TBI-FORENSIC SERVICES DIVISION
PERFORMANCE VERIFICATION FORM

Instrument/Method to Verify:

added short 5 meter GC column along with new methods

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 Ben Hubert Title SAFS Initials BH

Completed: Signature/Date [signature] 2/3/21

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: 2021.02.03 15:41:00 -06'00'

Unit Supervisor/Date _____

Unit Supervisor/Date _____

Crime Laboratory Regional Supervisor/Date [signature] 2.4.21

Crime Laboratory Regional Supervisor/Date _____

Crime Laboratory Regional Supervisor/Date _____

Quality Assurance Manager/Date [signature] 02/03/21

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: 2021.02.03 15:41:17 -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.

Revalidation and Performance check for Thermo Trace 1310 GC Nicolet iS50 FTIR Hogwarts

2-1-21

Introduction

This validation and performance check is designed to demonstrate the effectiveness of Hogwarts. This instrument will be evaluated on method functionality and previously determined acceptance criteria to determine suitability for the analysis of legally significant compounds.

In order to provide optimal utility to the laboratory a new column was installed and new methods were developed for Hogwarts. As a result, Hogwarts required a limited revalidation to demonstrate that it still produces acceptable data for casework. This was done by running specific standards on each approved method. These standards include, fentanyl, heroin, and buprenorphine in order to demonstrate the instrument's effectiveness over a variety of compounds. The data obtained from these runs was then evaluated for instrument response and spectral accuracy. This data can be found attached to this memo.

Materials

Column:

Agilent

J&W GC HP-5 5 meter, 0.32 ID, 0.25 µm

Liner:

Restek Split/ Splitless straight with glass wool liner

Drug Standards

Fentanyl Citrate Standard

USPC lot # 1275-F

Heroin Standard

Cerilliant #FE06151603

Buprenorphine

Sigma Aldrich #SLBQ94554V

Results

Analysis of the standards run on Hogwarts have consistently shown compliance with standard operating procedures 22.3 and 22.6.1. All methods have been utilized in the analysis of known drug standards. The data obtained from these standards is consistent with previously verified standards in the Nashville forensic chemistry standard library. The instrument response was compared to older data taken from before the new column and new methods. The chromatography, peak shape, and spectra all appear to be consistent to the data that the instrument was generating previously.

Conclusions

After monitoring parameters specified in Forensic Chemistry Standard Operating Procedure found in chapter 22 and verifying the functionality of previously utilized methods with known drug standards, it has been demonstrated that Hogwarts produced comparable results to previous instrument response and GC-FTIR libraries.

After performing theses runs, the instrument showed comparable results to its previous state. Using the instrument will not require new competency training, though I do recommend that scientists in the Forensic Chemistry Unit read the Addendum in the instructions for using the instrument, which describes the parameters of all new methods, and the instrument be returned to service.

Hogwarts

GC-FTIR

Chromeleon®7 Software

Dionex Chromeleon version 7.2.10

Ominc 9.11.745 software

Ominc Series 9.11.727

Driver version 9.11.709

Nicolet iS50

Firmware version 1.11

Thermo Scientific Hogwarts GC-FTIR Operating Procedures

Each GC-FTIR system will be identified from all other GC-FTIR systems by use of a unique identifier. This identifier could be a reference to a particular number, model number, serial number, name, etc. All GC-FTIR systems employ OMNIC software. The Hogwart's GC-FTIR additionally employs Chromeleon 7 GC software. See the instrument's maintenance logbook for the specific OMNIC and Chromeleon 7 software version.

General Operations:

1. Ensure that the power is on to all components
2. Open the Chromeleon 7 application by double clicking the icon on the computer desktop (This may take a few moments)
3. Once the Chromeleon 7 application has successfully opened, open the OMNIC application by double clicking the icon on the computer desktop

NOTE: IT IS IMPORTANT THAT YOU FIRST OPEN CHROMELEON AND THEN OMNIC. OMNIC WILL NOT COLLECT DATA IF YOU DO NOT OPEN CHROMELEON FIRST.

To Set Up for Analysis:

Make sure that the **Default iS50 GC-IR** experiment is selected on the OMNIC **Experiment** tool bar and that the blue button is lit up on the iS50 GC-IR accessory.

This should be selected automatically by the instrument. The instrument should be set to a Gain of 1, Resolution of 8 cm-1, 4 Scans, 64 Scans for the background and a spectral range of 4000 to 800 cm-1.

Data Acquisition:

1. All parameters for analysis on the Hogwart's GC-FTIR are electronically stored in the Chromeleon 7 software under the **Data** tab within the folder name **Chromeleon Local.** The method parameters for an analysis run will be noted in the analyst's case file.

NOTE: Remember that the column on the Hogwart's GC-FTIR has a longer column and thinner film thickness than GC/IR #1 and #2. This should be taken into consideration for certain analytes, using the necessary methods as needed.

2. A sample blank must be run each day per each case file, method, and extraction prior to running a case sample.
3. If the reservoir on the GC-FTIR is not cold, fill the reservoir with liquid nitrogen.
4. In the **OMNIC** application window select the **Series** tab and select **Heater Status…**

5. Make sure the heaters are turned on (checked box) and set the **Flow cell setpoint (deg. C):** and **Transfer line setpoint (deg. C):** to **280°C** in the white box and select the **Update Heaters** button.
6. To the right of the white box where the temperature values are set it will show the actual temperature of the flow cell and transfer line. When the values have not reached the desired set temperature, the filament background picture will become yellow. Once the values of the set temperatures have been reached the filament background will turn green.
7. Exit the **Heater Status…** window once the set temperatures have been reached.

Creating a Sequence:

8. Select the **Data** tab within the **Chromeleon Console** window.
9. Find the file titled **_Series Template_ (COPY AND PASTE)** and copy and paste it to your personal Chromeleon sequence folder.
10. Once the file has been pasted to your folder rename it with the date and your initials.
11. Fill out and select the **Name, Position, Volume, Instrument Meth, and Comment** boxes for the samples on the displayed sequence. The **Instrument Meth** boxes will have drop down arrows to select each method.
12. It is the analyst's discretion as to which method to use.
13. Make sure that in the **Name** box provides detailed sample information and the user's initials (This is how the file information will be saved in **OMNIC**)
14. **Click here to add a new injection** to add more samples to the sequence.
15. Once all of the samples have been added and the sequence is ready to run select the **OMNIC** application window.
16. Select the "Collect Ser" button on the **OMNIC** taskbar.

NOTE: IT WILL TAKE A FEW MOMENTS FOR OMNIC TO LOAD THE COLLECT SERIES IF THE SOFTWARE HAS NOT ALREADY BEEN IN USE.

17. The background will collect once the **OMNIC** software has finished loading and an **External Trigger** window will pop open stating "Ready to start data collection at external trigger.".
18. Select the **Chromeleon Console** window and highlight the beginning of the sequence run (or the sample you wish to run).
19. Click the "Start" button at the top of the sequence.
20. After a few moments the sequence toolbar should load from yellow to green (New→Running) and where the "Start" button appeared it will now state "Stop".

Auto-sampler Injection:

The auto-sampler will automatically inject your sample once the run has been started in the **Chromeleon Console** and the TRACE 1310 instrument is at ready status.

OMNIC will be triggered to start collecting data once the auto-sampler has injected the sample.

Manual Injection:

The TRACE 1310 instrument has touchscreen capabilities that allow for you to monitor your run, obtain information about the instrument, and manually inject. When manually injecting, the touchscreen will provide the status of the instrument (Not Ready/Ready). When a green play/arrow button pops up on the screen, the instrument is ready for manual injection. Inject your sample and select the green play/arrow button. The **Chromeleon Console** and TRACE 1310 instrument will start collecting, triggering **OMNIC** to start collecting data.

21. Once the sample or sequence has finished, the toolbar in the sequence of the **Chromeleon Console** will state that the "Run Finished".

Analyzing data in OMNIC:

22. Open the **OMNIC** application window and select "File" and then "Open…" in the toolbar.
23. An "Open" window will appear and in the "Files of type:" box, click the down arrow and select the "Series Files (*.SRS)" option.
24. Select the data file you wish to open and click the "Open" button.
25. Data file will display in **OMNIC**.
26. Use the bottom tools or taskbar to analyze the spectra.
27. To add a spectra region to a new window, right mouse click the bottom screen (spectra) and select "Copy To > New Window" and then click the "OK" button
28. To view a window, select the "Window" tab in the toolbar and click on the window you wish to display.

To Set Up for iS50 ATR Analysis:

Make sure that **iS50 ATR** experiment is selected on the OMNIC **Experiment** tool bar and that the blue button is lit up on the iS50 ATR accessory.

The parameters for using the iS50 ATR accessory should be set to Autogain, Resolution of 4 cm^{-1}, 16 Scans, and a spectral range of 4000 to 600.

iS50 ATR Operating Instructions:

1. At **Experiment** on the tool bar, load the **iS50 ATR** parameter file.
2. Select **Report** on the menu bar and select "Template…".
3. Select the ATRTEMPLATE.RPT at the very top of the scrolled window and click the "Select" button below.
4. Clean ATR stage and underneath ATR accessory.
5. Collect background and add to window.
6. Add sample and turn down ATR accessory.
7. Collect sample, add to window, select stack spectra, fill out sample information in text box, and select print option on taskbar.
8. Clean ATR stage and underneath ATR accessory.
9. Select **Report** on menu bar and select "Template…".
10. Select WILLIENEWGCFTIR.RPT template at very bottom of scrolled window and click the "Select" button below to switch template back.
11. Make sure **Default iS50 GC-IR** parameter file is switched back and loaded in **Experiment** tool bar.

MONTHLY MAINTENANCE

Alignment:

1. At **Experiment** on the tool bar, load the **Transmission E.S.P.** parameter file.
2. Select **Collect** from the menu bar and select **Experiment Setup…**
3. After the window loads go to the **Bench** tab and make sure that the Gain is set to 1.0.
4. Then select the **Diagnostic** tab and select the "Align…" button. When the alignment is complete record the number in the appropriate GC/IR maintenance log.
5. Click "OK" button to exit out.
6. Next, check and make sure the desiccant on the instrument is blue (If pink, moisture is present).

Report & Main, ATR, GC iS50 Performance Tests (KBr)

1. Make sure that the main sample compartment is empty.
2. From the menu bar select **Collect** then select **Advanced Diagnostics….**
3. After "Nicolet iS50 Diagnostics" window opens, select **Performance Test.**
4. Check all the boxes for the **Main, ATR, GC iS50 Tests (KBr).**
5. Select the "Run Selected Test" button.
6. Fill out OMNIC with performance test values for each spectra (**Main, ATR, GC**) and print and place spectra in the appropriate GC/IR maintenance log book.

Example:

PERFORMANCE TEST (MAIN) 2200-2100 = 0.004 PASS RMH
PERFORMANCE TEST (ATR) 2800-2700 = 0.024 PASS RMH
PERFORMANCE TEST (GC) 2200-2100 = 0.012 PASS RMH

7. After tests are complete, select each spectra (**Main, ATR, GC**) and individually save by setting the filename to title under the "Monthly Performance Tests" folder under the "Spectra/Groups (*.SPA, *.SPG)" file type.
8. Select the back arrow button and select Report, Print, and then the back arrow button again. Place the print out in the GC/IR maintenance log book.
9. Exit out of "Nicolet iS50 Diagnostics" window.

ValPro Qualification:

1. Check to ensure the **Transmission E.S.P.** parameter file is loaded under **Experiment** from the tool bar.
2. Select **Analyze** on the menu bar and then **ValPro Qualification….**
3. Once the "ValPro Qualification" window appears use the drop down box under "Qualification test:" and select the "Nicolet iS50 system with DTGS in built-in position KBr-EP".
4. Select the "Qualify" button once the test has been loaded.
5. When the ValPro Qualification has completed, highlight the test that just completed in the "Energy ratio" tab and click the "Report…" button.
6. A window will pop up with the report. Select the "Print" button and fill out ValPro Qualification Report and initial and place in the GC/IR maintenance log book.
7. Select the "Close" button.

For iS50 ATR Accessory

1. In the "Qualification test:" drop down box select the "Nicolet iS50 system with integrated diamond ATR and built-in DTGS-EP" option.
2. Select the "Qualify" button once the test has been loaded and click "OK" when the confirmation window pops up for the background.
3. Retrieve the SMART iTR polystyrene standard "lollipop" from the second drawer near the IR #7.
4. When a window pops up stating "Place the polystyrene in the accessory and apply pressure. Choose OK when you are ready to collect the sample data", place the polystyrene standard "lollipop" on the sample compartment area with the "ATR STD 269-173000" words facing upwards and apply pressure.

NOTE: Be sure to place the iS50 ATR accessory on the "lollipop" polystyrene standard window in different locations when performing monthly maintenance so as to not place the iS50 ATR accessory on the same location on the "lollipop" window.

5. Select the "OK" button once the "lollipop" polystyrene standard is in place.
6. When the ValPro Qualification has completed, highlight the test that just completed in the "Wavenumber accuracy" tab and click the "Report…" button.
7. A window will pop up with the report. Select the "Print" button and place in the GC/IR maintenance log book.
8. Select the "Close" and then "Exit" button to close out of the ValPro Qualification.
9. Select and load the **Default iS50 GC-IR** parameter file under **Experiment** from the tool bar
10. Remove "lollipop" from iS50 ATR sample area and place back in Thermo box and return it to the second drawer near the IR #7.
11. Fill out ValPro Qualification Report and initial and place in the GC/IR maintenance log book.

To Run the Monthly Standard Check:

1. Check to ensure the **Default iS50 GC-IR** parameter file is loaded under **Experiment** from the tool bar.
2. Make sure the reservoir for the MCT detector is filled with liquid nitrogen.
3. Make sure that the **transfer line** and **flow cell** heaters are at 280°C.
4. Analyze the Monthly QC test standard (Amphetamine, Phentermine, Methamphetamine) that is kept refrigerated.
5. Check its expiration date. If it is past its expiration date, make up a new QC test standard following the correct procedure to ensure the proper concentrations.
6. Make sure that the **60@20AMIN** is loaded and used to run the Monthly QC standard.
7. Run this sample following the procedures for analyzing data from the GC/FTIR and place in the GC/IR maintenance log book.

This is not meant to be all-inclusive. There may be other ways to accomplish the same task.

Addendum

S/SL Injection Port with HP-5 5 meter column, 0.32 column ID, and 0.25 um film thickness:

*Stored Methods for **AUTOSAMPLE SPLIT INJECTION***

90TO270 70AMIN 10MIN Initial 90C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 5.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 10.00 minutes.

90TO270 70AMIN 30MIN Initial 90C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 5.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 30.00 minutes.

200TO270 70AMIN 10MIN Initial 200C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 5.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 10.00 minutes.

200TO270 70AMIN 20MIN Initial 200C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 5.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 20.00 minutes.

200TO270 70AMIN 30MIN Initial 200C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 5.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 30.00 minutes.

90TO270 35AMIN 20MIN Initial 90C degrees hold for 1 minute ramped to 270C degrees at 35C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 5.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 20.00 minutes.

