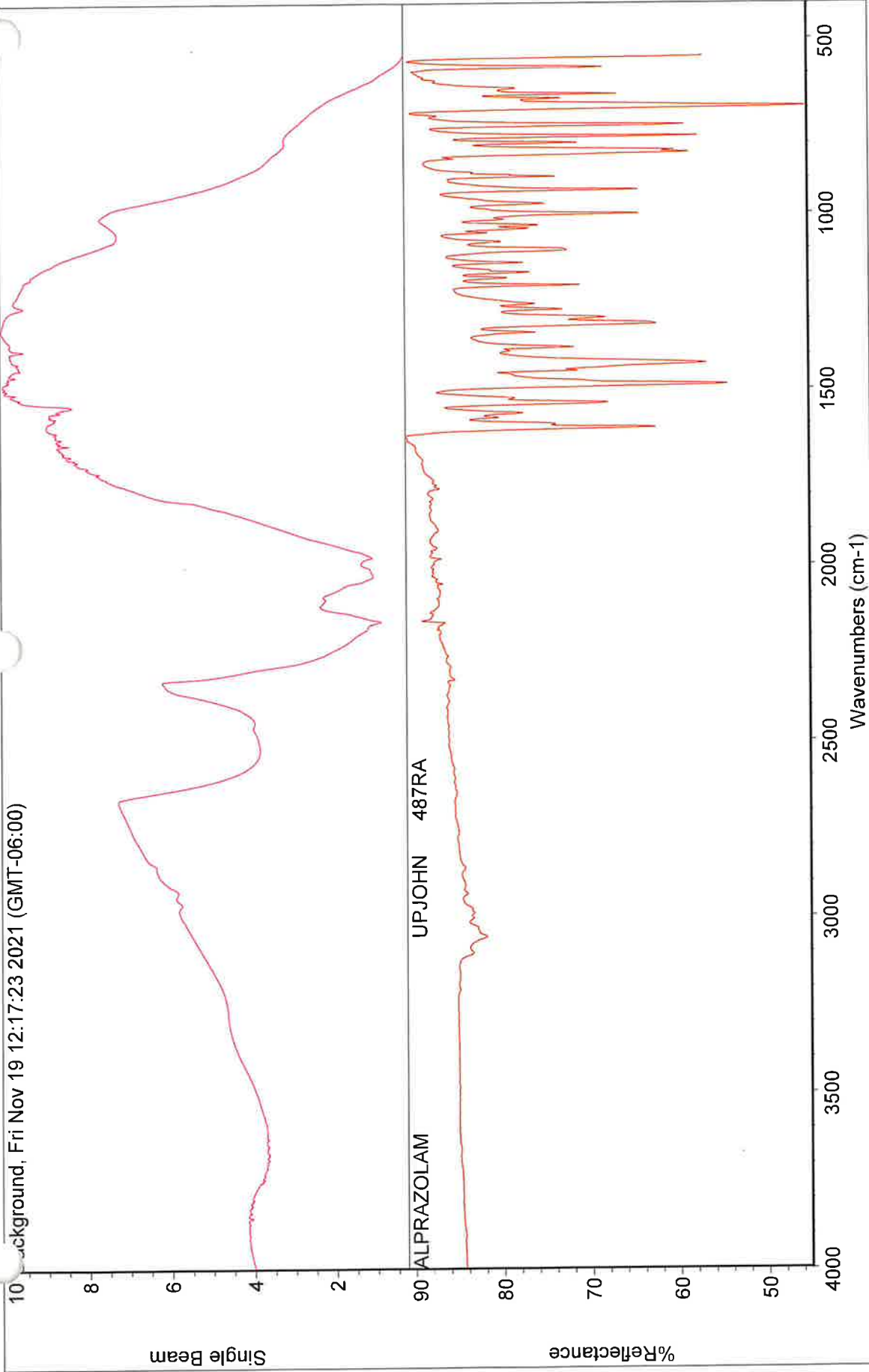


Search results list of matches

Index	Match	Compound Name	Library Name
1	98.58	ACETAMINOPHEN NEAT ZG SIGMA-ALDRICH LOT 088K0040	TBI ATR LIBRARY
2	98.58	ACETAMINOPHEN NEAT ZG SIGMA-ALDRICH LOT 088K0040	TBI ATR Drug Library
3	98.58	ACETAMINOPHEN NEAT ZG SIGMA-ALDRICH LOT 088K0040	TBI ATR #2
4	81.61	ACETAMINOPHEN NF REFERENCE STD PWF NEET WITH KBR 3MM PELLET	TBI Drug Library
5	28.16	Phenacetin USP Lot #F-4	TBI ATR LIBRARY
6	28.16	Phenacetin USP Lot #F-4	TBI ATR LIBRARY
7	28.16	Phenacetin USP Lot #F-4	TBI ATR Drug Library
8	28.16	Phenacetin USP Lot #F-4	TBI ATR #2
9	26.19	STD MDA HCL NEAT PWF	TBI Drug Library
10	25.10	3,4 METHYLENEDIOXYAMPHETAMINE HCL STD. .5NNAOH/CHCL3+HCL EX	TBI Drug Library

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Background, Fri Nov 19 12:17:23 2021 (GMT-06:00)



ALPRAZOLAM ~~NET~~ UPJOHN 487RA

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Detector: DTGS KBr
Sample gain: 8.0
Beamsplitter: KBr
Optical velocity: 0.4747
Source: IR
Aperture: 80.00

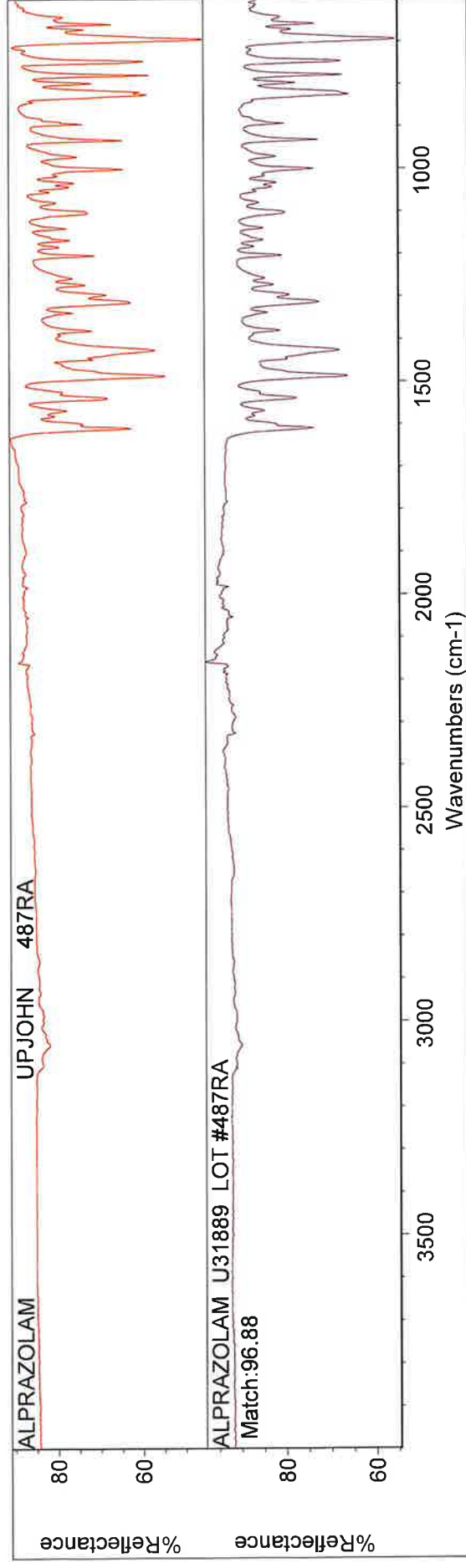
GADGET

Collection time: Fri Nov 19 12:19:51 2021 (GMT-06:00)

81

Search results for: ALPRAZOLAM
 Date: Fri Nov 19 12:20:10 2021 (GMT-06:00)
 Search algorithm: Correlation
 Regions searched: 3998.72-599.78