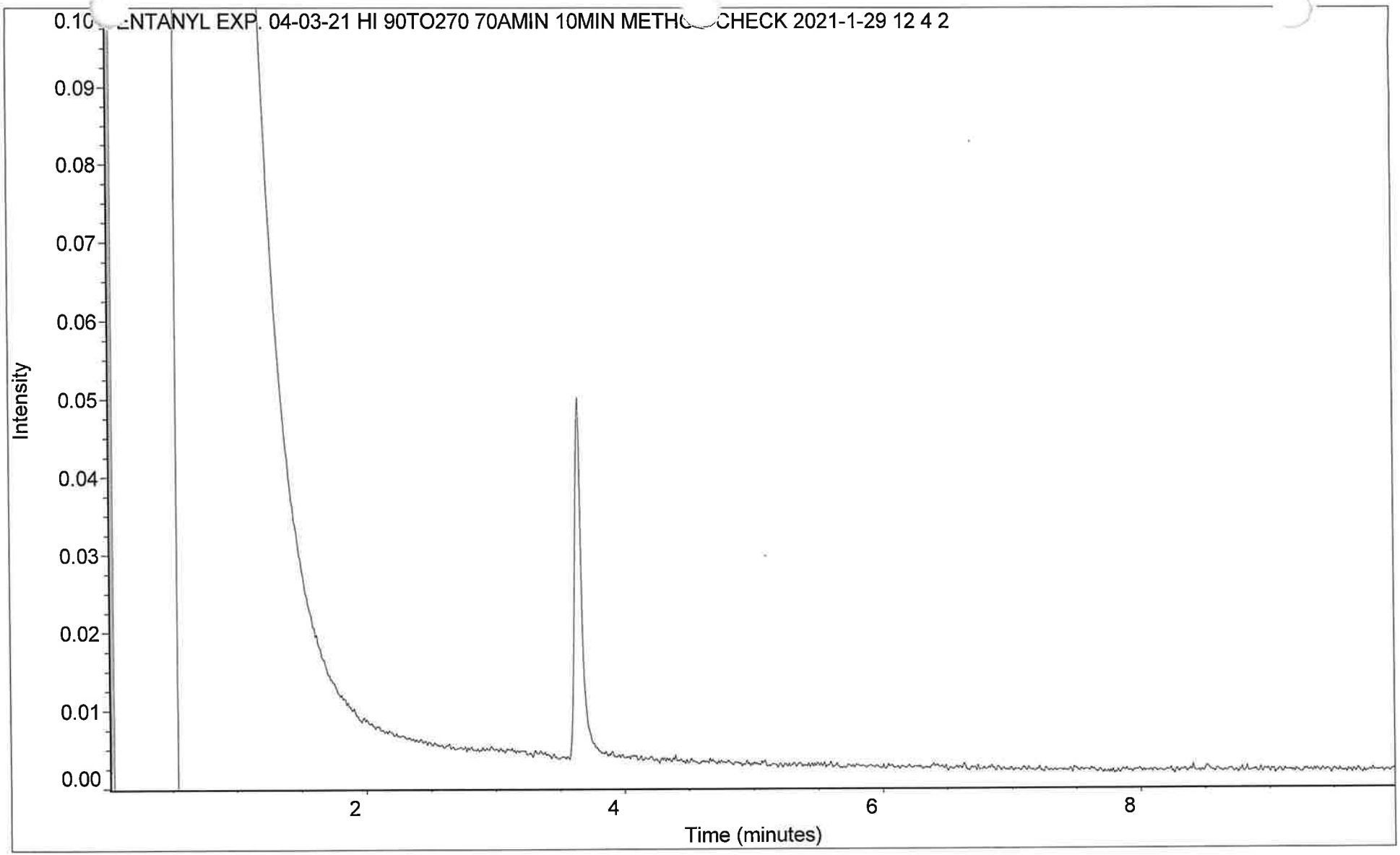
*Stored Methods for **HAND SPLIT INJECTION***

HI 90TO270 70AMIN 10MIN Initial 90C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split

flow 5.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 10.00 minutes.

HI 200TO270 70AMIN 30MIN Initial 200C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 5.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 30.00 minutes.

Always verify that the temperature for the GC interface is at least 10 degrees higher than the maximum temperature of the GC oven.



Linked spectrum at 3.648 min.

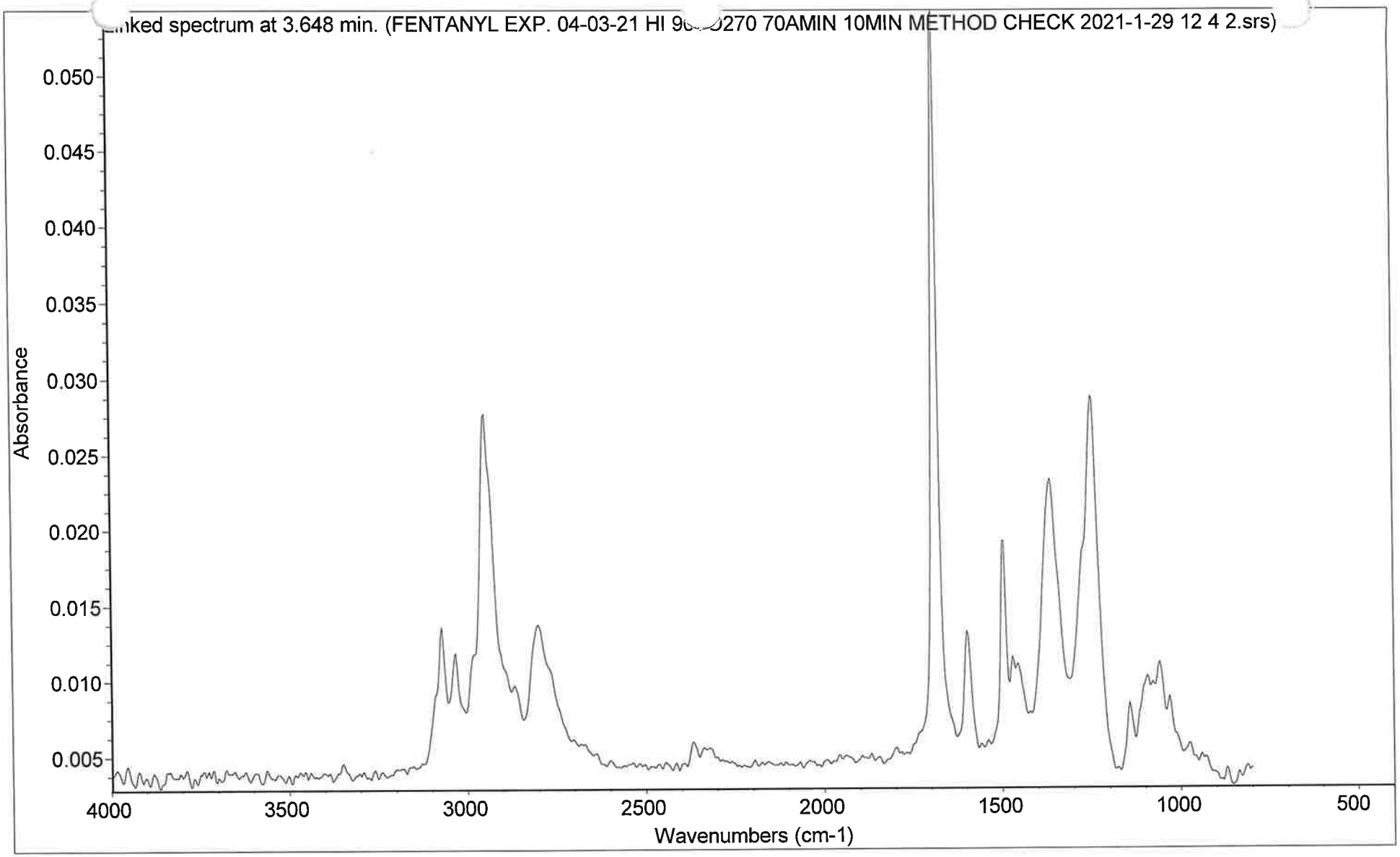
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Fri Jan 29 12:03:44 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 3.648 min. (FENTANYL EXP. 04-03-21 HI 90TO270 70AMIN 10MIN METHOD CHECK 2021-1-29 12 4 2.srs)

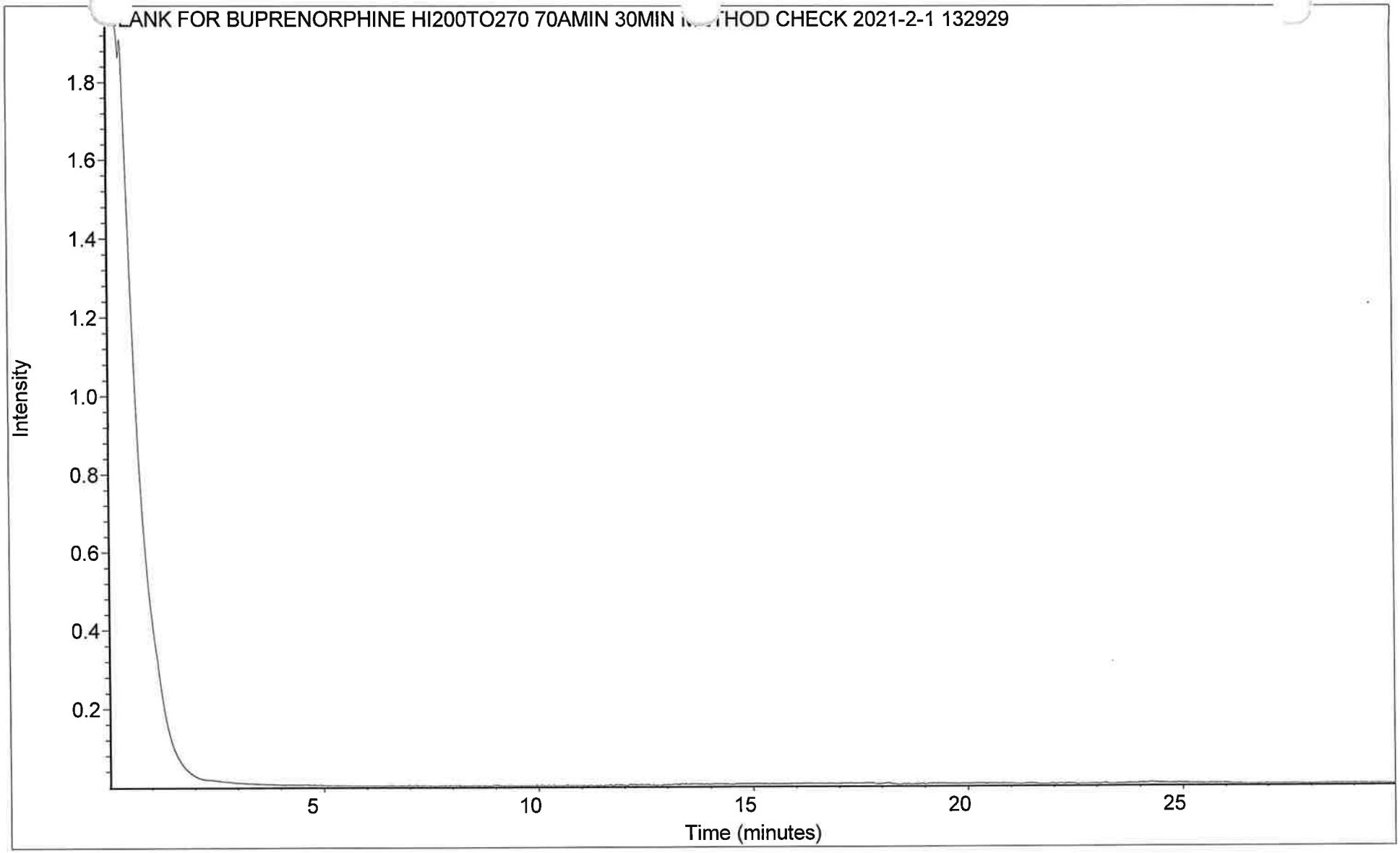
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Fri Jan 29 12:03:44 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

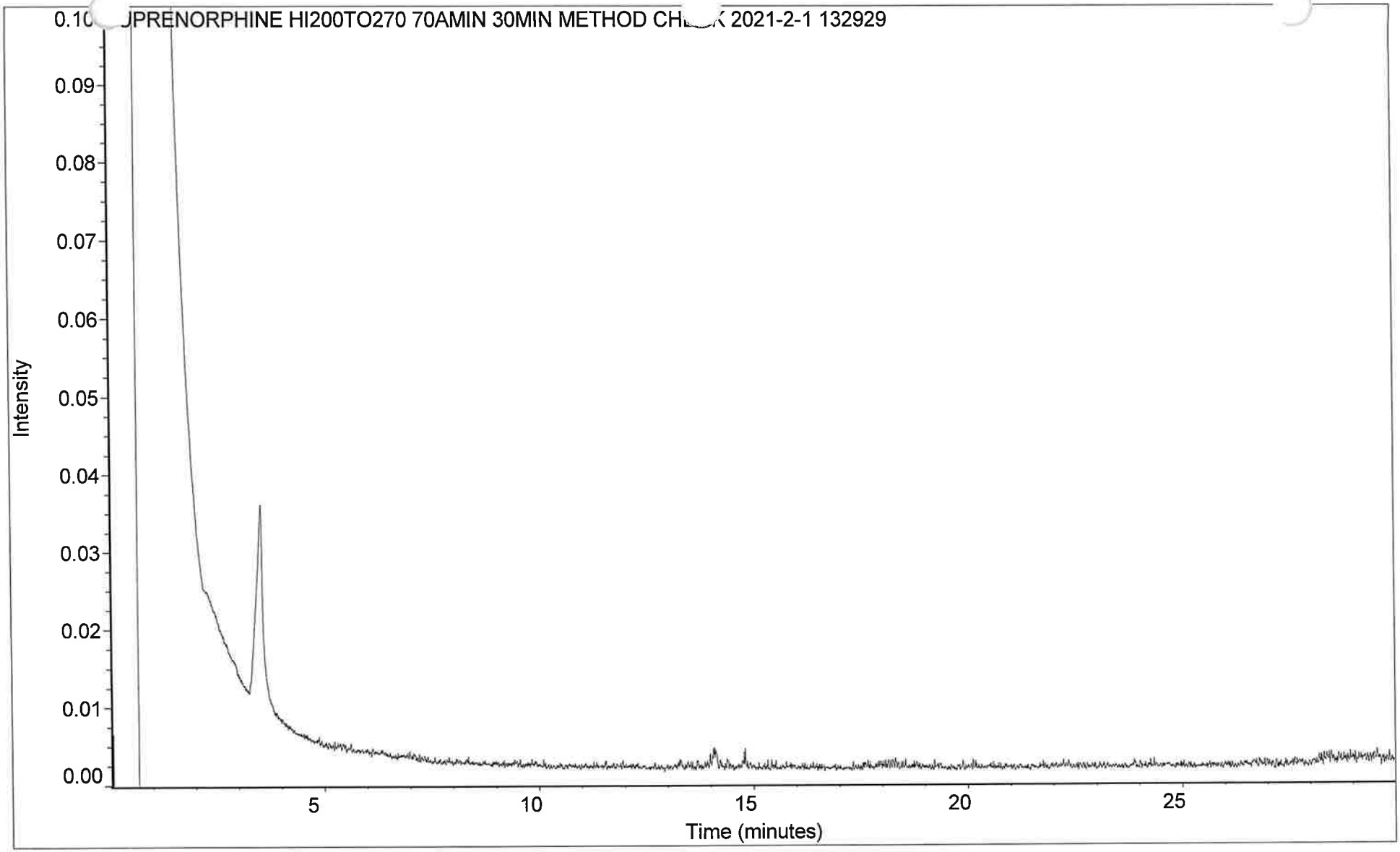
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Mon Feb 01 13:31:12 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 3.553 min.

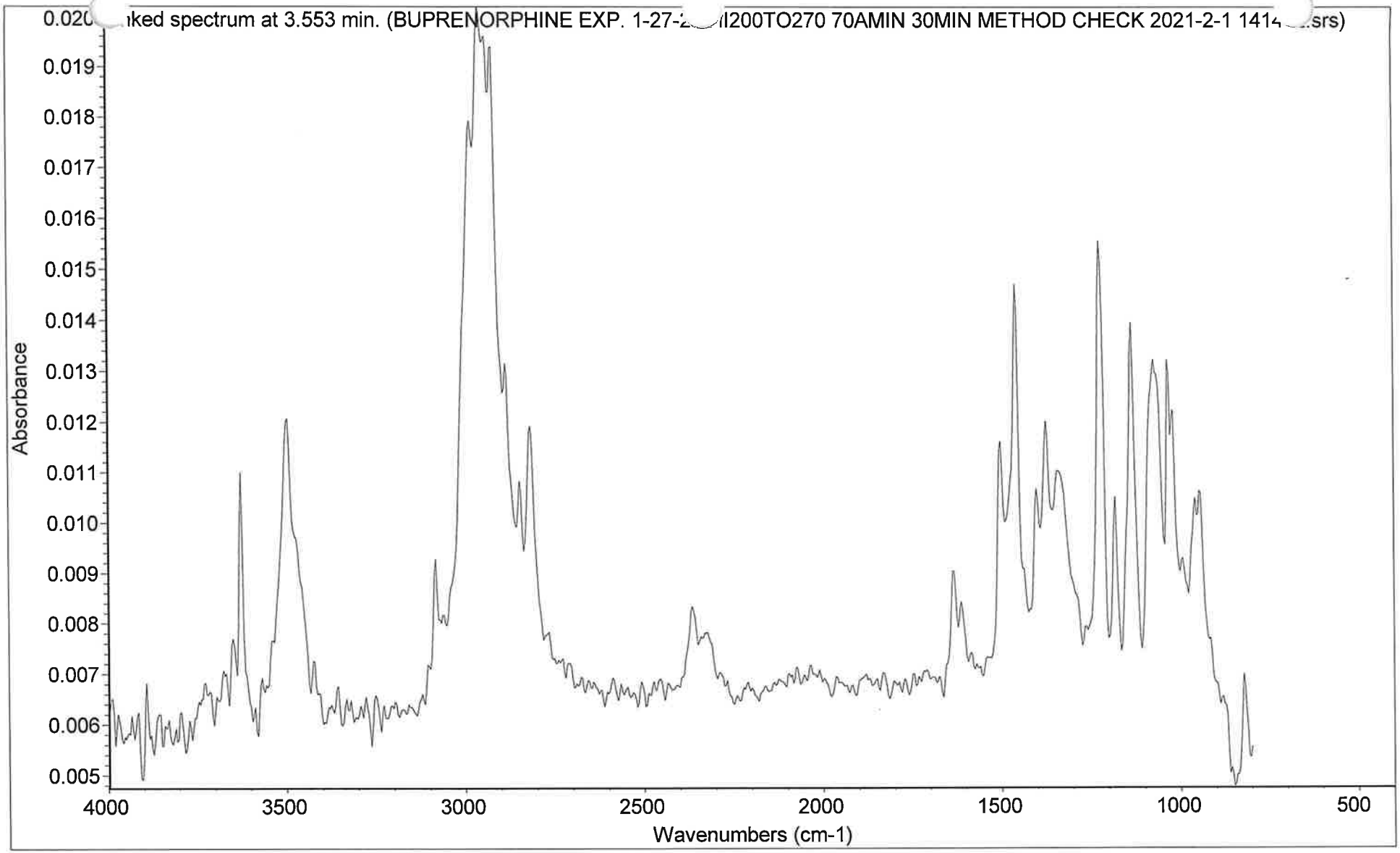
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Mon Feb 01 14:18:08 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 3.553 min. (BUPRENORPHINE EXP. 1-27-22 HI200TO270 70AMIN 30MIN METHOD CHECK 2021-2-1 141442.sr

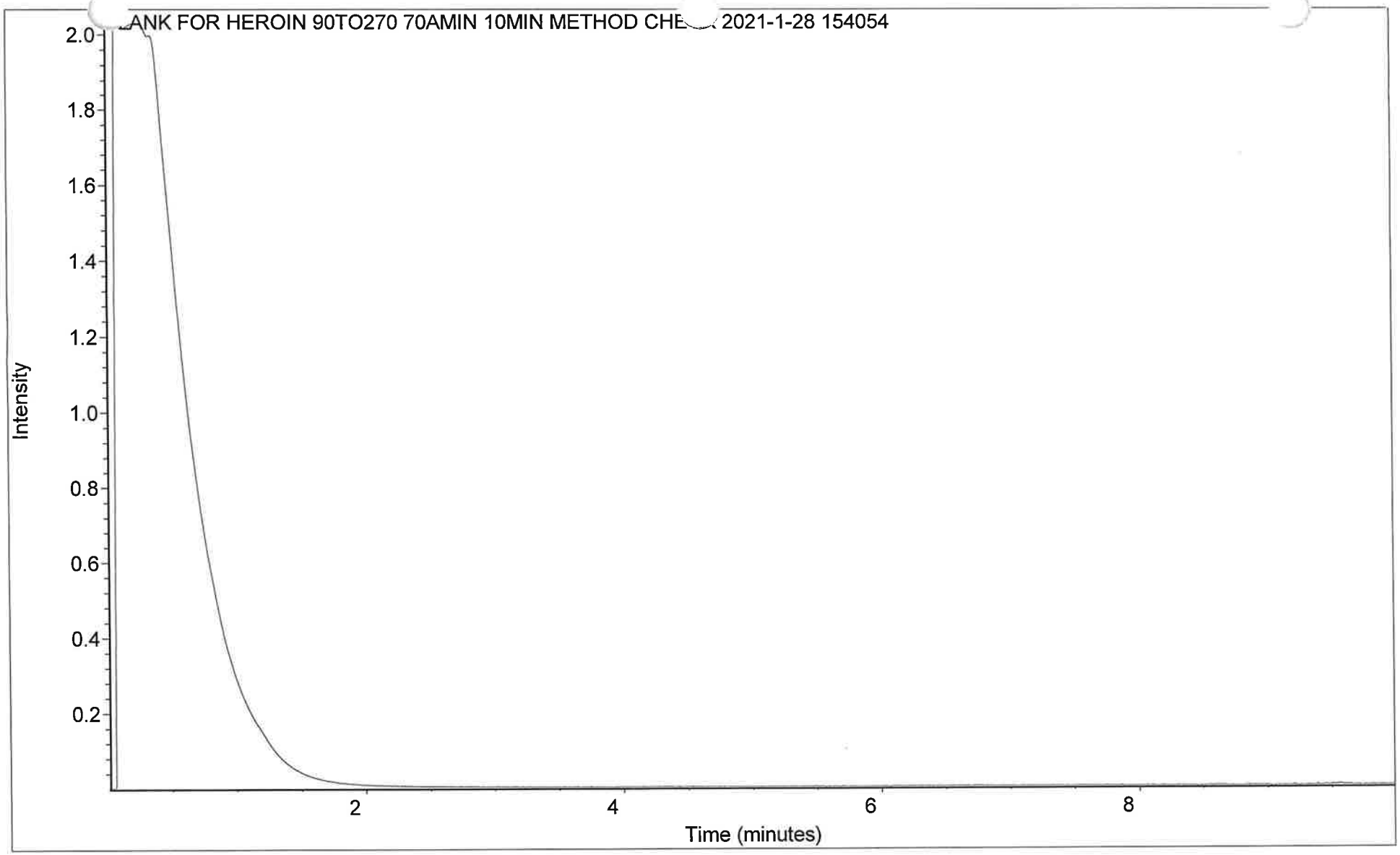
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Mon Feb 01 14:18:08 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

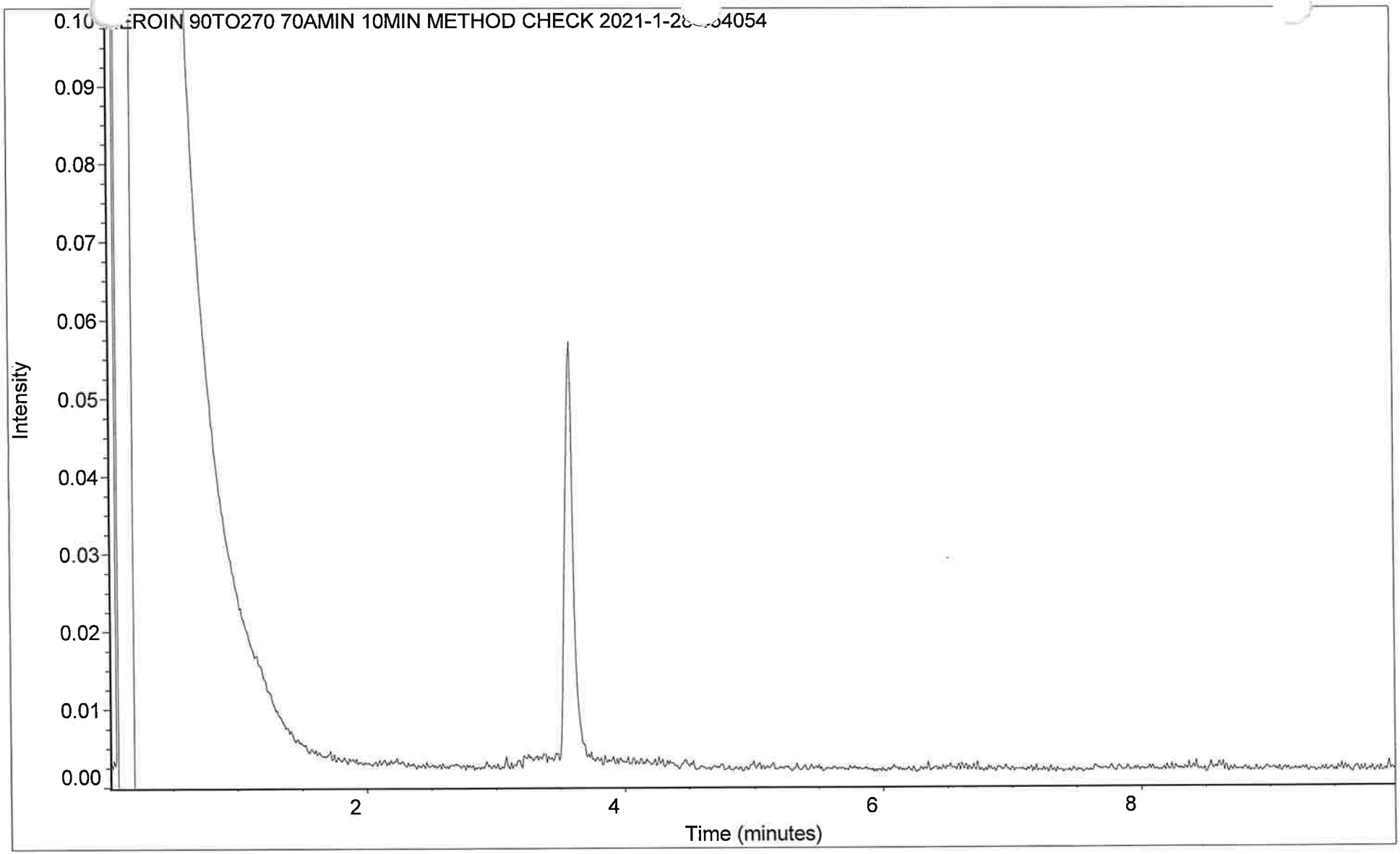
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Jan 28 14:52:16 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 3.582 min.

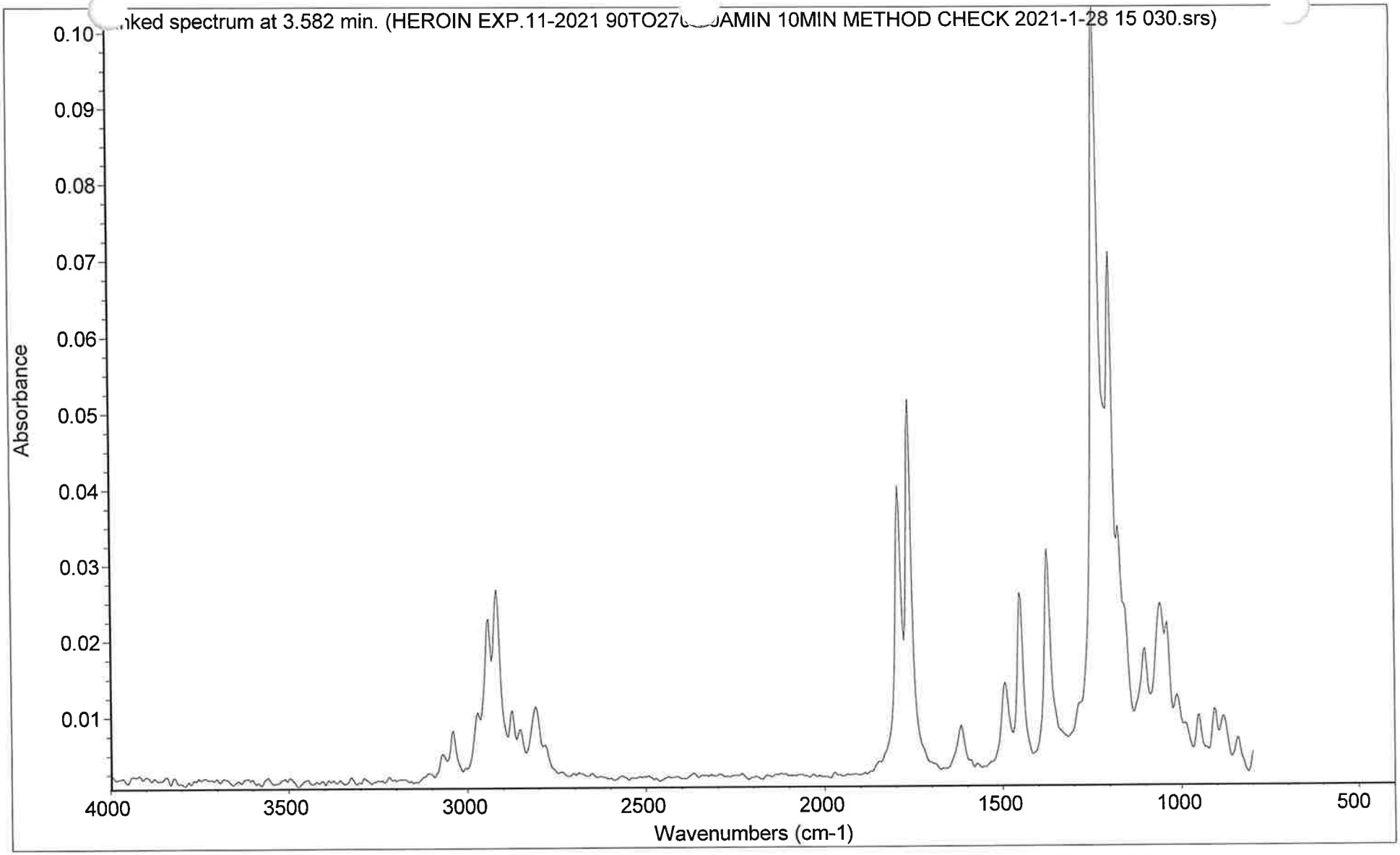
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Jan 28 15:05:04 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 3.582 min. (HEROIN EXP.11-2021 90TO270 70AMIN 10MIN METHOD CHECK 2021-1-28 15 030.srs)