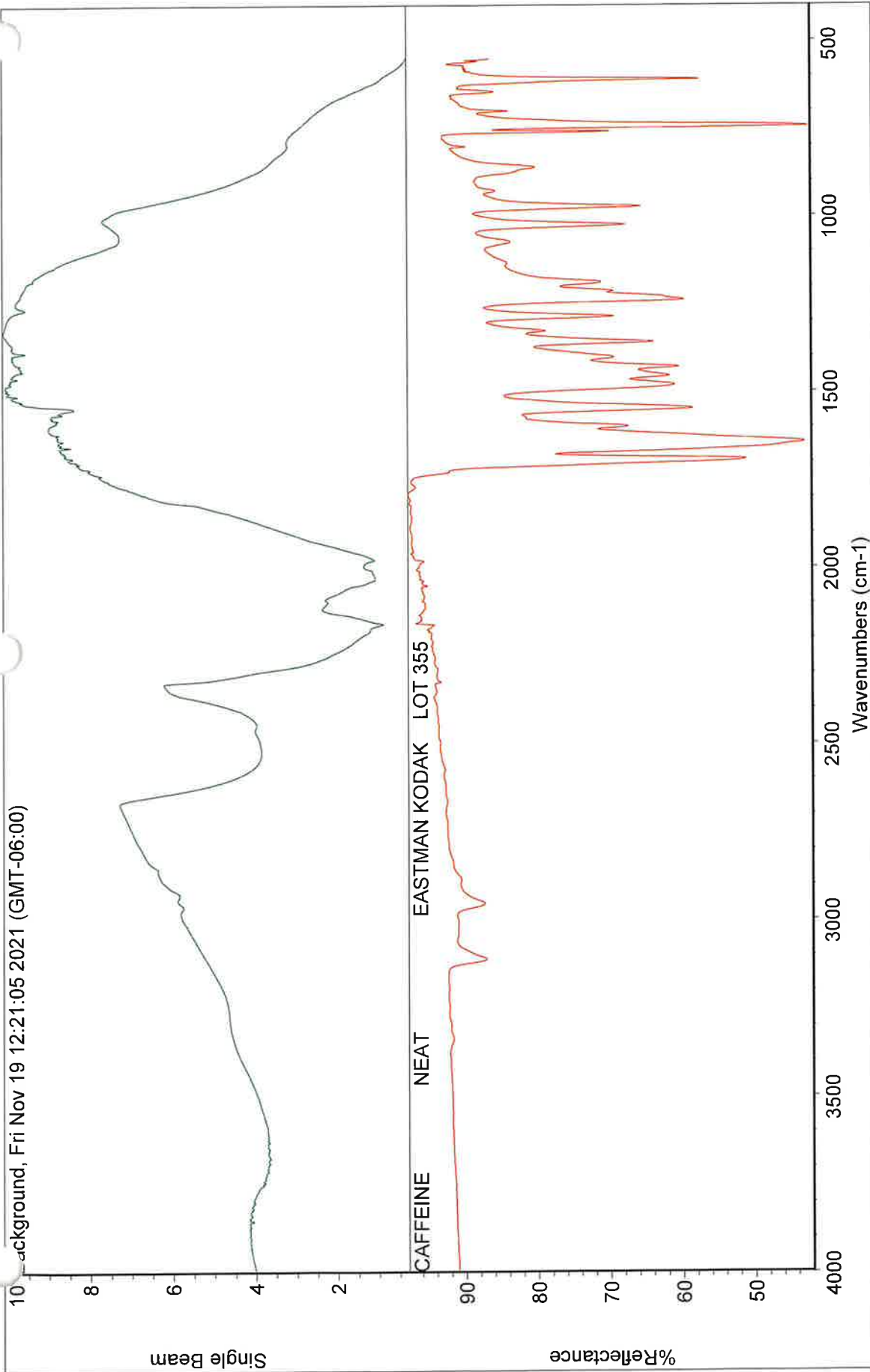
UPJOHN 487RA



Search results list of matches

Index	Match	Compound Name	Library Name
1	96.88	ALPRAZOLAM U31889 LOT #487RA	TBI ATR LIBRARY
2	96.88	ALPRAZOLAM U31889 LOT #487RA	TBI ATR LIBRARY
3	96.88	ALPRAZOLAM U31889 LOT#487RA	TBI ATR Drug Library
4	96.88	ALPRAZOLAM U31889 LOT #487RA	TBI ATR #2
5	76.51	ALPRAZOLAM STD LOT#487RA UPJOHN NEET WITH KBR 3MM PELLET PWF	TBI Drug Library
6	39.25	FLUALPRAZOLAM CAYMAN CHEMICAL LOT 0526790-23 NEAT EMC	TBI ATR LIBRARY
7	39.25	FLUALPRAZOLAM CAYMAN CHEMICAL LOT 0526790-23 NEAT EMC	TBI ATR Drug Library
8	39.25	FLUALPRAZOLAM CAYMAN CHEMICAL LOT 0526790-23 NEAT EMC	TBI ATR #2
9	34.93	Adinazolam Cayman Lot 0579199-6 NEAT LMN 4-1-20	TBI ATR LIBRARY
10	34.93	Adinazolam Cayman Lot 0579199-6 NEAT LMN 4-1-20	TBI ATR Drug Library

Background, Fri Nov 19 12:21:05 2021 (GMT-06:00)



CAFFEINE

NEAT

EASTMAN KODAK LOT 355

Number of sample scans: 16

Number of background scans: 16

Resolution: 4.000

Sample gain: 8.0

Detector: DTGS KBr

Beamsplitter: KBr

Optical velocity: 0.4747

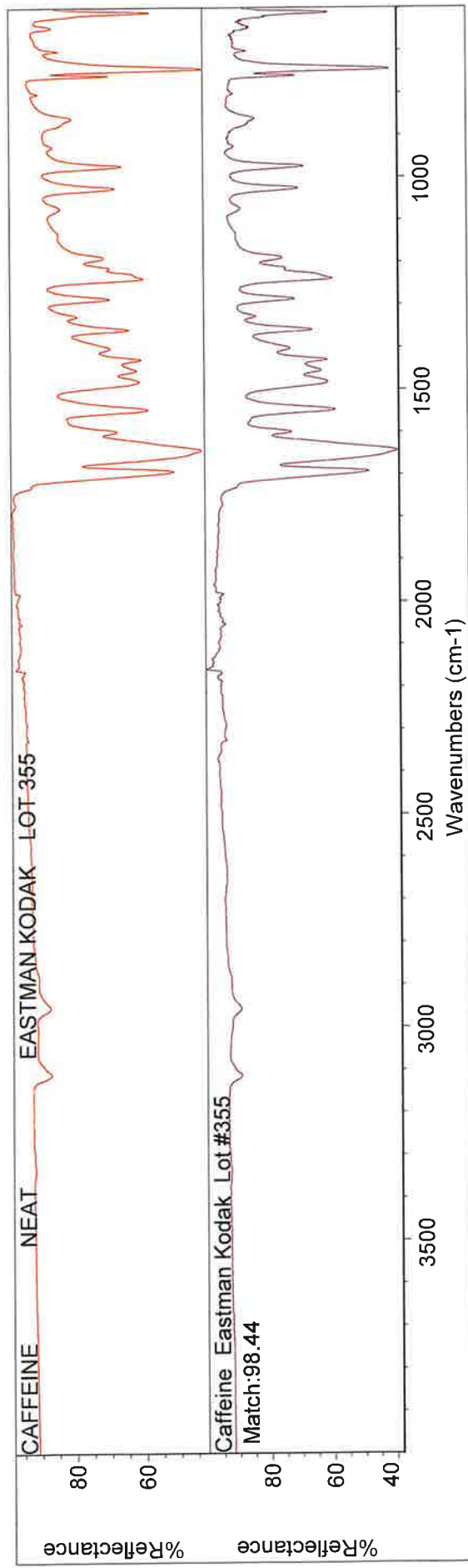
Aperture: 80.00

Collection time: Fri Nov 19 12:23:29 2021 (GMT-06:00)

GADGET

28

Search results for: CAFFEINE NEAT EASTMAN KODAK LOT 355
 Date: Fri Nov 19 12:24:08 2021 (GMT-06:00)
 Search algorithm: Correlation
 Regions searched: 3998.72-599.78

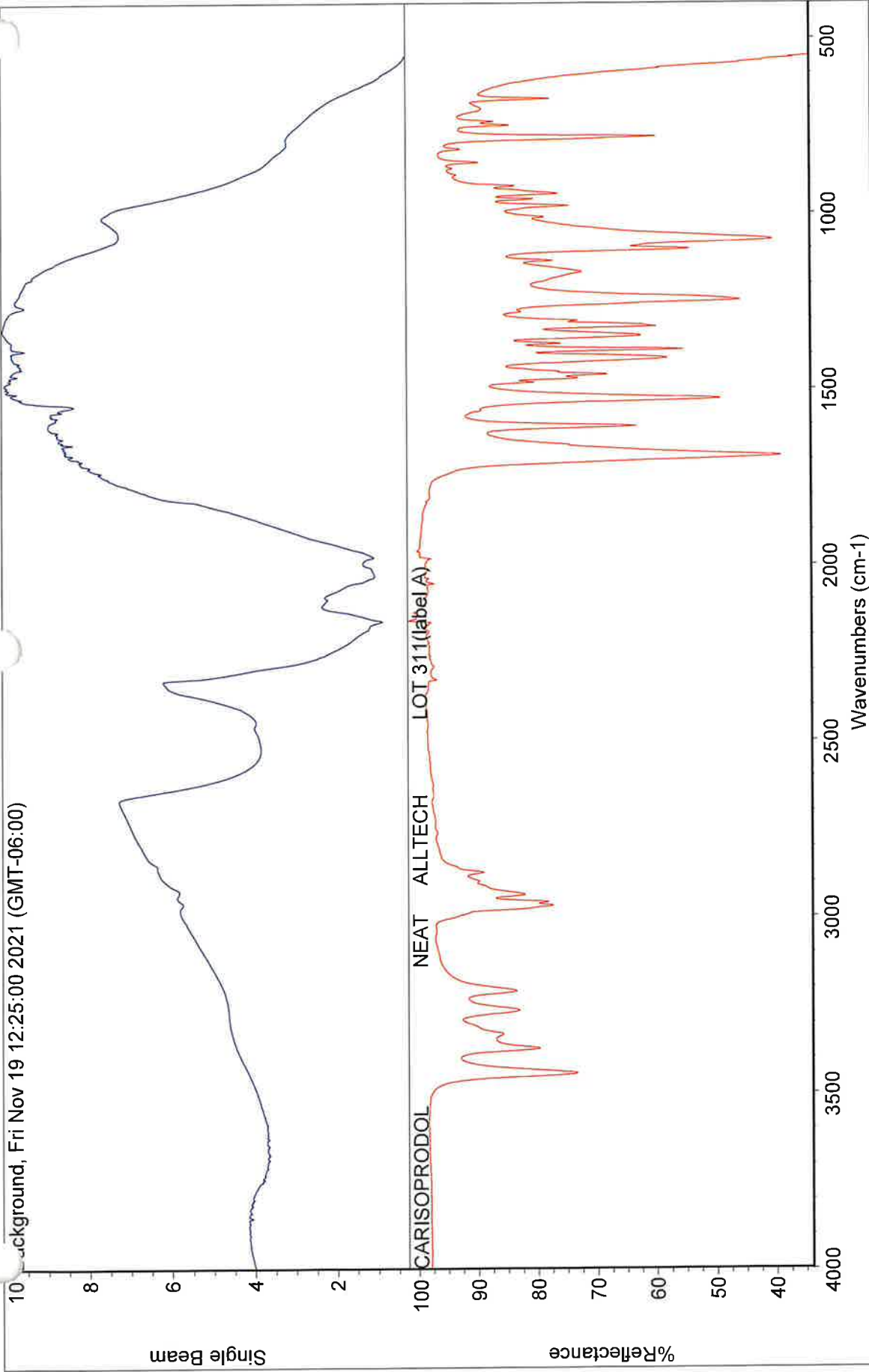


Search results list of matches

Index	Match	Compound Name	Library Name
1	98.44	Caffeine Eastman Kodak Lot #355	TBI ATR LIBRARY
2	98.44	Caffeine Eastman Kodak Lot #355	TBI ATR LIBRARY
3	98.44	Caffeine Eastman Kodak Lot #355	TBI ATR Drug Library
4	98.44	Caffeine Eastman Kodak Lot #355	TBI ATR #2
5	62.62	STD CAFFEINE	TBI Drug Library
6	39.30	Brorphine HCl Cayman Lot 0567046-8 NEAT LMN	TBI ATR Drug Library
7	39.30	Brorphine HCl Cayman Lot 0567046-8 NEAT LMN	TBI ATR #2
8	36.25	Chloroform Fisher Lot #024586	TBI ATR LIBRARY
9	36.25	Chloroform Fisher Lot #024586	TBI ATR LIBRARY
10	36.25	Chloroform Fisher Lot #024586	TBI ATR Drug Library

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Background, Fri Nov 19 12:25:00 2021 (GMT-06:00)