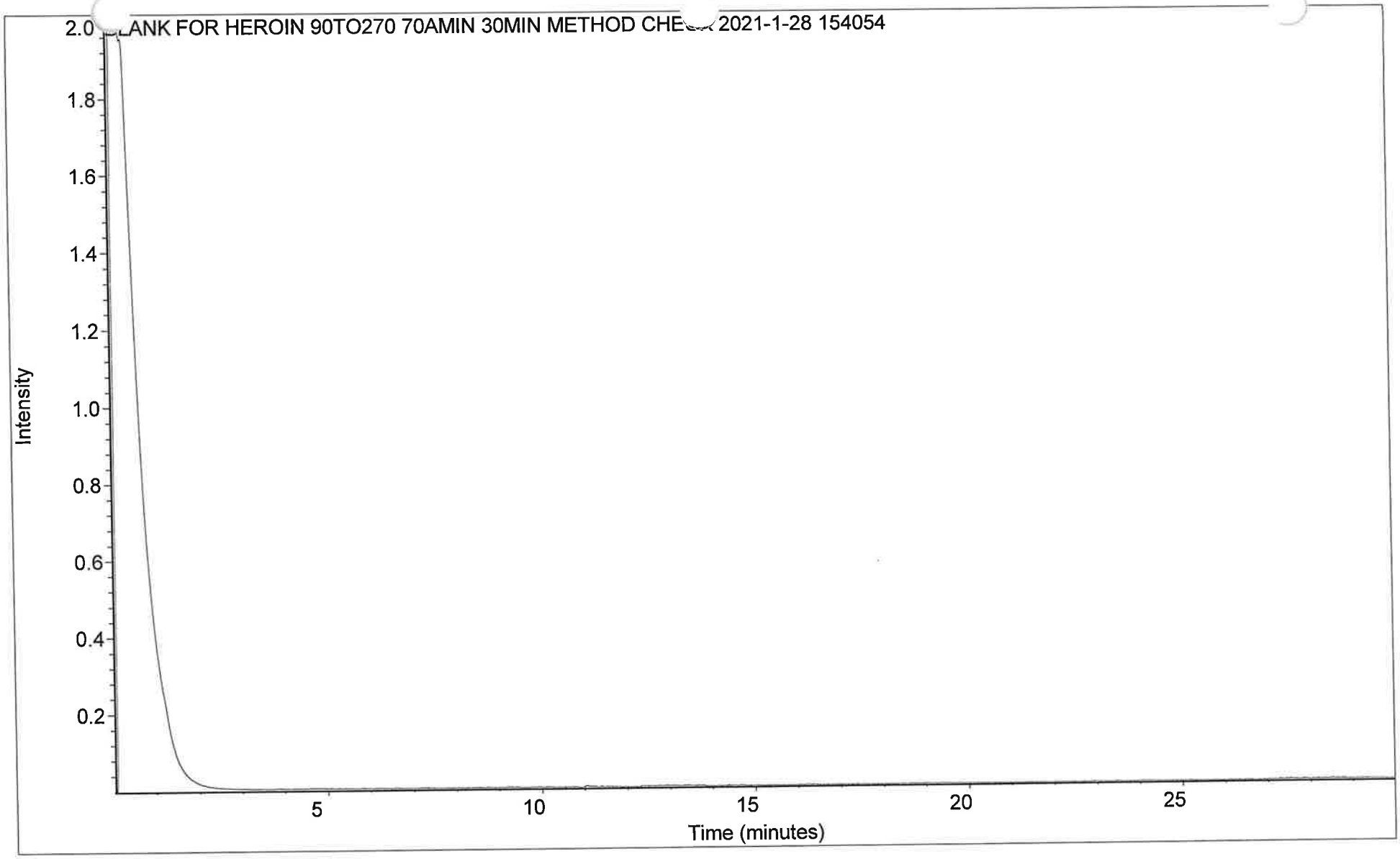
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Jan 28 15:05:04 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

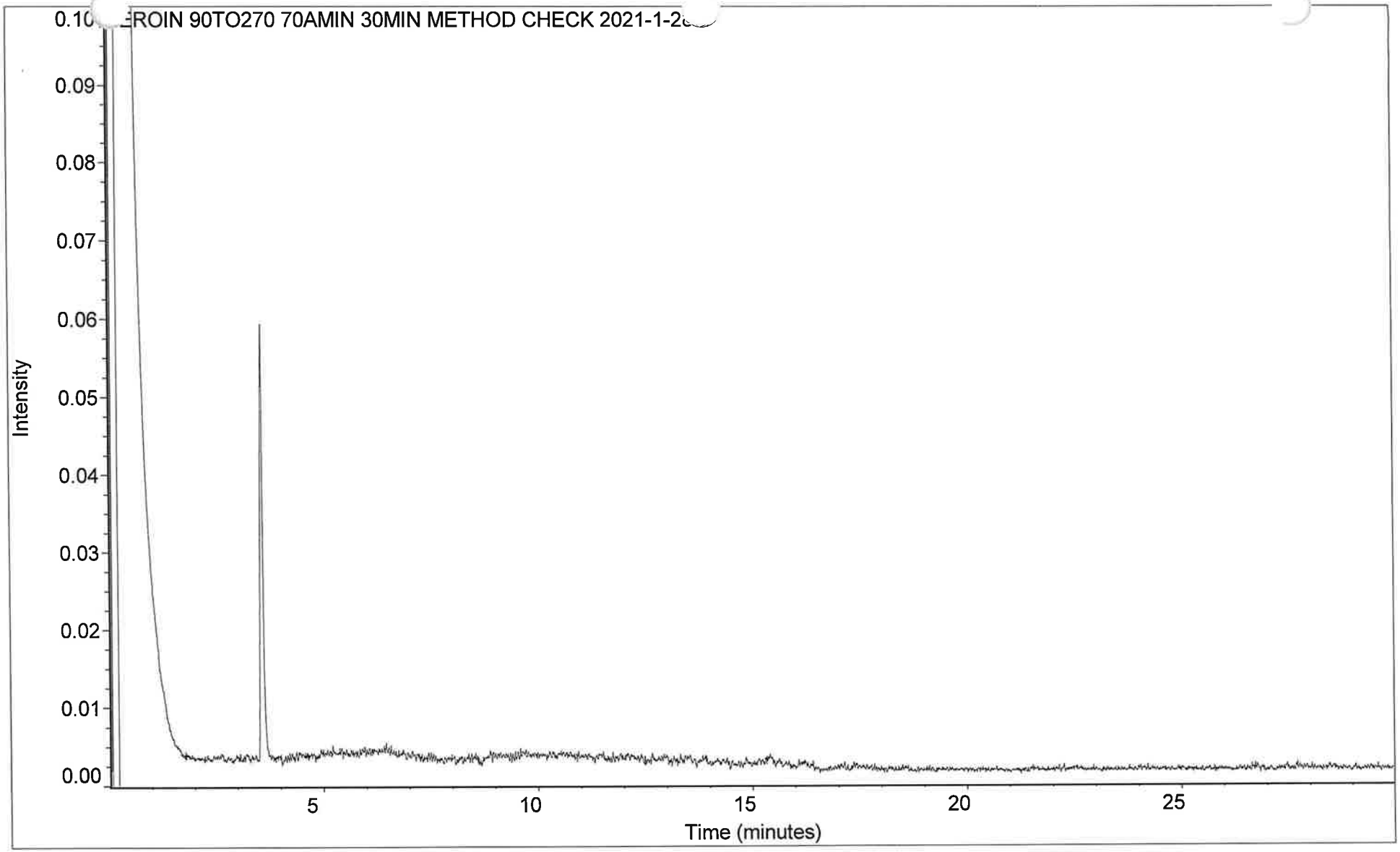
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Jan 28 15:43:28 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

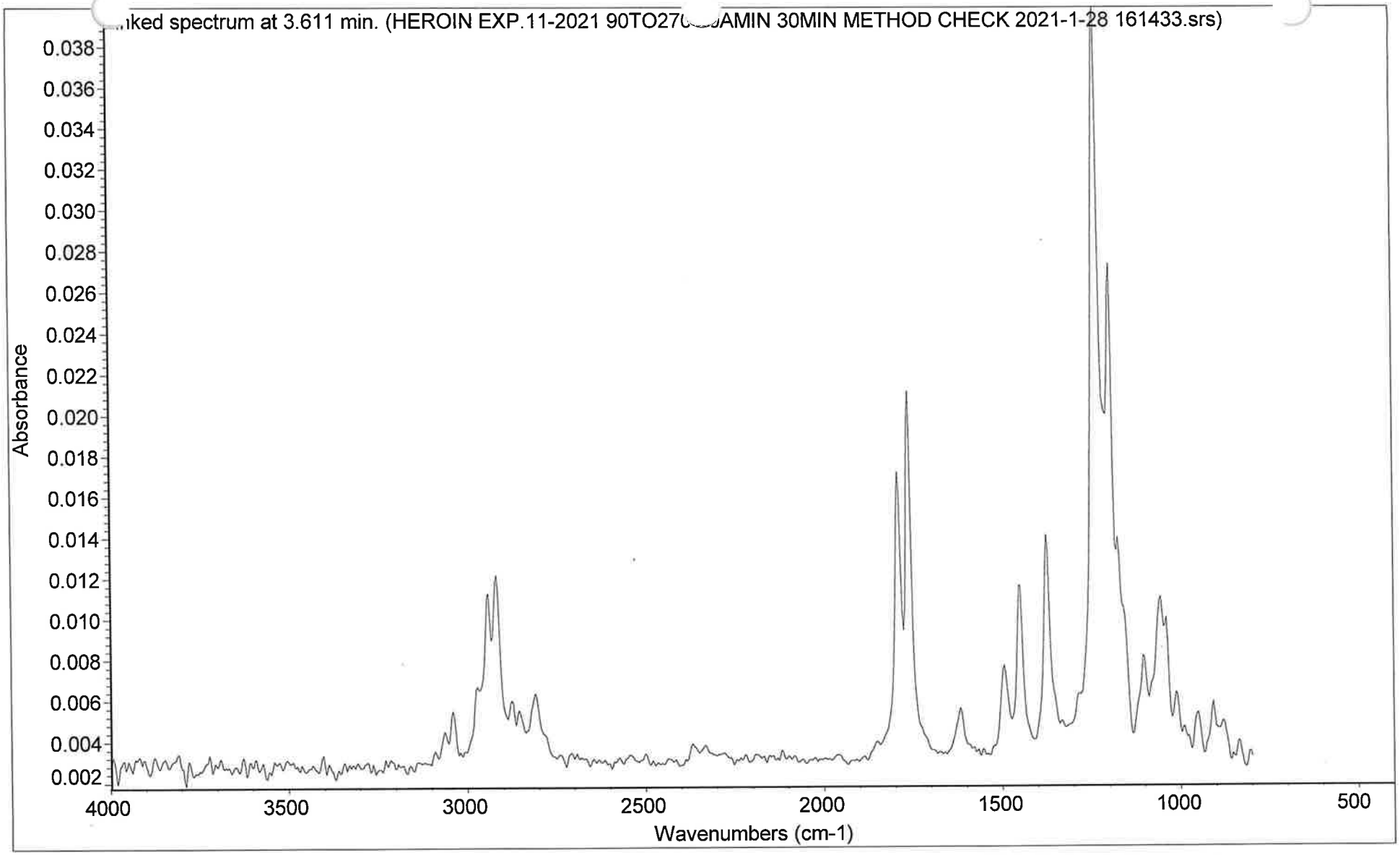
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Jan 28 16:17:36 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 3.611 min. (HEROIN EXP.11-2021 90TO270 70AMIN 30MIN METHOD CHECK 2021-1-28 161433.srs)

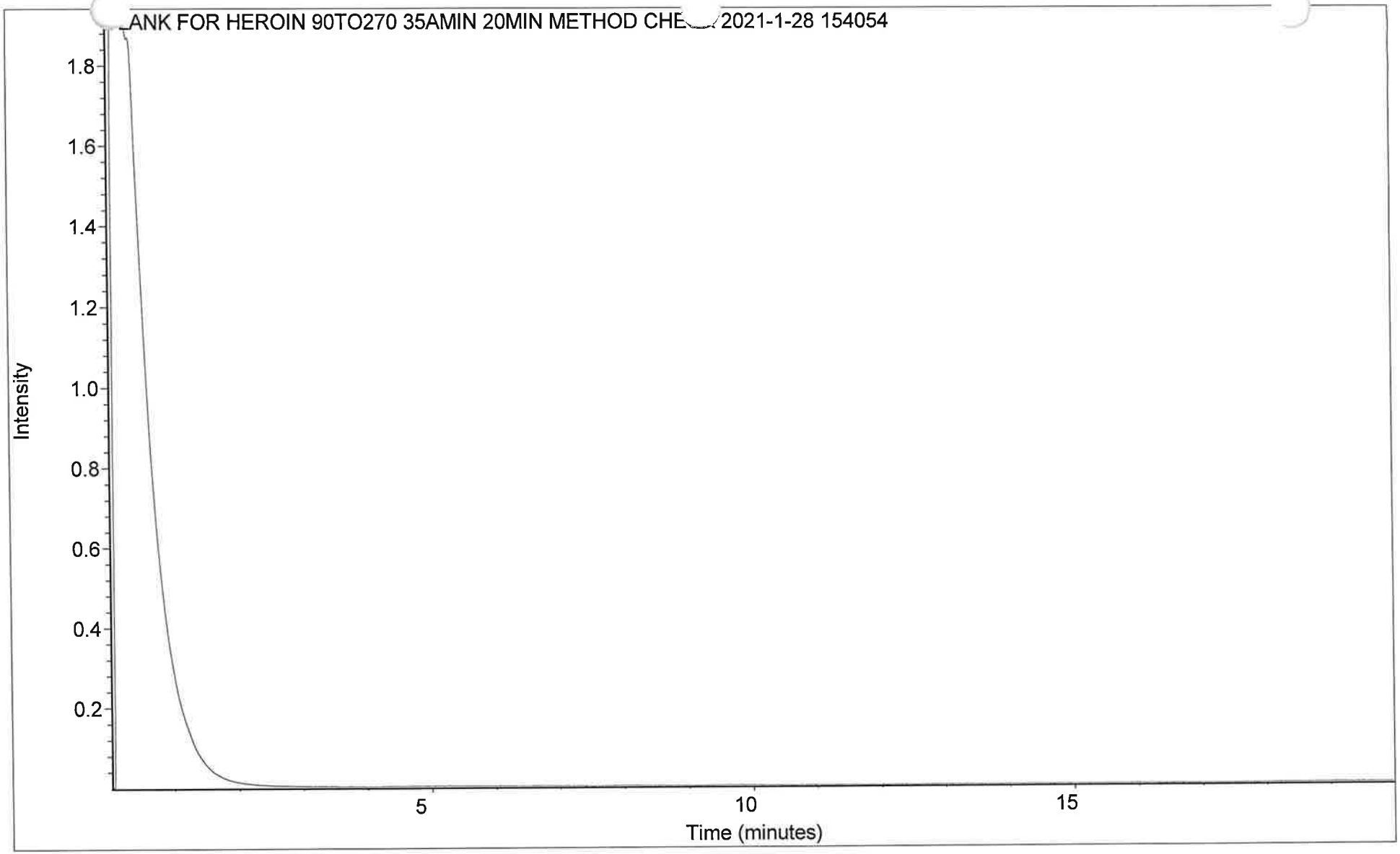
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Jan 28 16:17:36 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