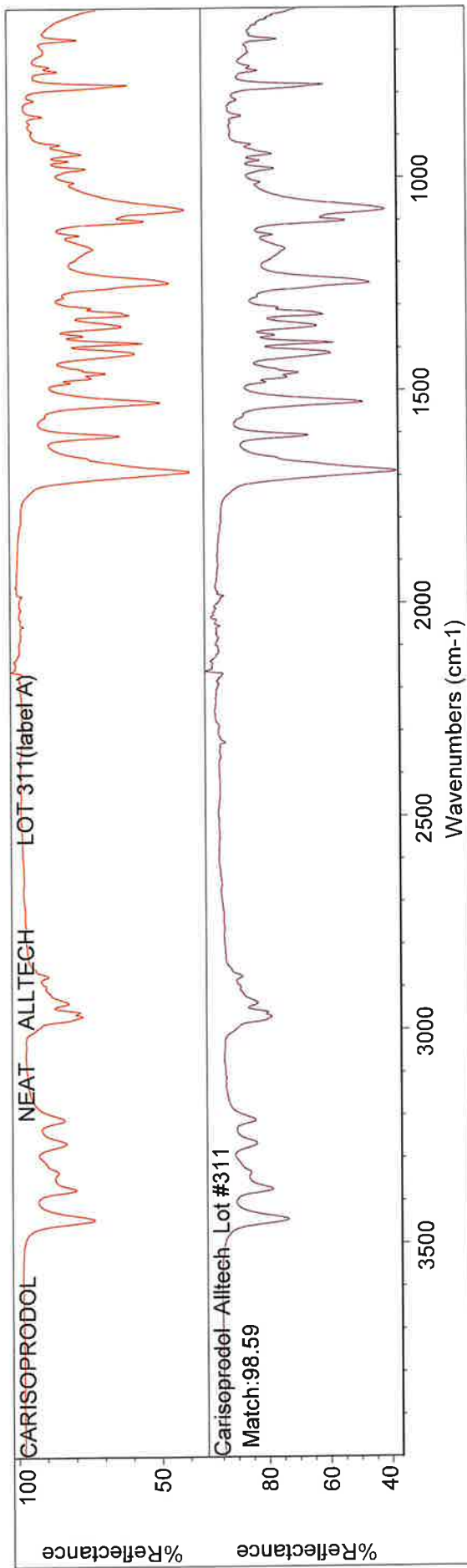


CARISOPRODOL NEAT ALLTECH LOT 311(label A) Number of sample scans: 16
Collection time: Fri Nov 19 12:28:13 2021 (GMT-06:00) GADGET Number of background scans: 16
Detector: DTGS KBr Sample gain: 8.0 Resolution: 4.000
Beamsplitter: KBr Optical velocity: 0.4747
Source: IR Aperture: 80.00

18

Search results for: CARISOPRODOL
 Date: Fri Nov 19 12:28:37 2021 (GMT-06:00)
 Search algorithm: Correlation
 Regions searched: 3998.72-599.78

NEAT ALLTECH LOT (label A)

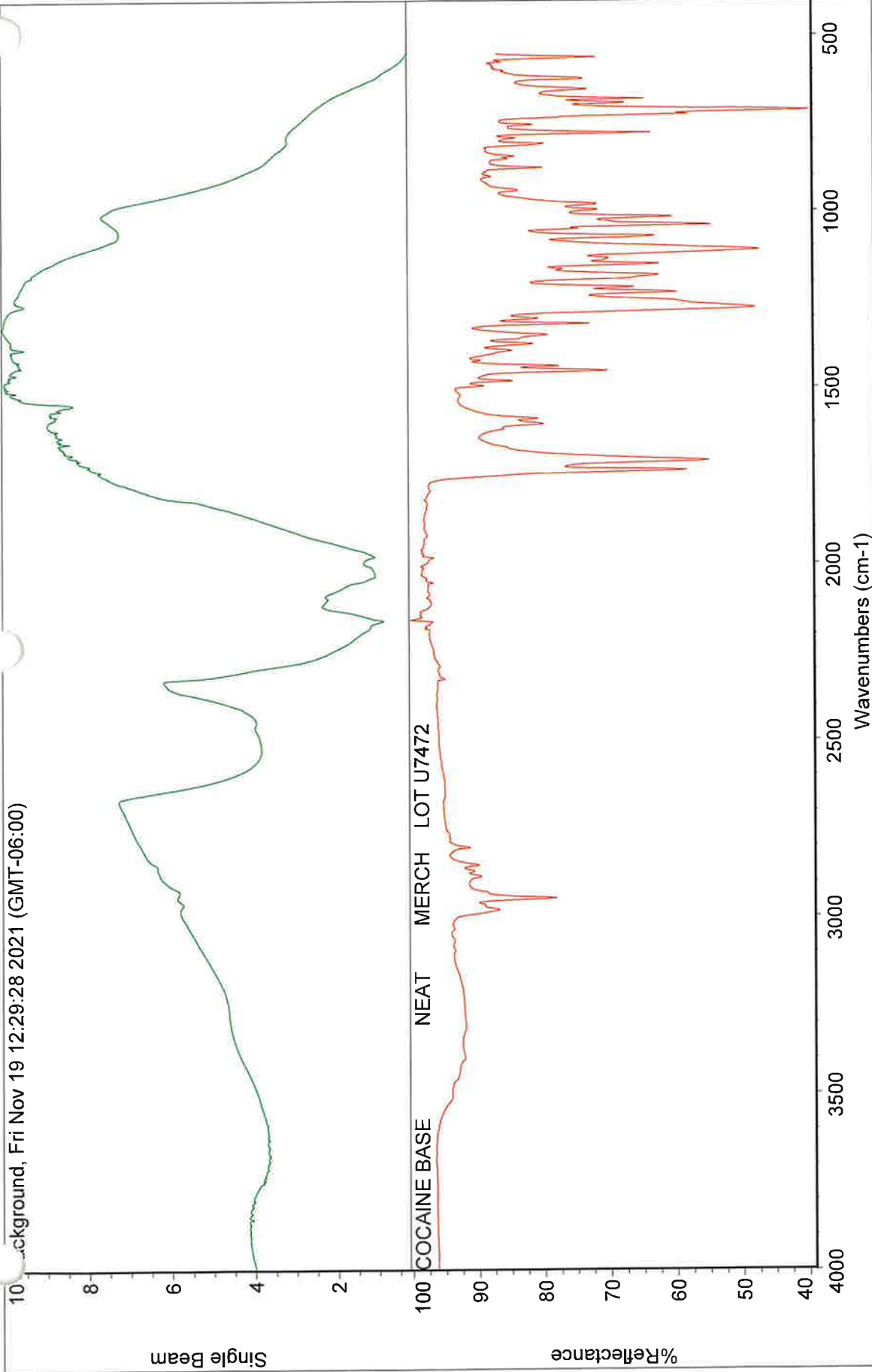


Search results list of matches

Index	Match	Compound Name	Library Name
1	98.59	Carisoprodol Alltech Lot #311	TBI ATR LIBRARY
2	98.59	Carisoprodol Alltech Lot #311	TBI ATR LIBRARY
3	98.59	Carisoprodol Alltech Lot #311	TBI ATR Drug Library
4	98.59	Carisoprodol Alltech Lot #311	TBI ATR #2
5	40.62	FLUNITRAZEPAM STD HOFFMANN LA-ROCHE LOT PP-1 NEAT PWF	TBI Drug Library
6	33.76	STD. MEPROBAMATE USP REF. STD	TBI Drug Library
7	31.10	METHCATHINONE HCL STANDARD SIGMA LOT 42H36051 PWF	TBI Drug Library
8	29.47	NITRAZEPAM STD ALLTECH APPLIED SCIENCE LOT PP271 NEET WITH K	TBI Drug Library
9	28.48	HALAZEPAM STD. NEET WHS	TBI Drug Library
10	27.81	DIAZEPAM (RO 5-2807) LOT# 677038 REFERENCE STD. WHS	TBI Drug Library

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Background, Fri Nov 19 12:29:28 2021 (GMT-06:00)



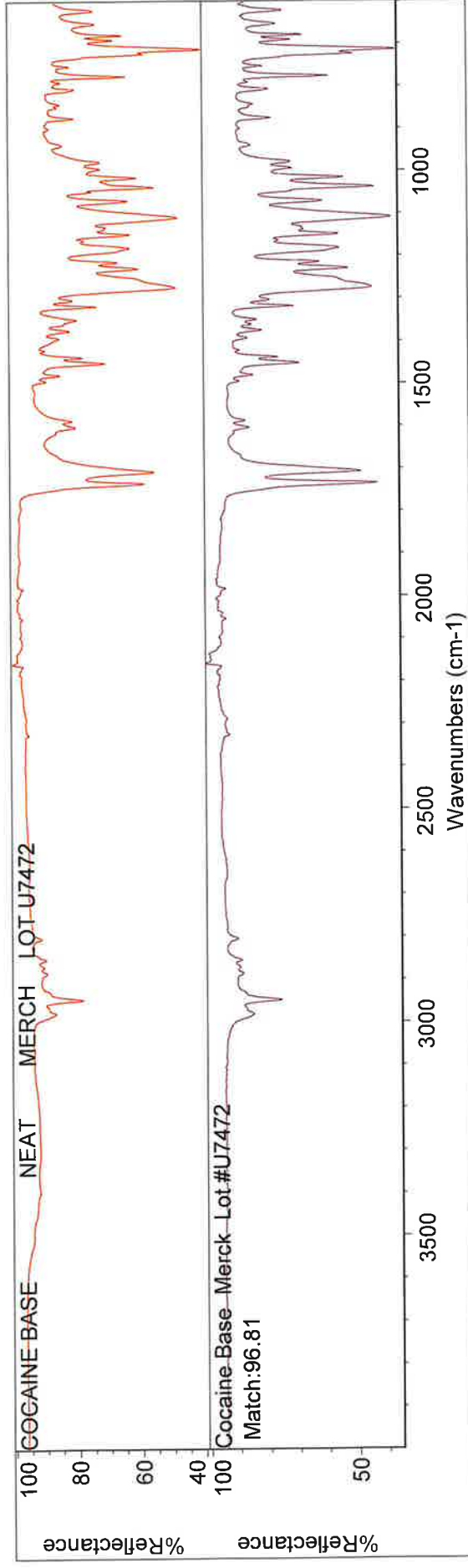
COCAINE BASE NEAT MERCH LOT U7472

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Detector: DTGS KBr
Sample gain: 8.0
Beamsplitter: KBr
Optical velocity: 0.4747
Source: IR
Aperture: 80.00

Collection time: Fri Nov 19 12:32:03 2021 (GMT-06:00) GADGET

28

Search results for: COCAINE BASE NEAT MERCH LOT U7472
 Date: Fri Nov 19 12:32:17 2021 (GMT-06:00)
 Search algorithm: Correlation
 Regions searched: 3998.72-599.78