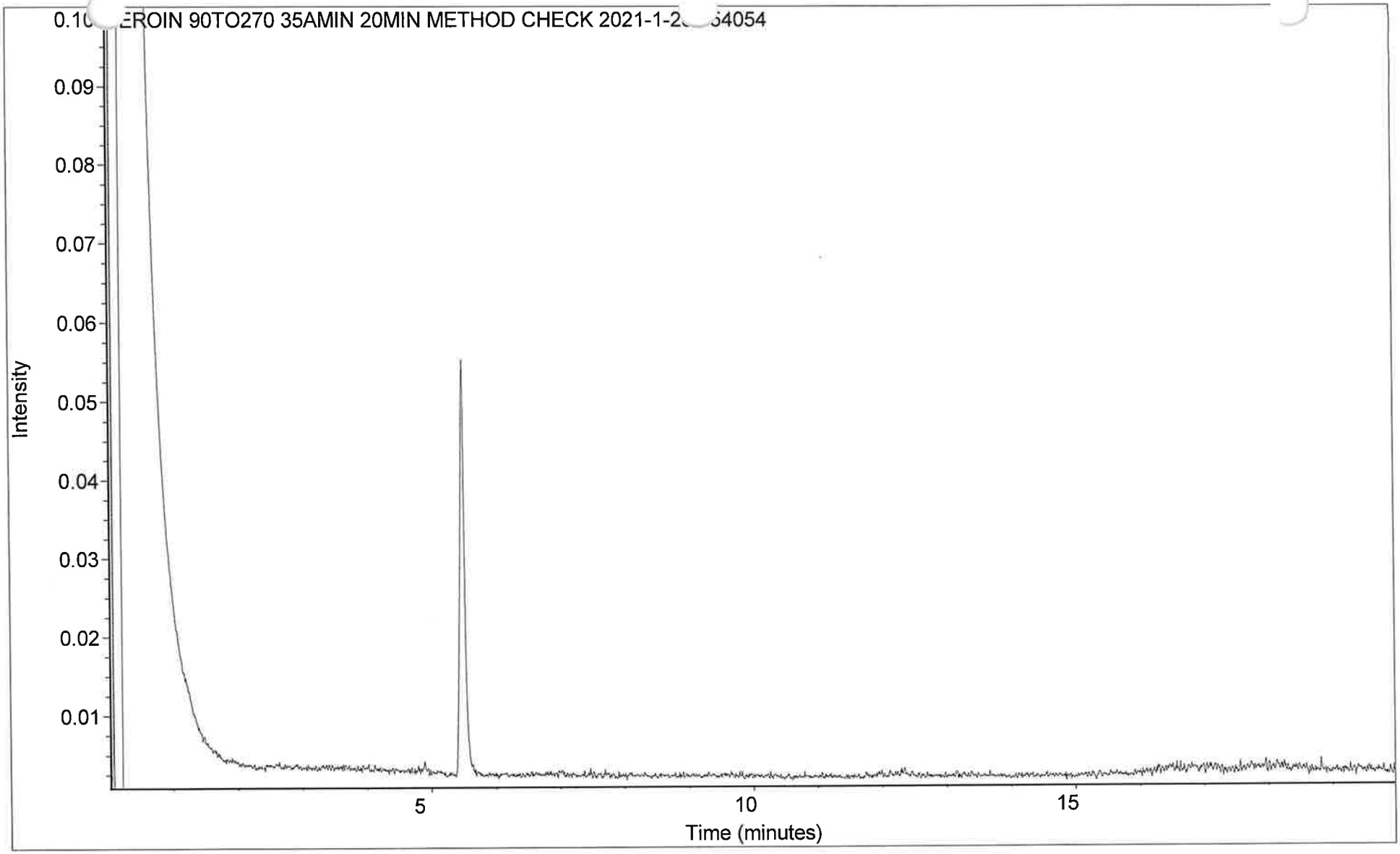
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Jan 28 14:01:04 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 5.525 min.

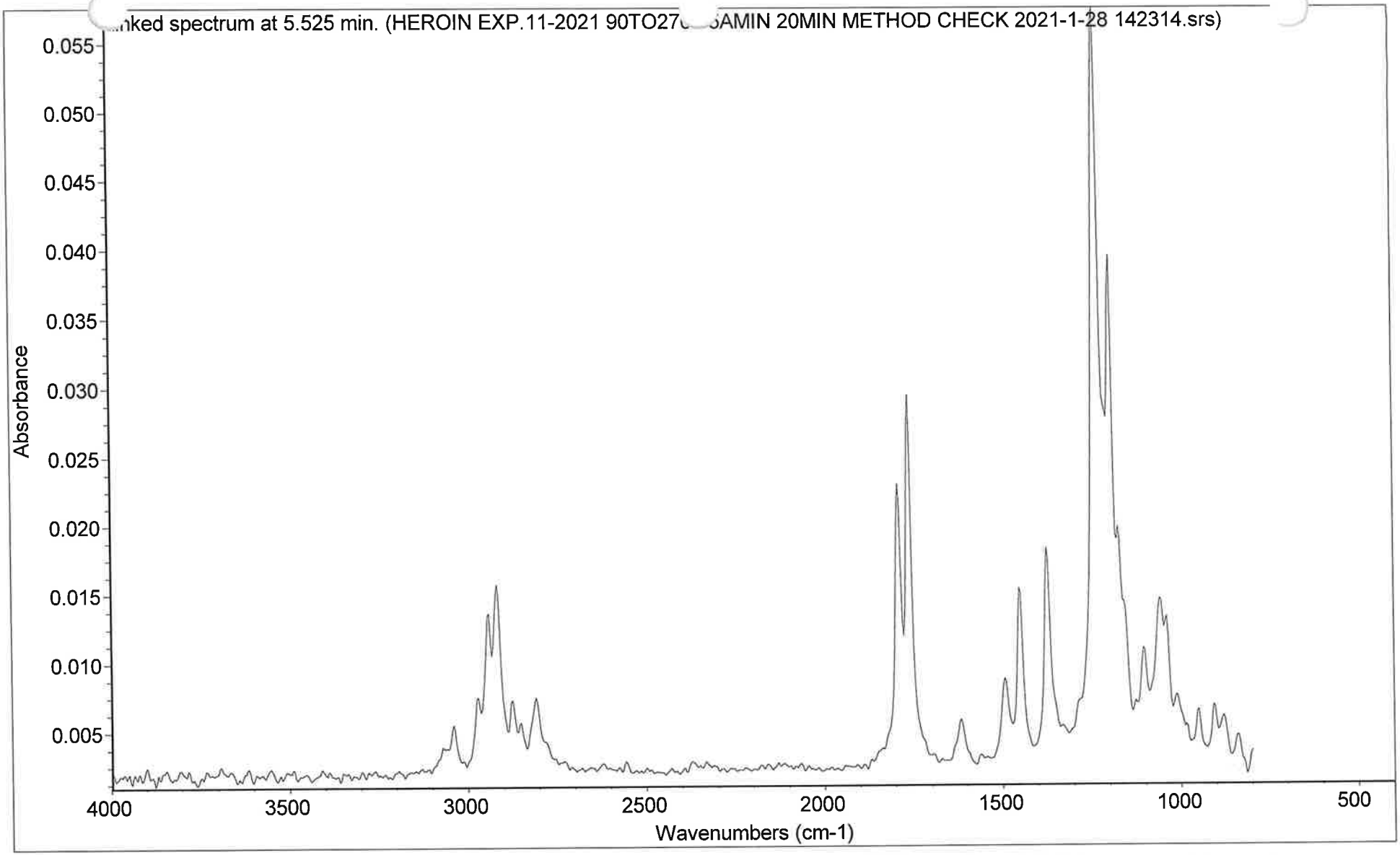
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Jan 28 14:26:40 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 5.525 min. (HEROIN EXP.11-2021 90TO270 35AMIN 20MIN METHOD CHECK 2021-1-28 142314.srs)

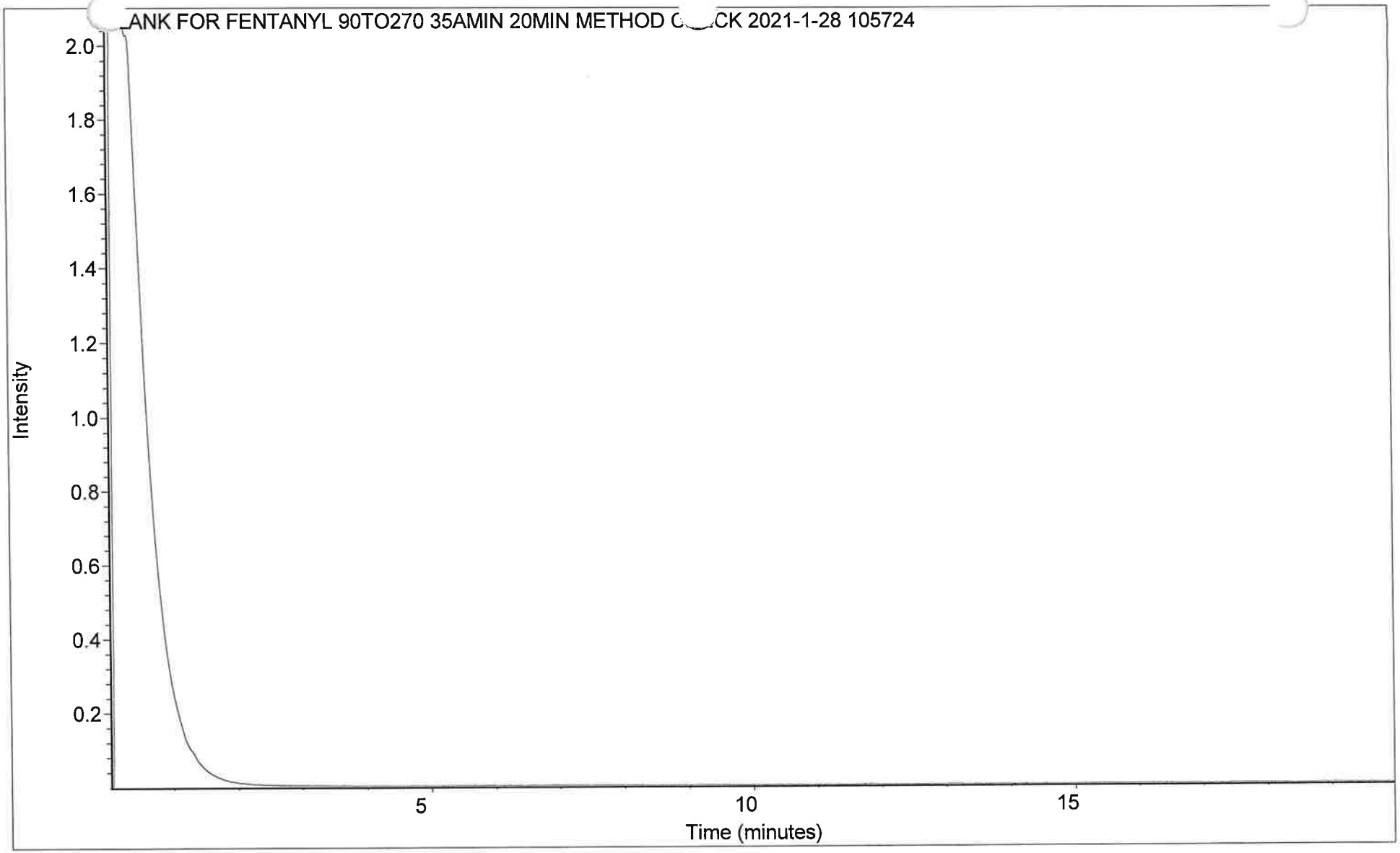
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Jan 28 14:26:40 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

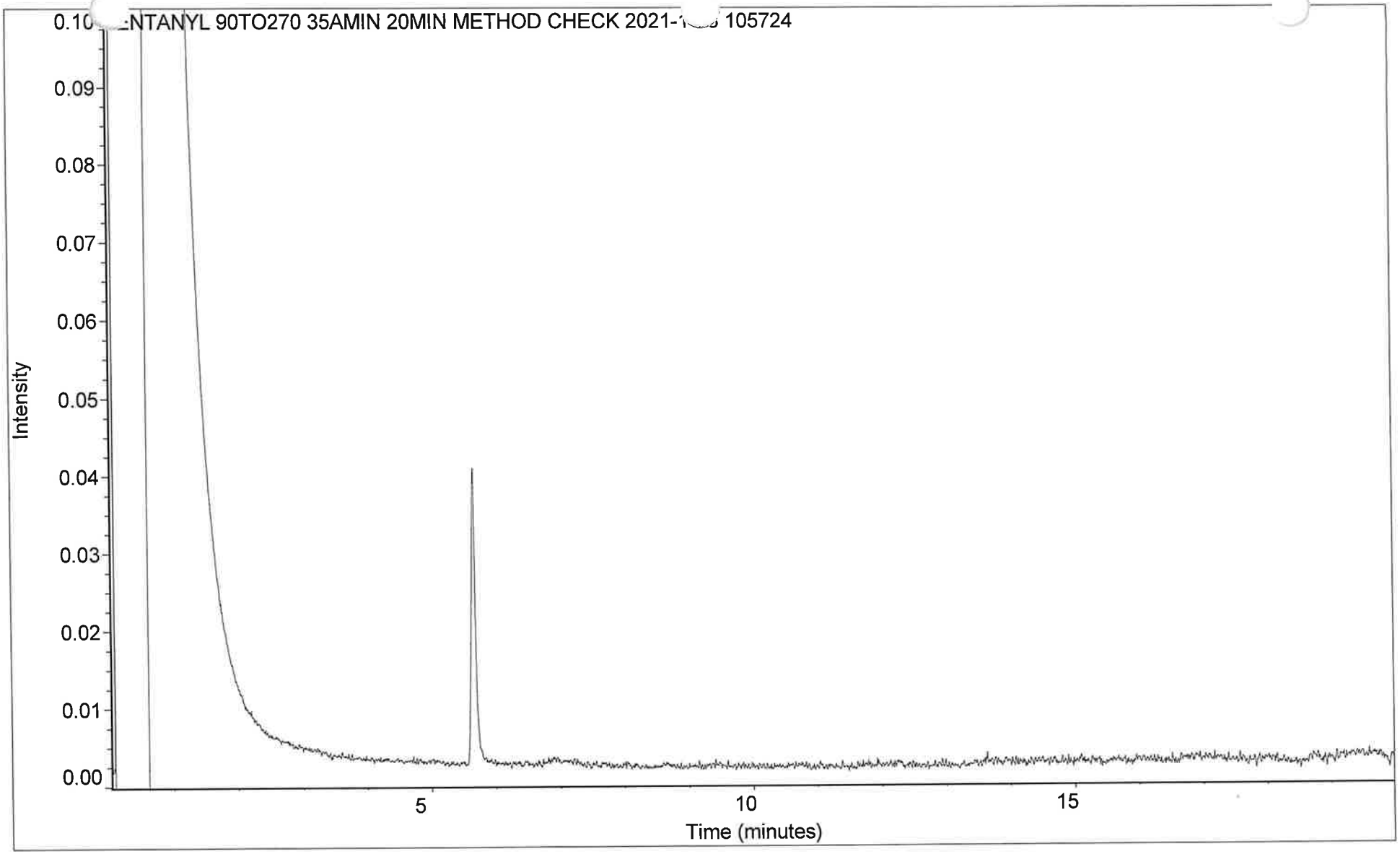
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Jan 28 11:01:52 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