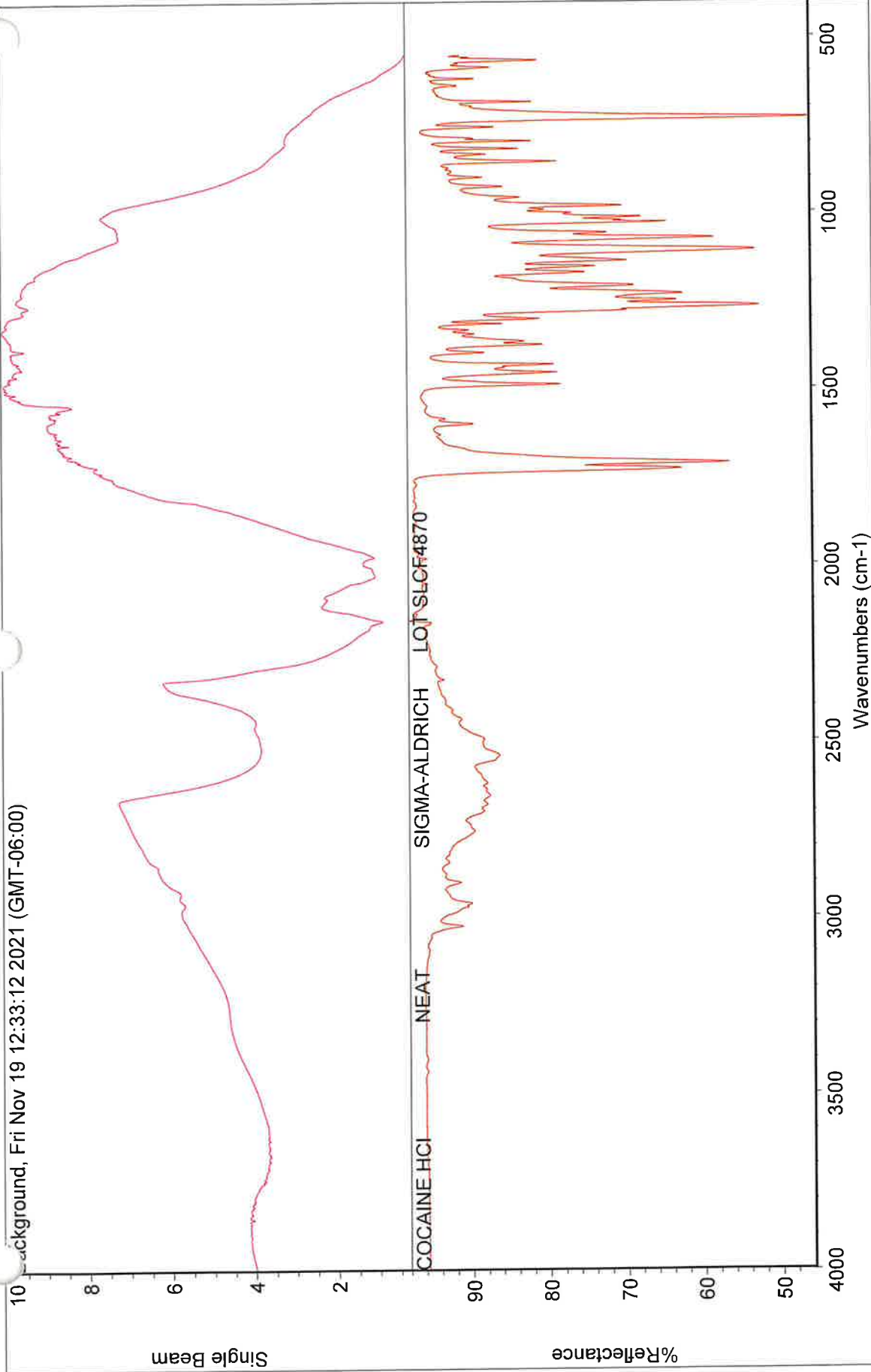


Search results list of matches

Index	Match	Compound Name	Library Name
1	96.81	Cocaine Base Merck Lot #U7472	TBI ATR LIBRARY
2	96.81	Cocaine Base Merck Lot #U7472	TBI ATR LIBRARY
3	96.81	Cocaine Base Merck Lot #U7472	TBI ATR Drug Library
4	96.81	Cocaine Base Merck Lot #U7472	TBI ATR #2
5	73.16	STD COCAINE FREE BASE (MERCK) PWF	TBI Drug Library
6	42.68	NANDROLONE BENZOATE STERALOIDS LOT# B0650 NEAT GBE	TBI ATR LIBRARY
7	42.68	NANDROLONE BENZOATE STERALOIDS LOT# B0650 NEAT GBE	TBI ATR Drug Library
8	42.68	NANDROLONE BENZOATE STERALOIDS LOT# B0650 NEAT GBE	TBI ATR #2
9	37.92	(-)-COCAINE-(+)-TARTRATE	TBI Drug Library
10	30.91	Testosterone Benzoate Sigma Lot #49F0246	TBI ATR LIBRARY

28

Background, Fri Nov 19 12:33:12 2021 (GMT-06:00)



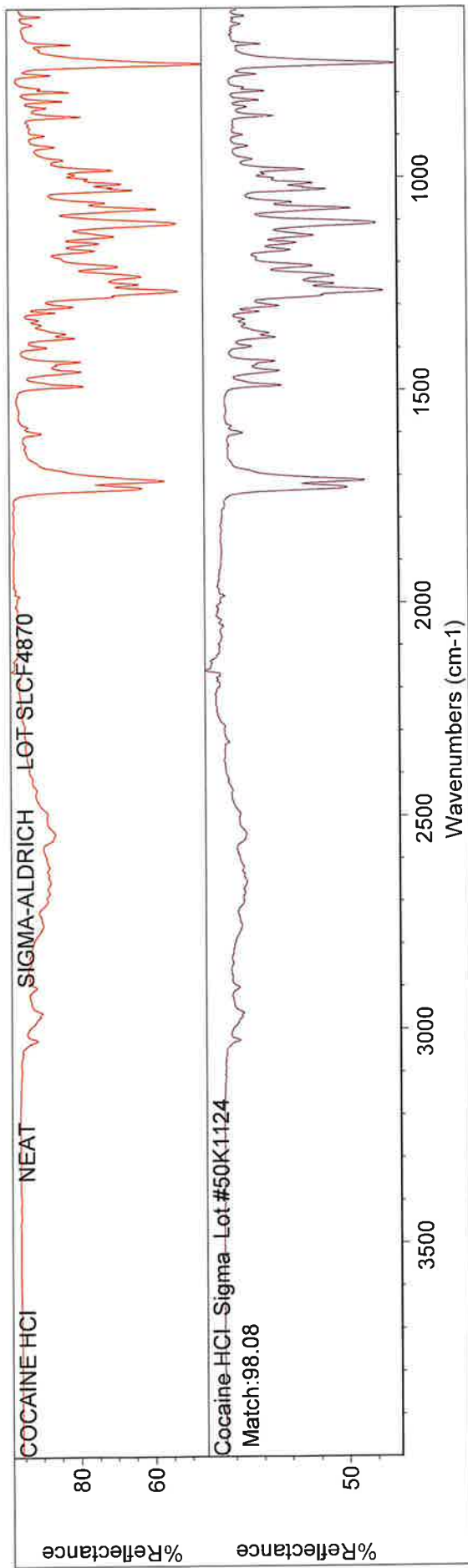
COCAINE HCl	NEAT	SIGMA-ALDRICH	LOT SLCF4870	Number of sample scans: 16
				Number of background scans: 16
				Resolution: 4.000
				Detector: DTGS KBr
				Sample gain: 8.0
				Beamsplitter: KBr
				Optical velocity: 0.4747
				Source: IR
				Aperture: 80.00

Collection time: Fri Nov 19 12:36:20 2021 (GMT-06:00)

GADGET

lg

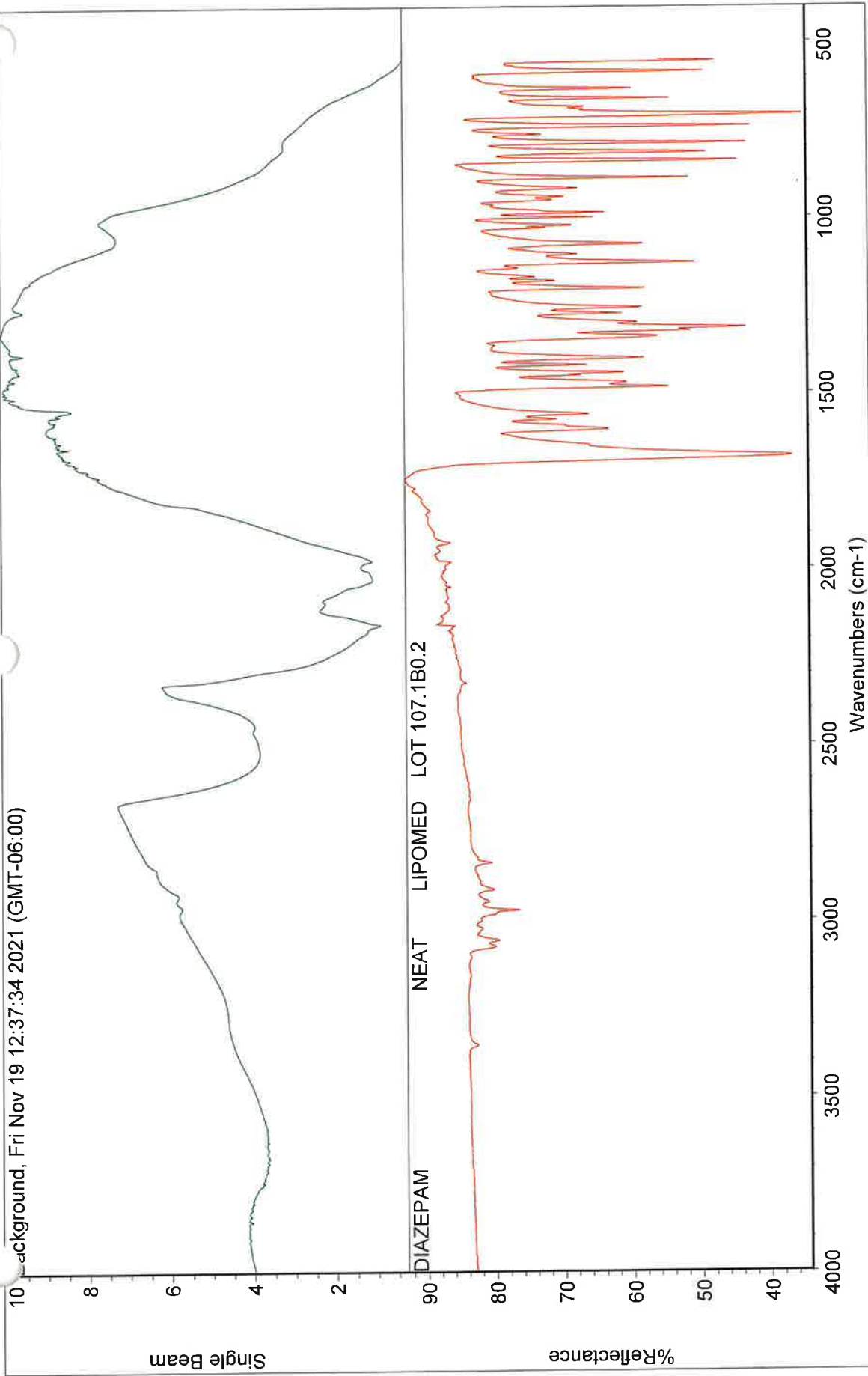
Search results for: COCAINE HCl NEAT SIGMA-ALDRICH LOT SLCF4870
 Date: Fri Nov 19 12:36:40 2021 (GMT-06:00)
 Search algorithm: Correlation
 Regions searched: 3998.72-599.78