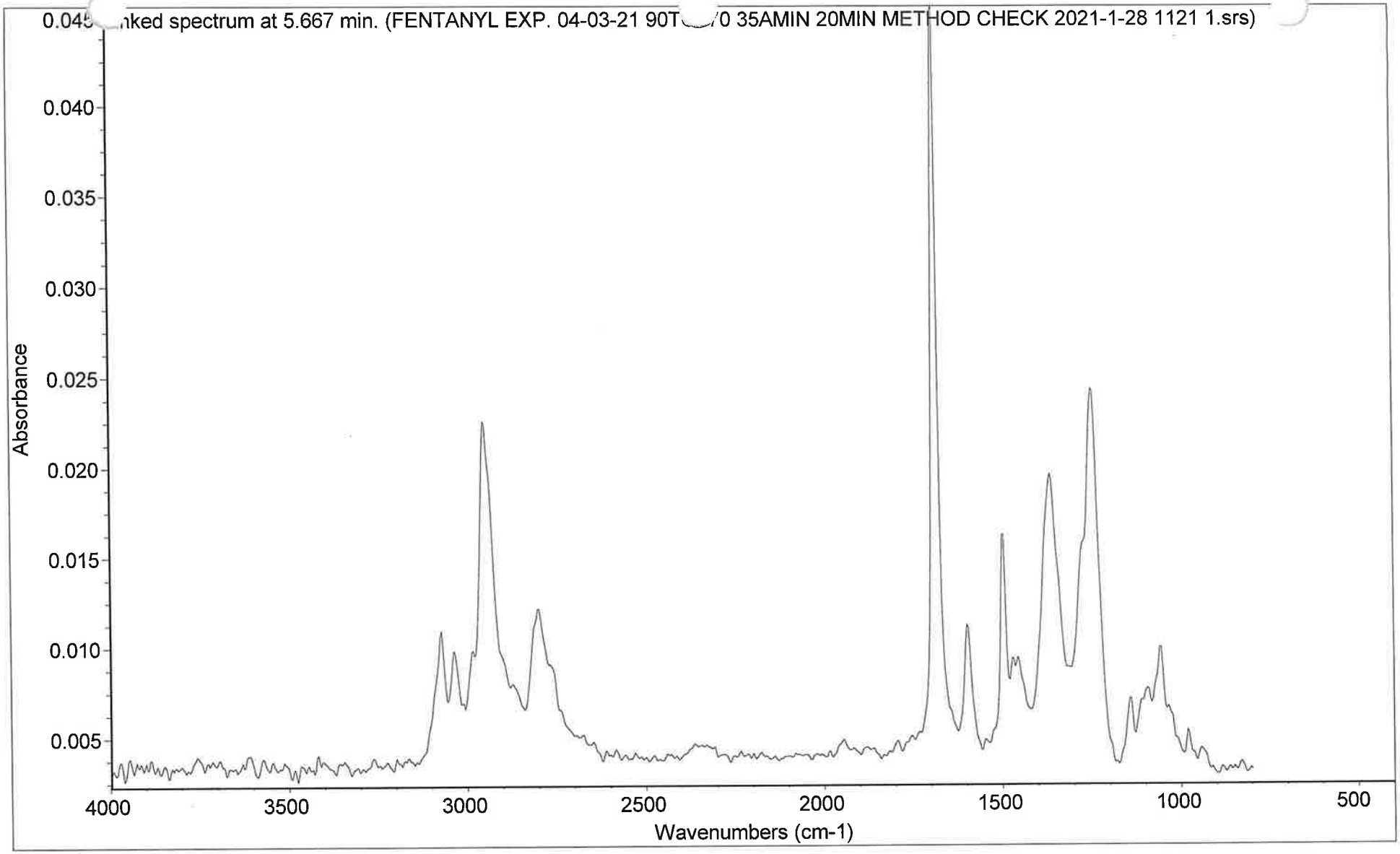
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Jan 28 11:23:12 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 5.667 min. (FENTANYL EXP. 04-03-21 90TO270 35AMIN 20MIN METHOD CHECK 2021-1-28 1121 1.srs)

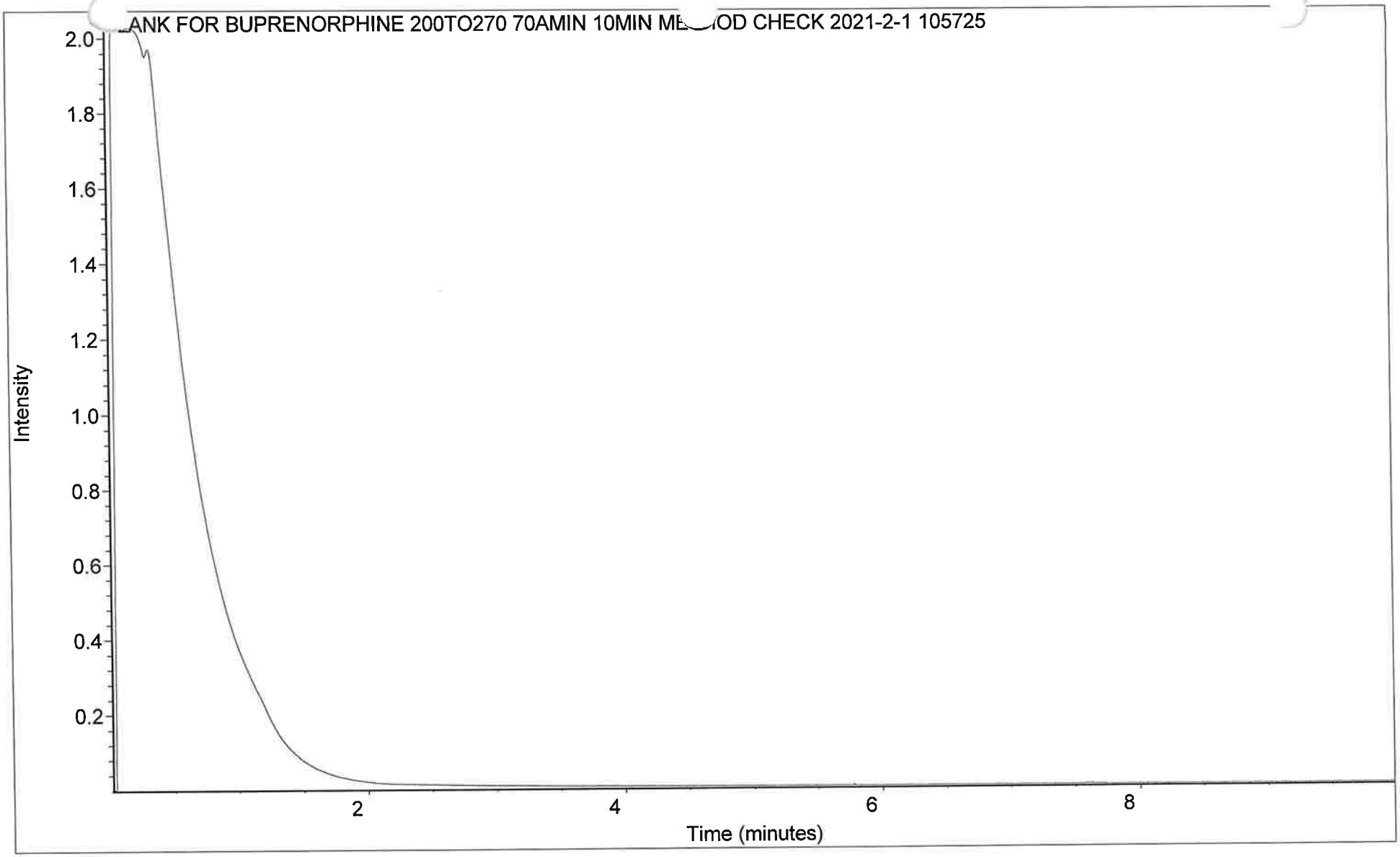
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Jan 28 11:23:12 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

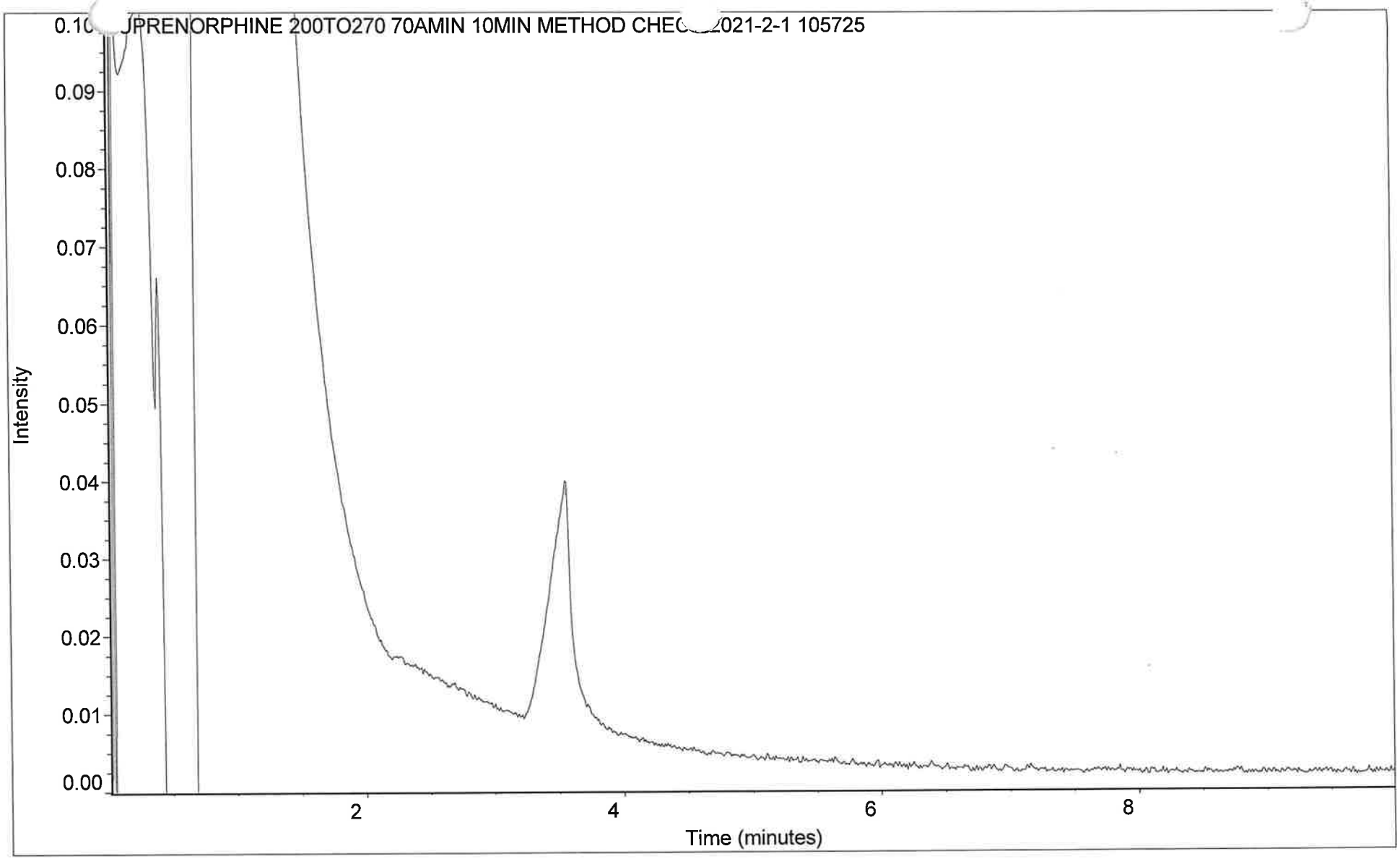
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Mon Feb 01 11:01:52 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



BUPRENORPHINE 200TO270 70AMIN 10MIN METHOD CHECK 2021-2-1 105725

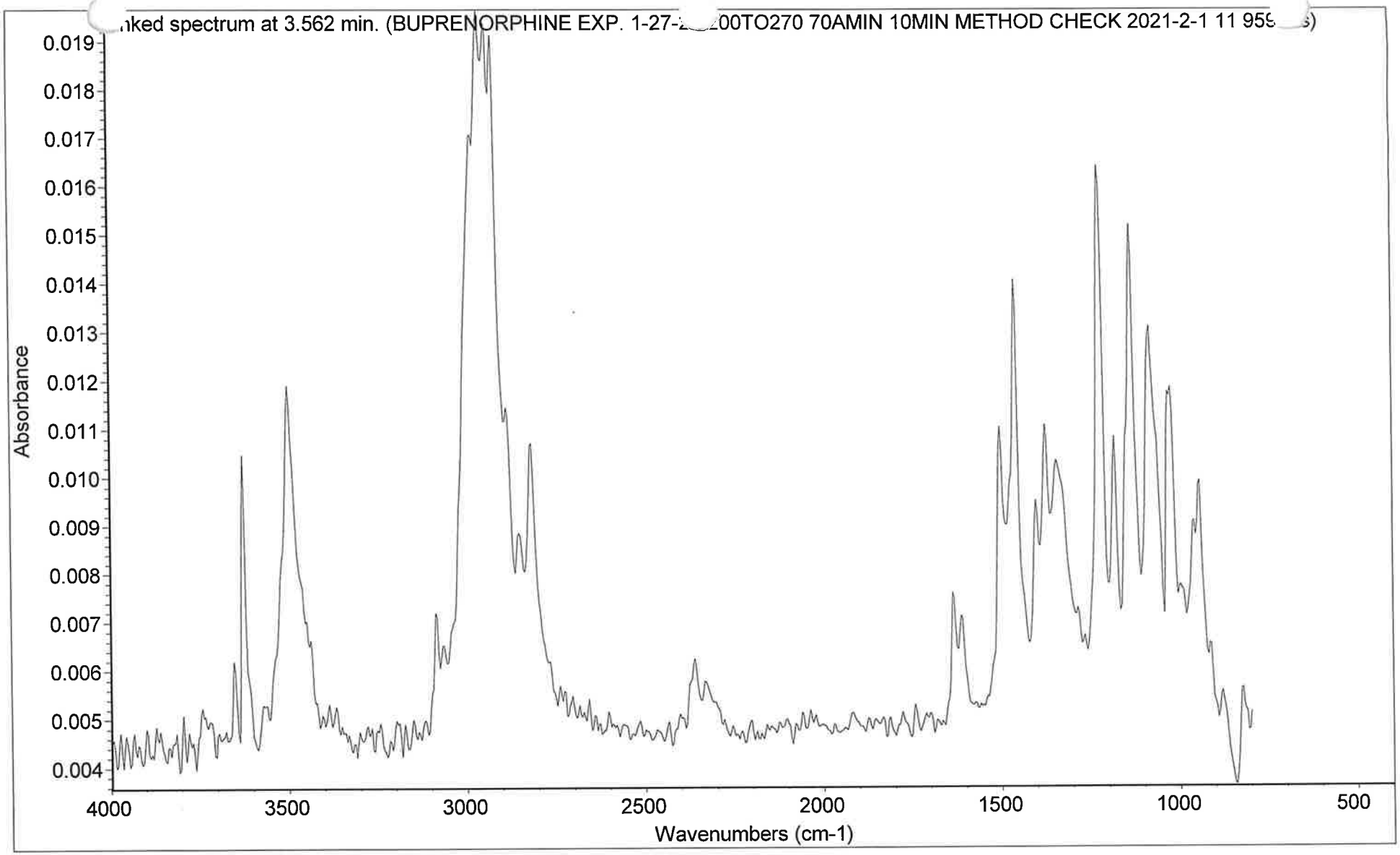
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

HOGWARTS

Collection time: Unknown

Detector: MCT/A
Beamsplitter: KBr
Source: Off

Number of sample scans: 1
Number of background scans: 0
Resolution: Unknown
Sample gain: 0.0
Optical velocity: 0.0000
Aperture: 0.00