Search results list of matches

Index	Match	Compound Name	Library Name
1	308	Cocaine HCl Sigma Lot #50K1124	TBI ATR LIBRARY
2	31	Cocaine HCl Sigma Lot #50K1124	TBI ATR LIBRARY
3	31	Cocaine HCl Sigma Lot #50K1124	TBI ATR Drug Library
4	80	Cocaine HCl Sigma Lot #50K1124	TBI ATR #2
5	33	STD COCAINE HCL (MALINCKRODT)PWF	TBI Drug Library
6	36	COCAINE HCL STD SIGMA 48F0208 NEAT PWF	TBI Drug Library
7	38	STD COCAINE HCL NEAT WITH KBR 3MM (MALINCKRODT)	TBI Drug Library
8	37	COCAINE HCL MANITOL 50:50 MIXTURE PWF	TBI Drug Library
9	243	TILETAMINE STD USP LOT#F0C019	TBI ATR LIBRARY
10	242	TILETAMINE STD USP LOT#F0C019	TBI ATR Drug Library

Background, Fri Nov 19 12:37:34 2021 (GMT-06:00)



DIAZEPAM

NEAT LIPOMED LOT 107.1B0.2

Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Detector: DTGS KBr
Sample gain: 8.0
Beamsplitter: KBr
Optical velocity: 0.4747
Source: IR
Aperture: 80.00

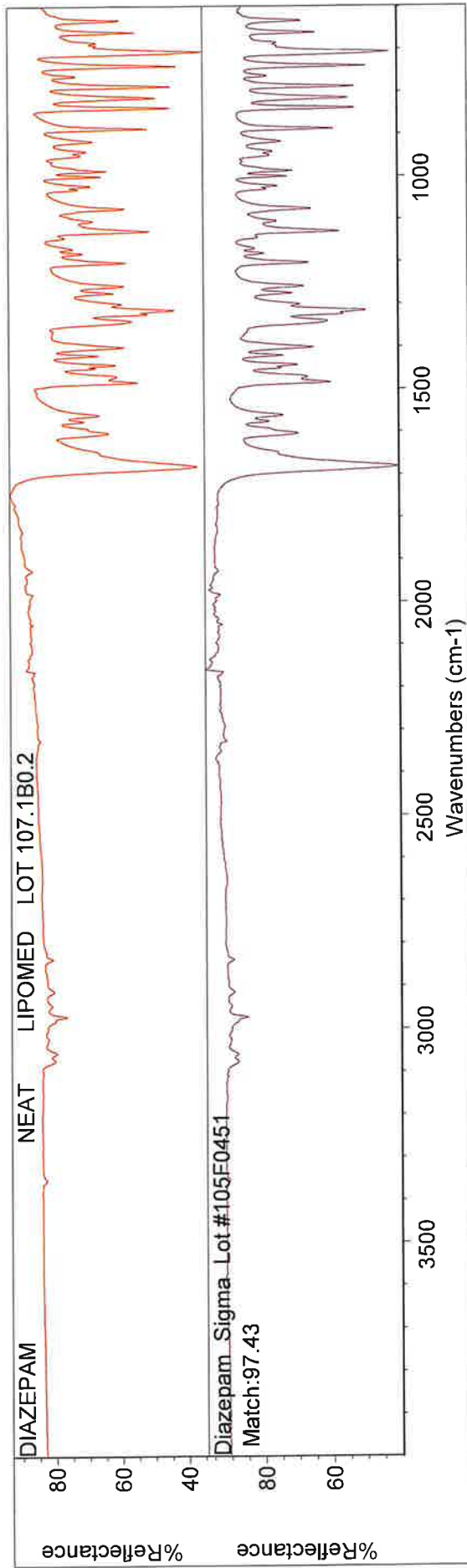
Collection time: Fri Nov 19 12:39:46 2021 (GMT-06:00)

GADGET

pg

Search results for: DIAZEPAM
 Date: Fri Nov 19 12:40:02 2021 (GMT-06:00)
 Search algorithm: Correlation
 Regions searched: 3998.72-599.78

NEAT LIPOMED LOT 107.1B0.2

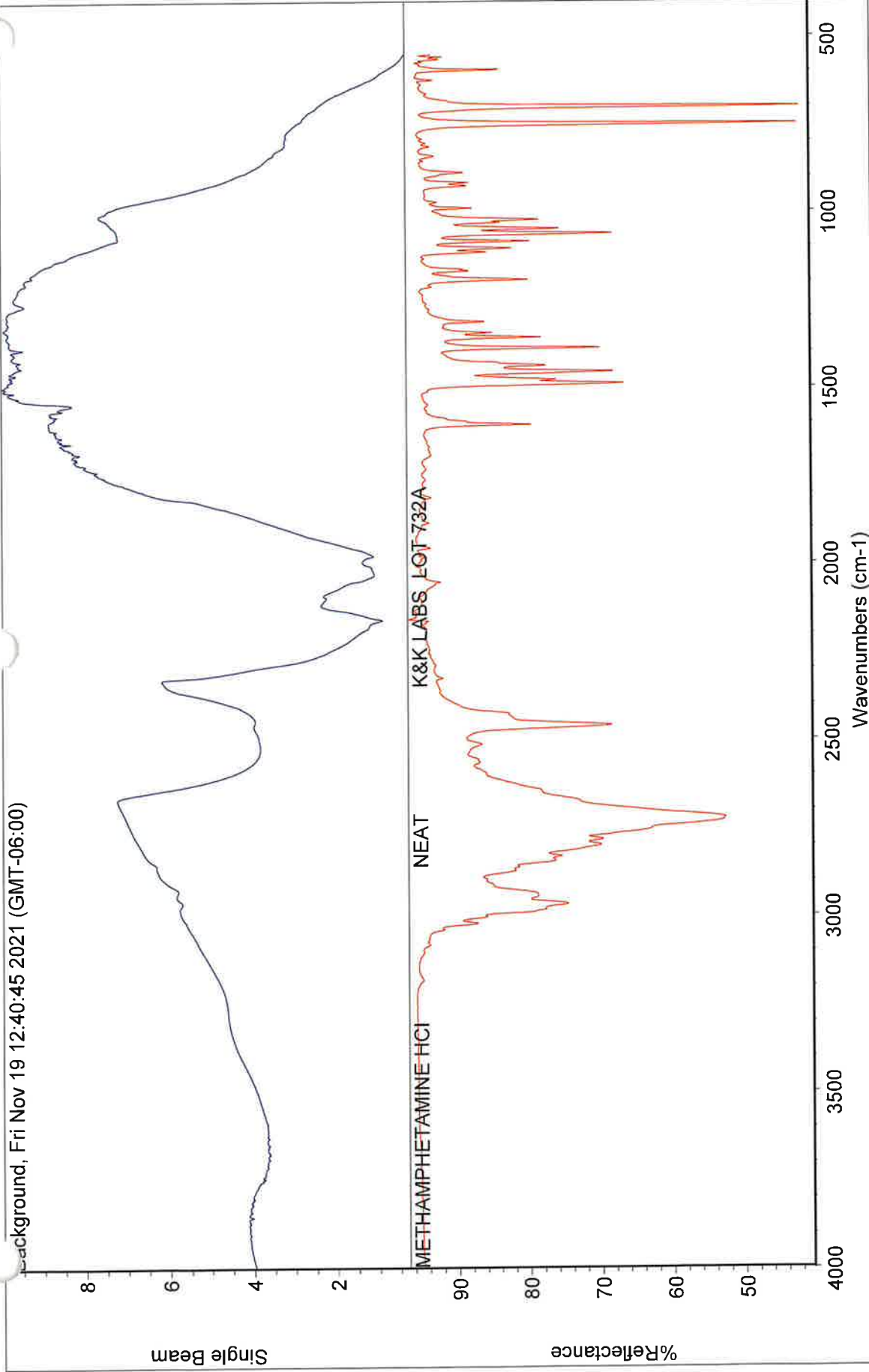


Search results list of matches

Index	Match	Compound Name	Library Name
1	315	Diazepam Sigma Lot #105F0451	TBI ATR LIBRARY
2	38	Diazepam Sigma Lot #105F0451	TBI ATR LIBRARY
3	38	Diazepam Sigma Lot #105F0451	TBI ATR Drug Library
4	87	Diazepam Sigma Lot #105F0451	TBI ATR #2
5	43	DIAZEPAM(RO 5-2807) LOT# 677038 REFERENCE STD. WHS	TBI Drug Library
6	147	STD PRAZEPAM WARNER-LAMBERT LOT32 NEAT WITH KBR3MM PWF	TBI Drug Library
7	556	alpha-PYRROLIDINOHEXANOPHENONE CAYMAN CHEMICAL LOT 0457893-	TBI ATR LIBRARY
8	374	alpha-PYRROLIDINOHEXANOPHENONE CAYMAN CHEMICAL LOT 0457893-	TBI ATR Drug Library
9	319	alpha-PYRROLIDINOHEXANOPHENONE CAYMAN CHEMICAL LOT 0457893-	TBI ATR #2
10	10	BENZPHETAMINE HCL UPJOHN STD J-O441 NEET WITH KBR PWF	TBI Drug Library

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Background, Fri Nov 19 12:40:45 2021 (GMT-06:00)



METHAMPHETAMINE HCl

NEAT

K&K LABS LOT 732A

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

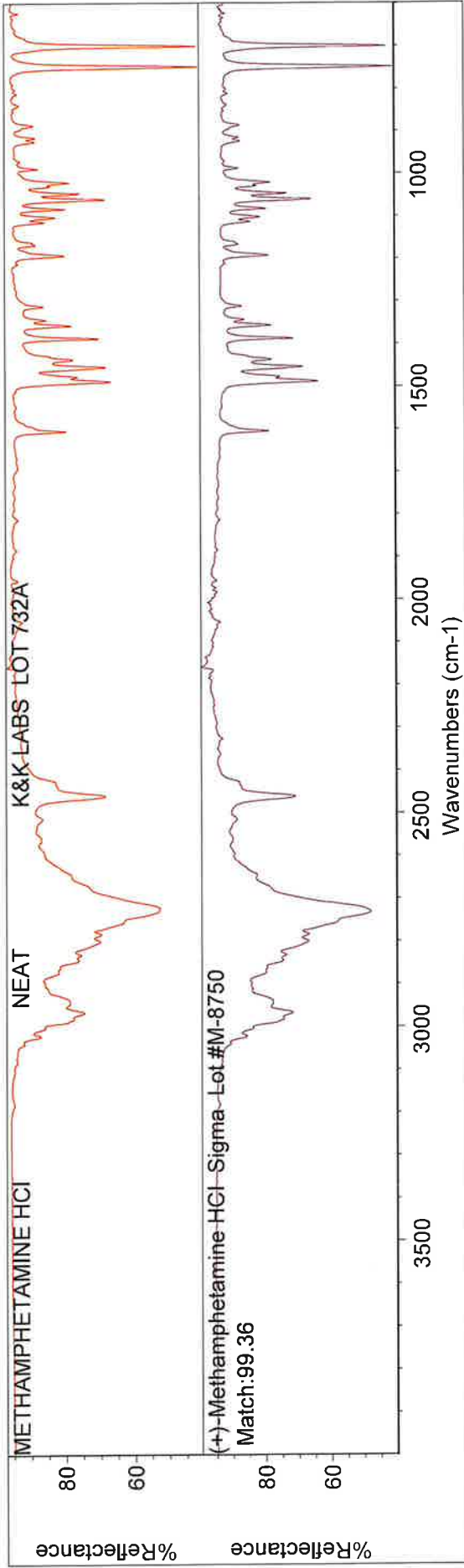
Collection time: Fri Nov 19 12:43:48 2021 (GMT-06:00)

GADGET

99

Search results for: METHAMPHETAMINE HCl
Date: Fri Nov 19 12:44:10 2021 (GMT-06:00)
Search algorithm: Correlation
Regions searched: 3998.72-599.78

NEAT K&K LABS LOT 732A

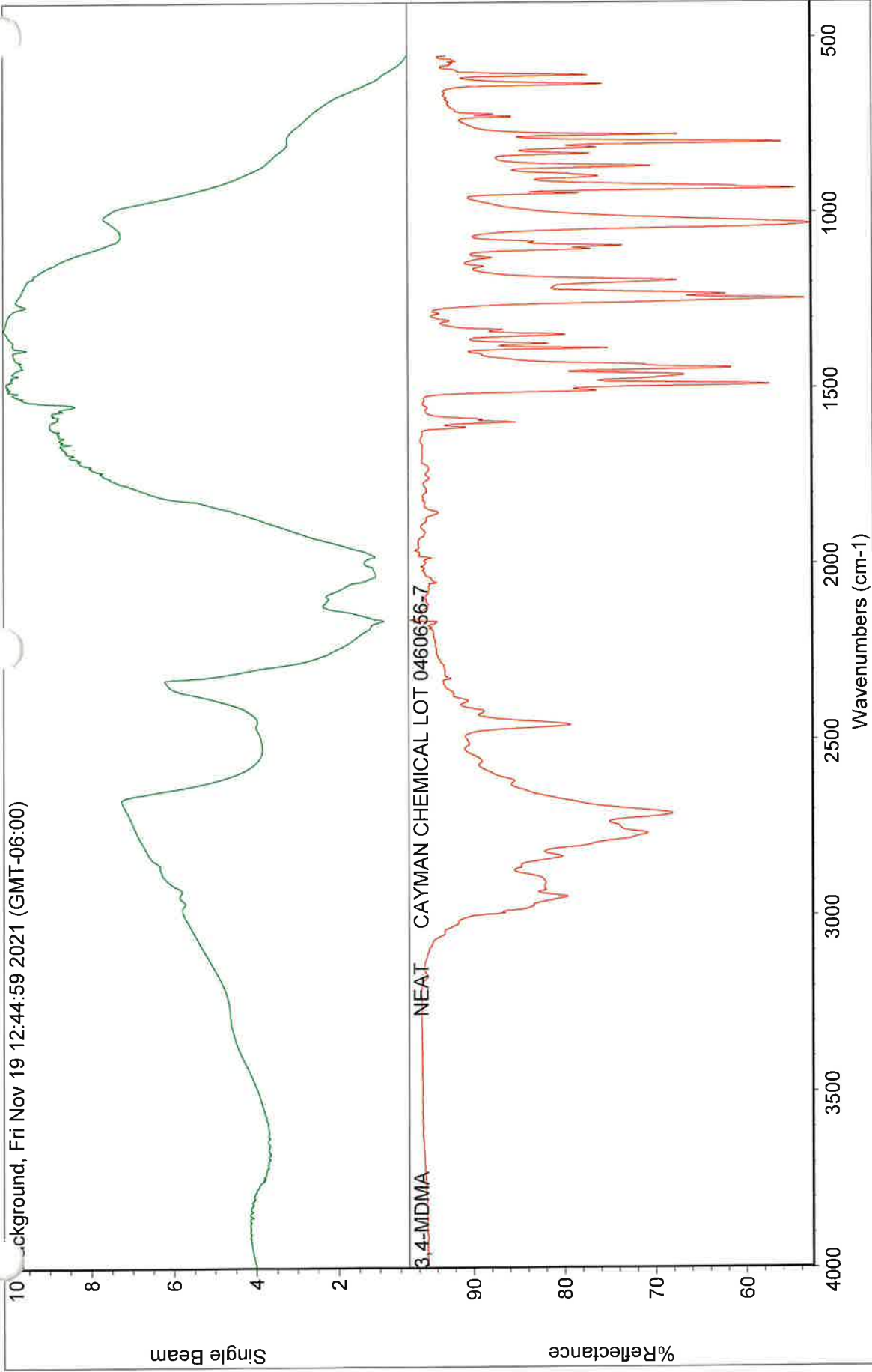


Search results list of matches

Index	Match	Compound Name	Library Name
1	99.36	(+)-Methamphetamine HCl Sigma Lot #M-8750	TBI ATR LIBRARY
2	99.36	(+)-Methamphetamine HCl Sigma Lot #M-8750	TBI ATR LIBRARY
3	99.36	(+)-Methamphetamine HCl Sigma Lot #M-8750	TBI ATR Drug Library
4	99.36	(+)-Methamphetamine HCl Sigma Lot #M-8750	TBI ATR #2
5	98.87	(D,L)-Methamphetamine HCl K & K Lot #732A	TBI ATR LIBRARY
6	98.87	(D,L)-Methamphetamine HCl K & K Lot #732A	TBI ATR LIBRARY
7	98.87	(D,L)-Methamphetamine HCl K & K Lot #732A	TBI ATR Drug Library
8	98.87	(D,L)-Methamphetamine HCl K & K Lot #732A	TBI ATR #2
9	98.70	(-)-Methamphetamine HCl Sigma Lot #44H0081	TBI ATR LIBRARY
10	98.70	(-)-Methamphetamine HCl Sigma Lot #44H0081	TBI ATR Drug Library

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Background, Fri Nov 19 12:44:59 2021 (GMT-06:00)



3,4-MDMA

NEAT CAYMAN CHEMICAL LOT 0460656-7

Number of sample scans: 16

Number of background scans: 16

Resolution: 4.000

Detector: DTGS KBr

Sample gain: 8.0

Beamsplitter: KBr

Optical velocity: 0.4747

Source: IR

Collection time: Fri Nov 19 12:47:40 2021 (GMT-06:00)

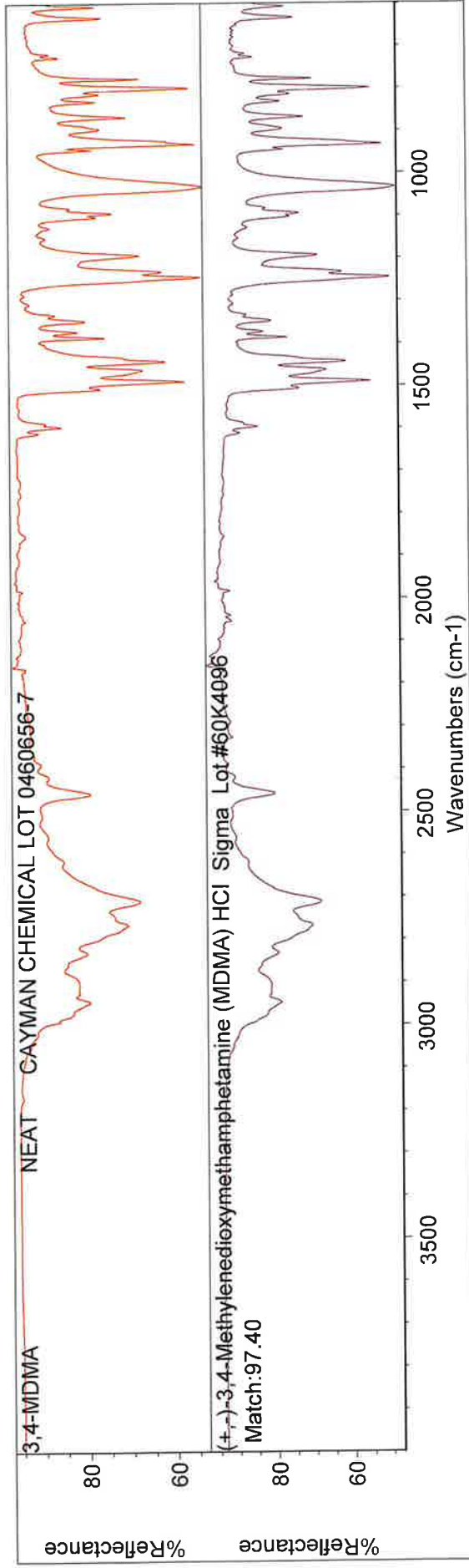
GADGET

22

Search results for: 3,4-MDMA
 Date: Fri Nov 19 12:47:55 2021 (GMT-06:00)
 Search algorithm: Correlation
 Regions searched: 3998.72-599.78