Linked spectrum at 3.562 min. (BUPRENORPHINE EXP. 1-27-22 200TO270 70AMIN 10MIN METHOD CHECK 2021-2-1 11 959.srs)

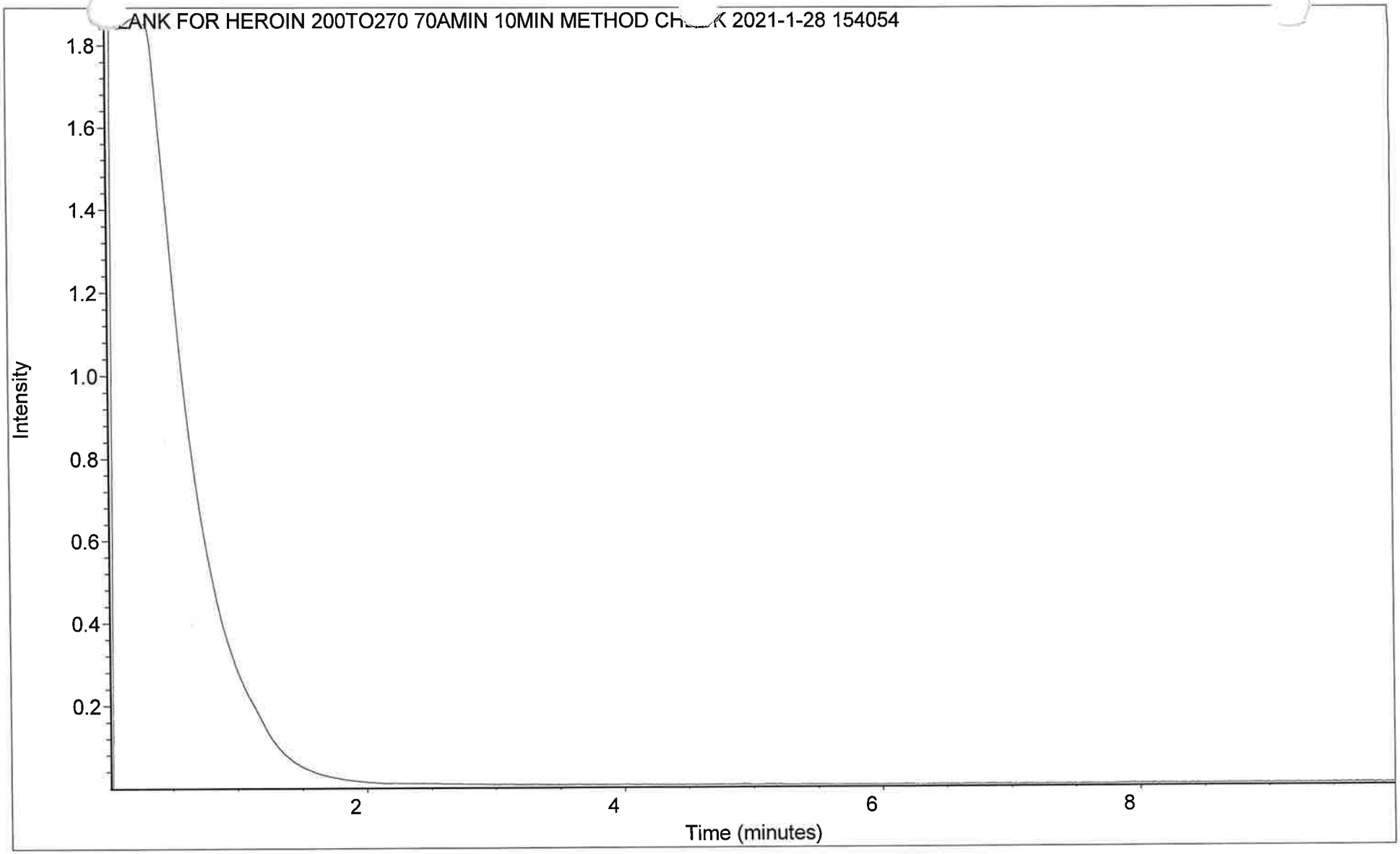
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Mon Feb 01 11:14:40 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

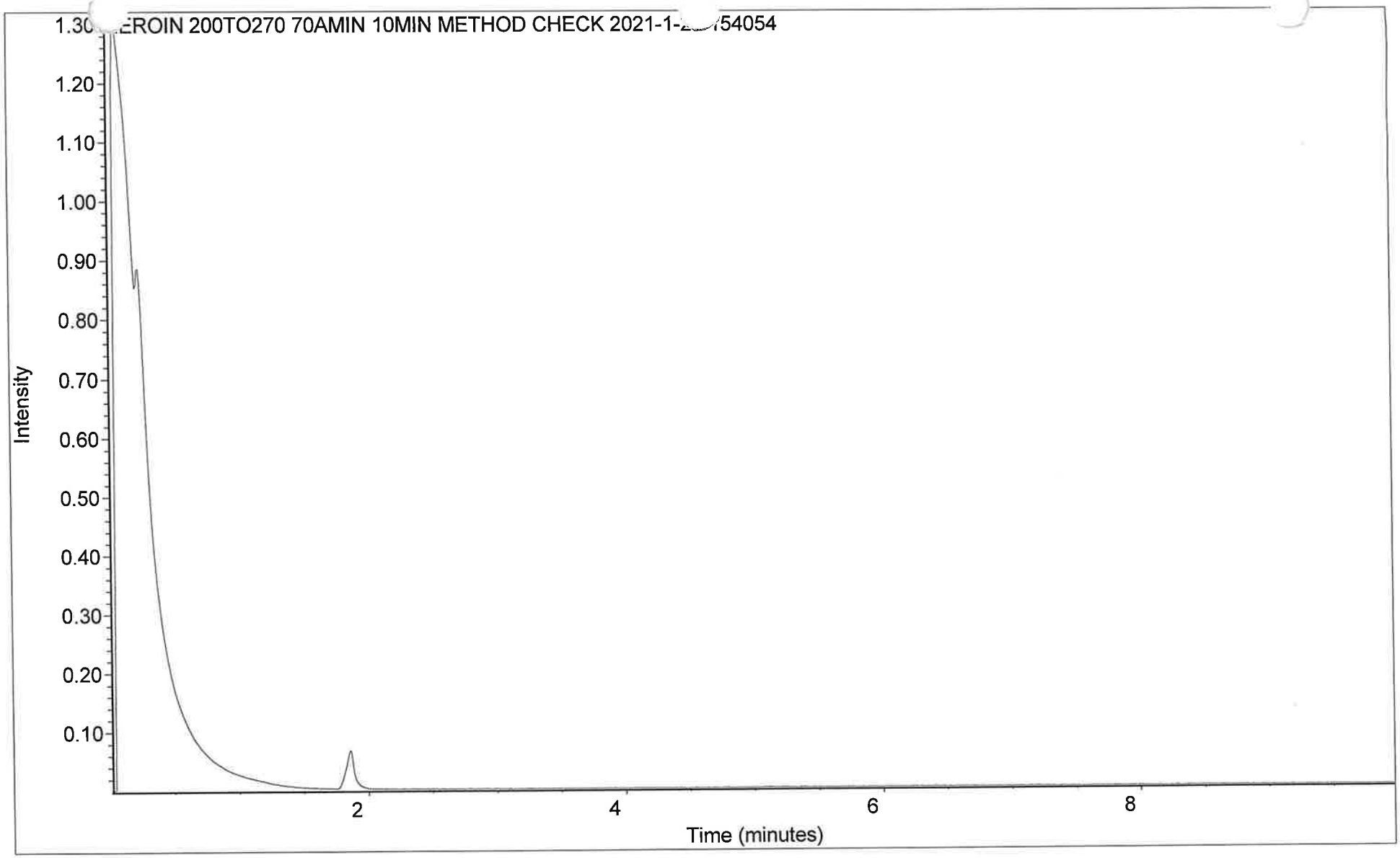
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Jan 28 15:17:52 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 1.858 min.

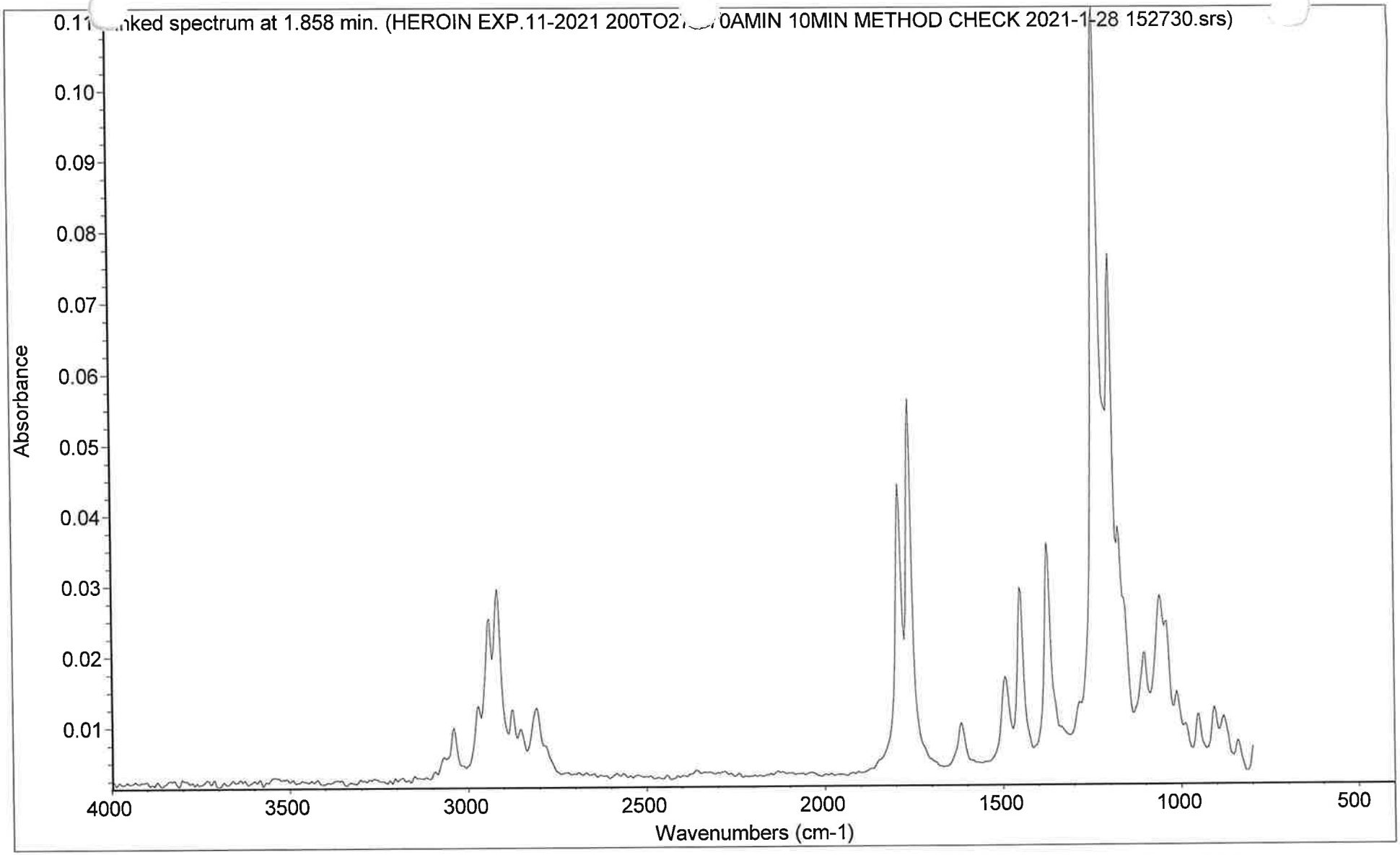
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Jan 28 15:30:40 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 1.858 min. (HEROIN EXP.11-2021 200TO270 70AMIN 10MIN METHOD CHECK 2021-1-28 152730.srs)

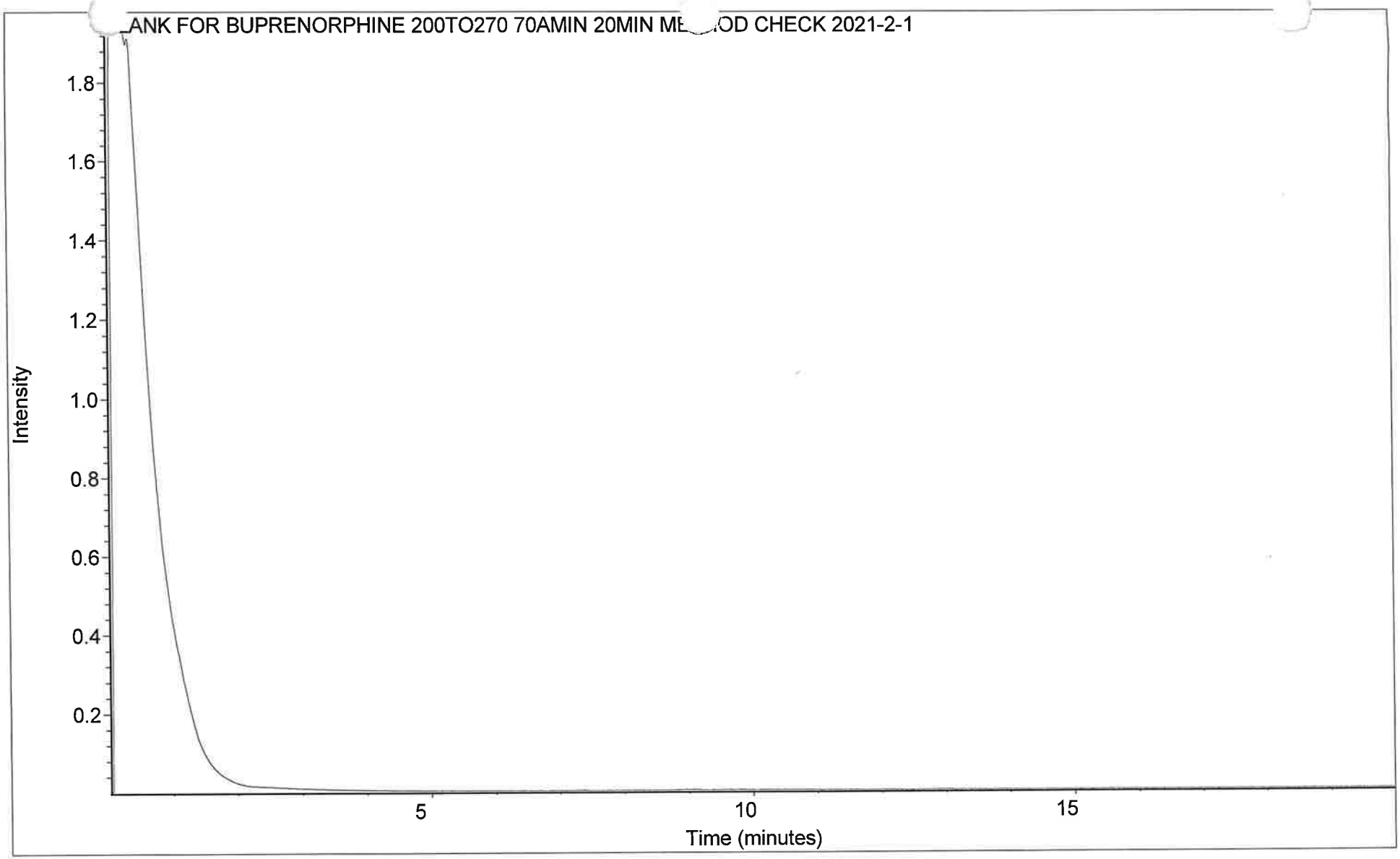
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Jan 28 15:30:40 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