NEAT

CAYMAN CHEMICAL LOT 0460656-7

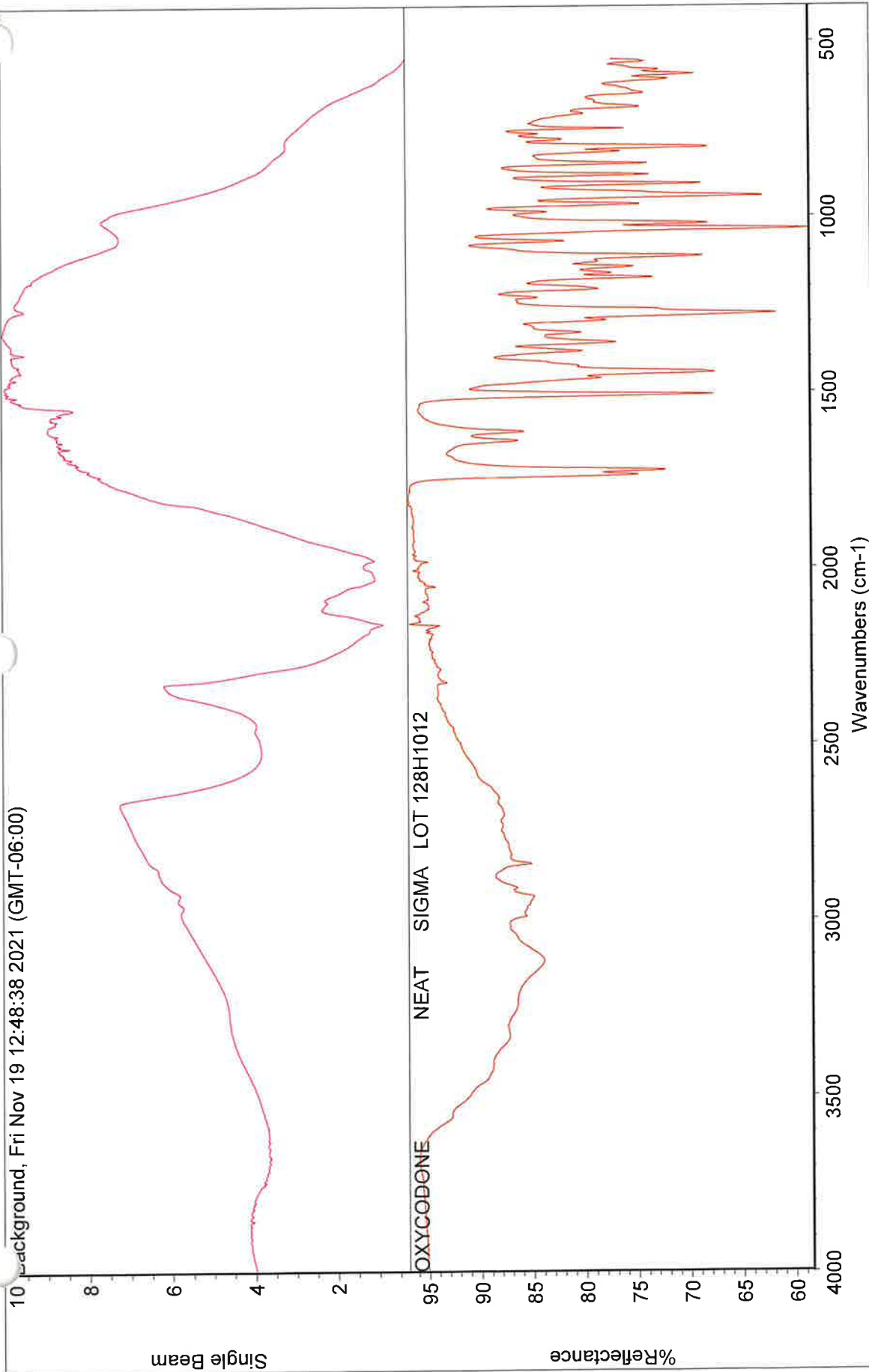


Search results list of matches

Index	Match	Compound Name	Library Name
1	97.40	(+,-)-3,4-Methylenedioxyamphetamine (MDMA) HCl	Sigma L
2	97.40	(+,-)-3,4-Methylenedioxyamphetamine (MDMA) HCl	Sigma L
3	97.40	(+,-)-3,4-Methylenedioxyamphetamine (MDMA) HCl	Sigma L
4	97.40	(+,-)-3,4-Methylenedioxyamphetamine (MDMA) HCl	Sigma L
5	77.72	MDMA HCL STD SIGMA LOT70H4000 NEAT PWF	TBI Drug Library
6	59.57	3,4-Methylenedioxypropylamphetamine (MDPA) HCl	Alltech Lot
7	59.57	3,4-Methylenedioxypropylamphetamine (MDPA) HCl	Alltech Lot
8	59.57	3,4-Methylenedioxypropylamphetamine (MDPA) HCl	Alltech Lot
9	59.57	3,4-Methylenedioxypropylamphetamine (MDPA) HCl	Alltech Lot
10	55.88	N-HYDROXY-MDA HCL STD ALLTECH LOT 5601 NEAT PWF	TBI Drug Library

lg

Background, Fri Nov 19 12:48:38 2021 (GMT-06:00)



OXYCODONE

NEAT SIGMA LOT 128H1012

Detector: DTGS KBr
Beamsplitter: KBr
Source: IR

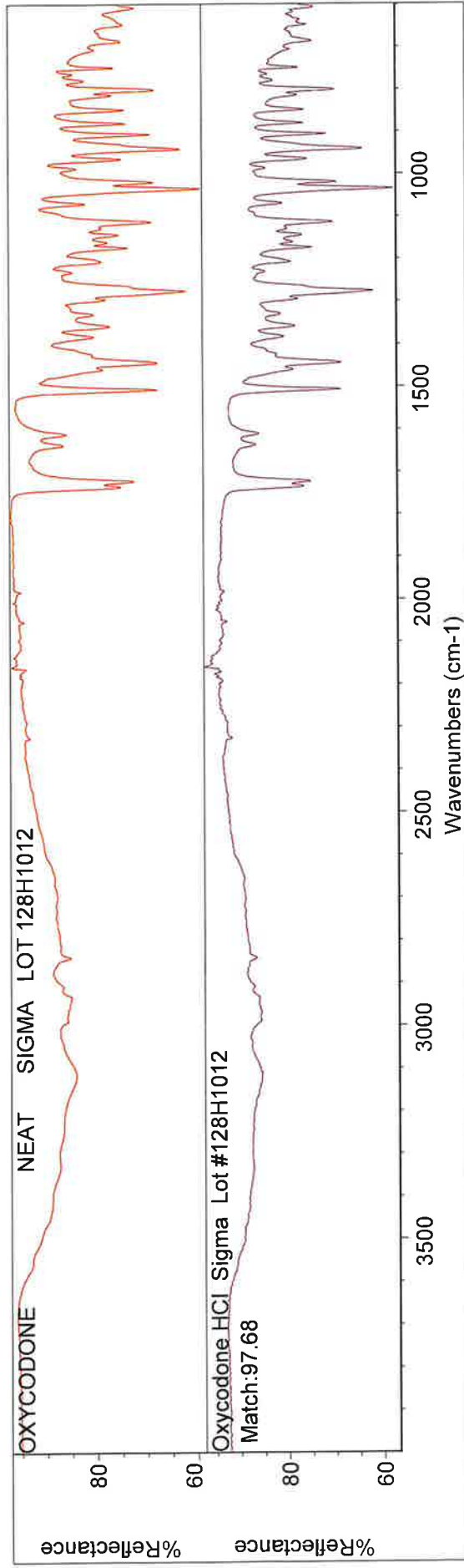
Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 8.0
Optical velocity: 0.4747
Aperture: 80.00

Collection time: Fri Nov 19 12:51:01 2021 (GMT-06:00)

GADGET

18

Search results for: OXYCODONE NEAT SIGMA LOT 128H1012
 Date: Fri Nov 19 12:51:21 2021 (GMT-06:00)
 Search algorithm: Correlation
 Regions searched: 3998.72-599.78



Search results list of matches

Index	Match	Compound Name	Library Name
1	97.68	Oxycodone HCl Sigma Lot #128H1012	TBI ATR LIBRARY
2	97.68	Oxycodone HCl Sigma Lot #128H1012	TBI ATR LIBRARY
3	97.68	Oxycodone HCl Sigma Lot #128H1012	TBI ATR Drug Library
4	97.68	Oxycodone HCl Sigma Lot #128H1012	TBI ATR #2
5	66.81	OXYCODONE HCL SIGMA LOT 128H1012 0.5N NaOH>CHCL3+HCL EXT GB	TBI ATR LIBRARY
6	66.81	OXYCODONE HCL SIGMA LOT 128H1012 0.5N NaOH>CHCL3+HCL EXT GB	TBI ATR Drug Library
7	66.81	OXYCODONE HCL SIGMA LOT 128H1012 0.5N NaOH>CHCL3+HCL EXT GB	TBI ATR #2
8	43.50	DIHYDROCODEINE STD. HCL+BASE/CHCL3 EXT. WHS	TBI Drug Library
9	37.16	DIHYDROCODEINE BASE CHCL3 EXT OF DIHYDROCODEINE STD. WHS	TBI Drug Library
10	35.38	DIHYDROCODEINE BASE FROM DIHYDROCODEINE BITARTRATE ALLTECH L	TBI Drug Library

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ATR Maintenance Log

Instrument ID

GADGET

[illegible]

Other Maintenance

[illegible]

ValPro Qualification Report

Qualification test: Nicolet iS20 system KBr - PV

Operator: Drugs ATR

Date: Friday, November 19, 2021 8:42:08 AM (GMT-06:00)

Instrument: Nicolet iS20 Serial number: BEP2110574

Filename: Nicolet iS20 system KBr - PV_20211119_084208.spg

Test description	High limit	Low limit	Measured	Result
Energy ratio				
Energy ratio 4000 / 2000	1.00	0.20	0.40	Pass
Energy ratio 2000 / 1000	4.00	0.80	1.45	Pass
Noise level				
P-P noise 4050 - 3950 (%T)	0.25	0.00	0.03	Pass
P-P noise 2050 - 1950 (%T)	0.221	0.00	0.034	Pass
P-P noise 1050 - 950 (%T)	0.10	0.00	0.03	Pass
P-P noise 550 - 450 (%T)	1.50	0.00	0.42	Pass
RMS noise 4050 - 3950	0.05	0.00	0.00	Pass
RMS noise 2050 - 1950	0.039	0.00	0.007	Pass
RMS noise 1050 - 950	0.014	0.00	0.008	Pass
RMS noise 550 - 450	0.30	0.00	0.08	Pass
Detector linearity				
Slope	1.10	0.90	1.05	Pass
Intercept (%T)	1.00	-1.00	0.05	Pass

Performed by: *Lg* Title: _____ Date: 11/19/21

Approved by: _____ Title: _____ Date: _____

Comments: _____

Digital comment(s):

No digital comments found.

ValPro Qualification Report

Qualification test: Nicolet iS20 system KBr - USP

Operator: Drugs ATR

Date: Friday, November 19, 2021 8:52:47 AM (GMT-06:00)

Instrument: Nicolet iS20 Serial number: BEP2110574

Filename: Nicolet iS20 system KBr - USP_20211119_085247.spg

Test description	High limit	Low limit	Measured	Result
Wavenumber accuracy				
Peak at 3060.0 (cm-1)	3061.0	3059.0	3059.7	Pass
Peak at 2849.5 (cm-1)	2850.5	2848.5	2849.3	Pass
Peak at 1942.9 (cm-1)	1943.9	1941.9	1942.6	Pass
Peak at 1601.2 (cm-1)	1602.2	1600.2	1601.1	Pass
Peak at 1583.0 (cm-1)	1584.0	1582.0	1583.0	Pass
Peak at 1154.5 (cm-1)	1155.5	1153.5	1154.5	Pass
Peak at 1028.3 (cm-1)	1029.3	1027.3	1028.4	Pass

Performed by:  Title: _____ Date: 11/19/21

Approved by: _____ Title: _____ Date: _____

Comments: _____

Digital comment(s):

No digital comments found.

TBI
BEP2110574

11/19/2021 8:57:53 AM
Nicolet iS20

SJ

em	Status	Current	Acceptable Range
Laser Current	Pass	0.20A	0.10A to 1.30A
Source Voltage	Pass	9.88V	4.00V to 13.00V
Source Current	Pass	1.95A	0.10A to 10.00A
Source Power		19.32W	
Temperature	Pass	45.01C	0.50C to 70.00C

Print

Return

TBI
BEP2110574

11/19/2021 8:57:53 AM
Nicolet iS20

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Power Supply	Status	Current	Acceptable Range
+ 5 Volt	Pass	4.97V	4.50V to 5.50V
+ 12 Volt	Pass	11.99V	10.80V to 13.20V
- 12 Volt	Pass	-12.01V	-13.20V to -10.80V
+3.3 Volt	Pass	3.33V	3.00V to 3.60V

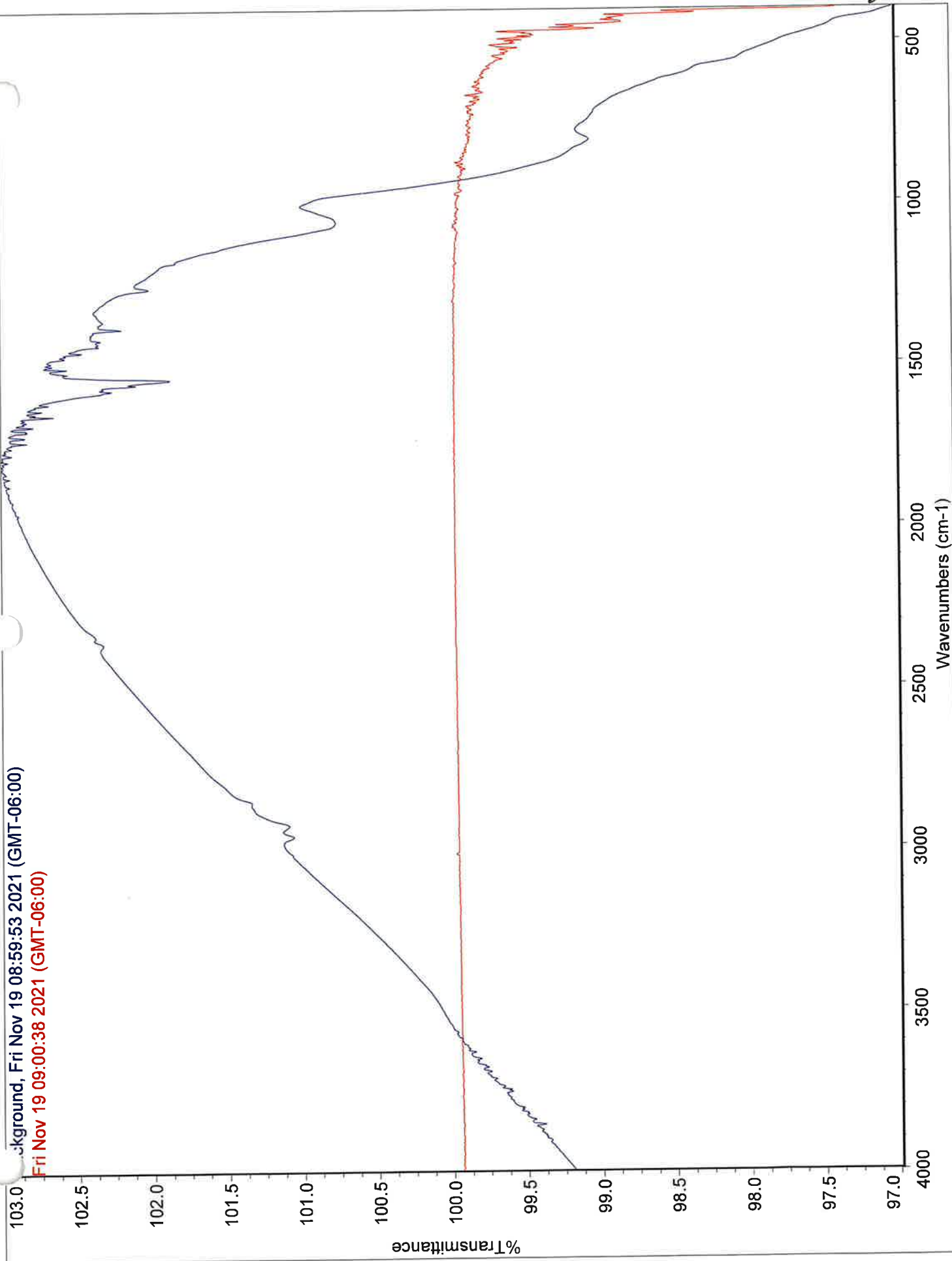
Print

View More

Return

Background, Fri Nov 19 08:59:53 2021 (GMT-06:00)

Fri Nov 19 09:00:38 2021 (GMT-06:00)





Qualification test: Quantification & Algorithms 2019 - ALL
 Date: Tuesday, November 16, 2021 2:37:03 PM (GMT-06:00)
 Operator: Drugs ATR

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.

ValPro Qualification Report

Qualification test: Nicolet iS20 KBr - Factory (CP,JP,PHEUR,PV,USP) - PV

Operator: Drugs ATR

Date: Tuesday, November 16, 2021 1:50:50 PM (GMT-06:00)

Instrument: Nicolet iS20 Serial number: BEP2110574

Filename: Nicolet iS20 KBr - Factory (CP,JP,PHEUR,PV,USP) - PV_20211116_135050.spg

Test description	High limit	Low limit	Measured	Result
CP Wavenumber accuracy				
Peak at 3027.0 (cm-1)	3032.0	3022.0	3025.6	Pass
Peak at 2851.0 (cm-1)	2856.0	2846.0	2849.3	Pass
Peak at 1601.0 (cm-1)	1602.0	1600.0	1601.1	Pass
Peak at 1028.0 (cm-1)	1029.0	1027.0	1028.4	Pass
Peak at 907.0 (cm-1)	908.0	906.0	906.5	Pass
CP Optical resolution				
Resolution 2870 - 2849.5 (%T)	100.00	18.00	37.00	Pass
Resolution 1589 - 1583 (%T)	100.00	12.00	22.00	Pass
CP Peak Resolution				
Peaks between 3120 and 2850 cm-1	7	7	7	Pass
JP Wavenumber accuracy				
Peak at 3060.0 (cm-1)	3061.5	3058.5	3059.7	Pass
Peak at 2849.5 (cm-1)	2851.0	2848.0	2849.3	Pass
Peak at 1942.9 (cm-1)	1944.4	1941.4	1942.6	Pass
Peak at 1601.2 (cm-1)	1602.2	1600.2	1601.1	Pass
Peak at 1583.0 (cm-1)	1584.0	1582.0	1583.0	Pass
Peak at 1154.5 (cm-1)	1155.5	1153.5	1154.5	Pass
Peak at 1028.3 (cm-1)	1029.3	1027.3	1028.4	Pass
JP Optical resolution				
Resolution 2870 - 2849.5 (%T)	100.00	18.00	37.00	Pass
Resolution 1589 - 1583 (%T)	100.00	12.00	22.00	Pass
JP Repeatability				
Peak at 3027.1 (cm-1)	5.00	-5.00	0.00	Pass
Peak at 1028.3 (cm-1)	1.00	-1.00	0.00	Pass
Intensity at 2849.5 (%T)	0.50	-0.50	-0.02	Pass
Intensity at 1028.3 (%T)	0.50	-0.50	-0.01	Pass
PHEUR Wavenumber accuracy				
Peak at 3060.0 (cm-1)	3061.0	3059.0	3059.7	Pass
Peak at 1601.2 (cm-1)	1602.2	1600.2	1601.1	Pass
Peak at 1028.3 (cm-1)	1029.3	1027.3	1028.4	Pass
Peak at 906.6 (cm-1)	907.6	905.6	906.5	Pass
PHEUR Optical resolution				
Resolution 2870 - 2849.5 (Abs)	10.00	0.33	0.39	Pass
Resolution 1589 - 1583 (Abs)	10.00	0.08	0.11	Pass
PV Energy ratio				
Energy ratio 4000 / 2000	1.00	0.20	0.42	Pass
Energy ratio 2000 / 1000	4.00	0.80	1.49	Pass

PV Noise level

P-P noise 4050 - 3950 (%T)	0.25	0.00	0.02	Pass
P-P noise 2050 - 1950 (%T)	0.221	0.00	0.016	Pass
P-P noise 1050 - 950 (%T)	0.10	0.00	0.02	Pass
P-P noise 550 - 450 (%T)	1.50	0.00	0.26	Pass
RMS noise 4050 - 3950	0.05	0.00	0.00	Pass
RMS noise 2050 - 1950	0.039	0.00	0.003	Pass
RMS noise 1050 - 950	0.014	0.00	0.004	Pass
RMS noise 550 - 450	0.30	0.00	0.04	Pass

PV Detector linearity

Slope	1.10	0.90	1.04	Pass
Intercept (%T)	1.00	-1.00	0.00	Pass

USP Wavenumber accuracy

Peak at 3060.0 (cm-1)	3061.0	3059.0	3059.7	Pass
Peak at 2849.5 (cm-1)	2850.5	2848.5	2849.3	Pass
Peak at 1942.9 (cm-1)	1943.9	1941.9	1942.6	Pass
Peak at 1601.2 (cm-1)	1602.2	1600.2	1601.1	Pass
Peak at 1583.0 (cm-1)	1584.0	1582.0	1583.0	Pass
Peak at 1154.5 (cm-1)	1155.5	1153.5	1154.5	Pass
Peak at 1028.3 (cm-1)	1029.3	1027.3	1028.4	Pass

Performed by: _____ Title: _____ Date: _____

Approved by: _____ Title: _____ Date: _____

Comments: _____

Digital comment(s):

No digital comments found.