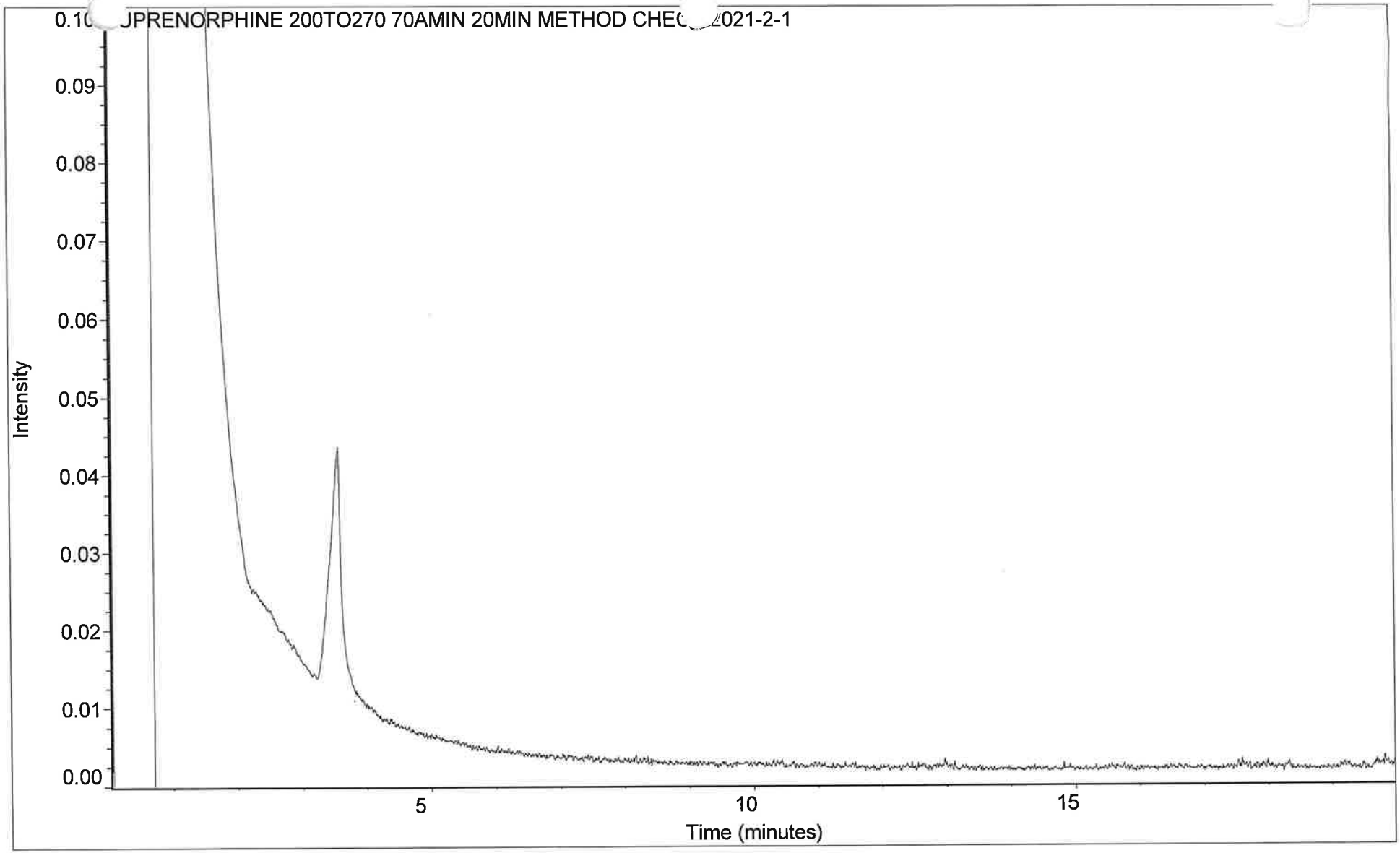
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Mon Feb 01 11:27:28 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 3.552 min.

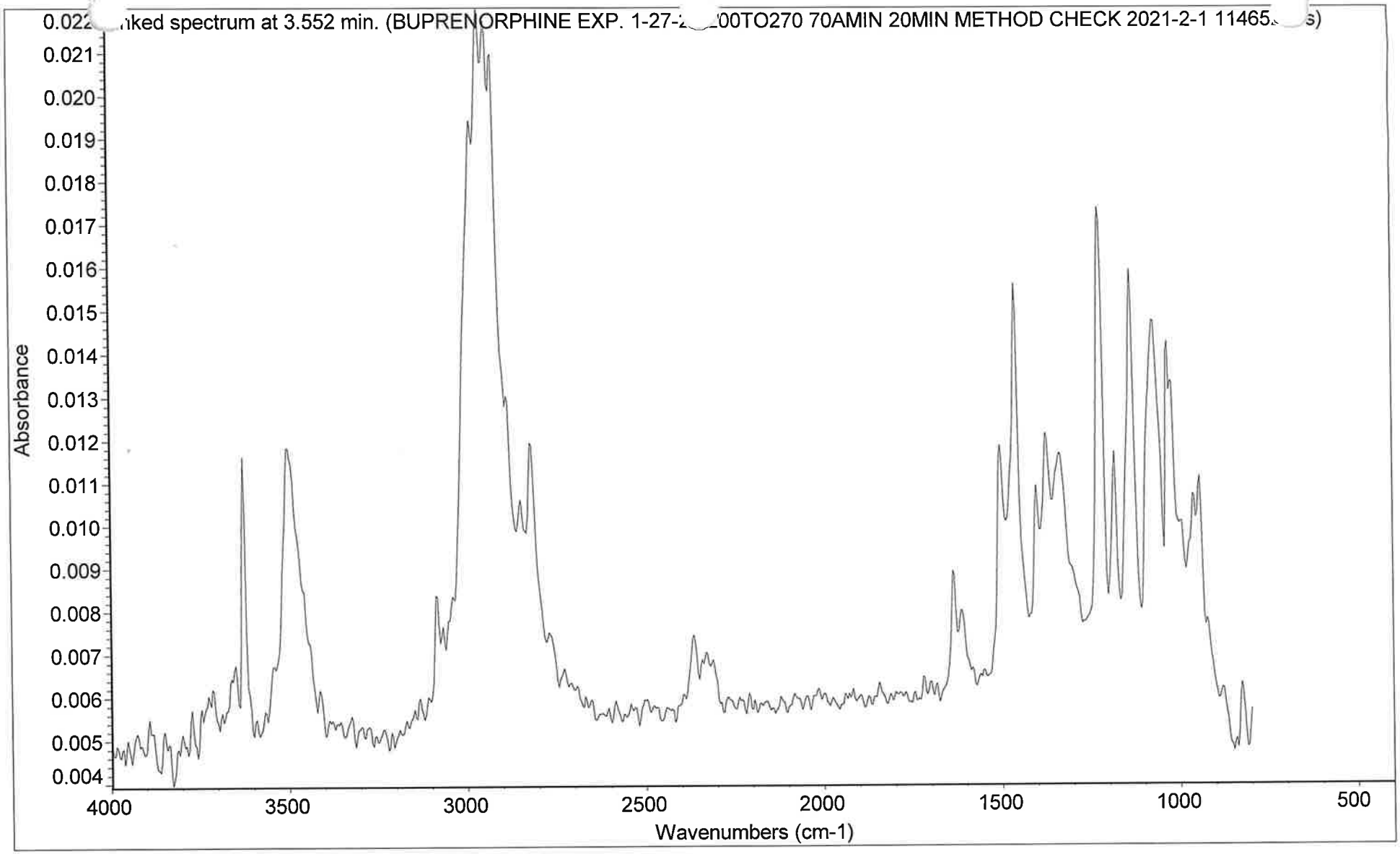
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Mon Feb 01 11:48:48 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 3.552 min. (BUPRENORPHINE EXP. 1-27-22 200TO270 70AMIN 20MIN METHOD CHECK 2021-2-1 114652.srs)

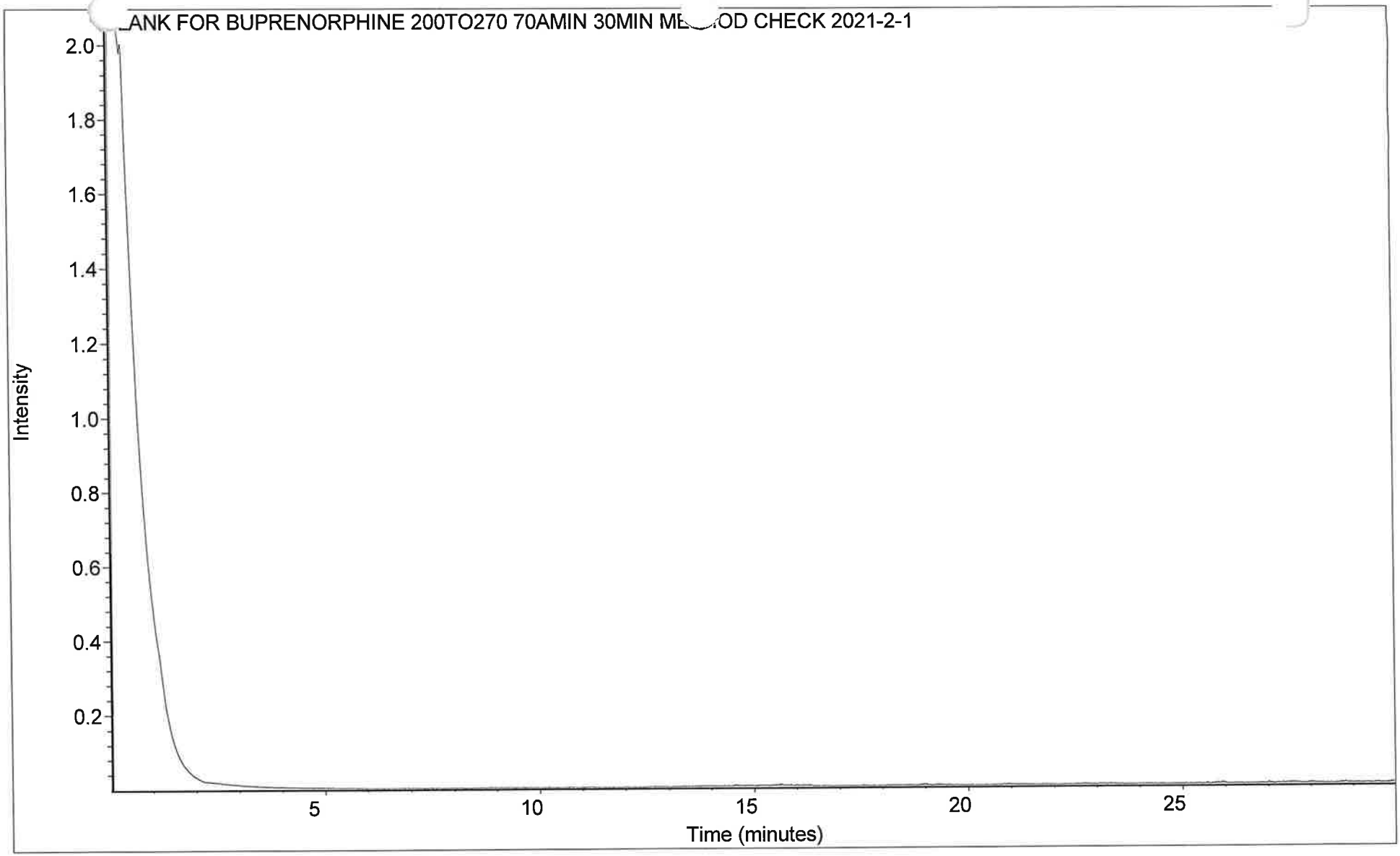
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Mon Feb 01 11:48:48 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

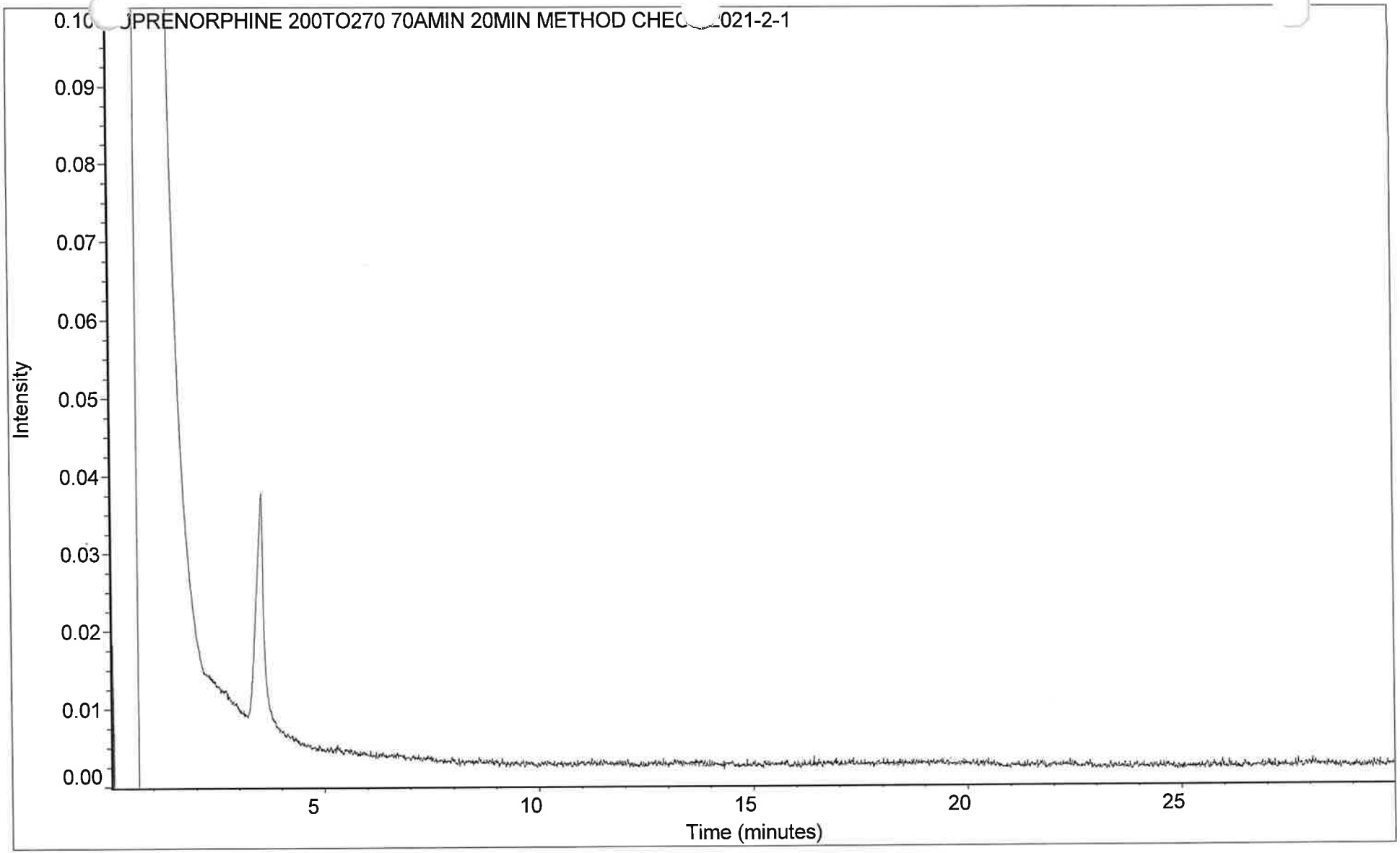
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Mon Feb 01 12:14:24 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 3.515 min.

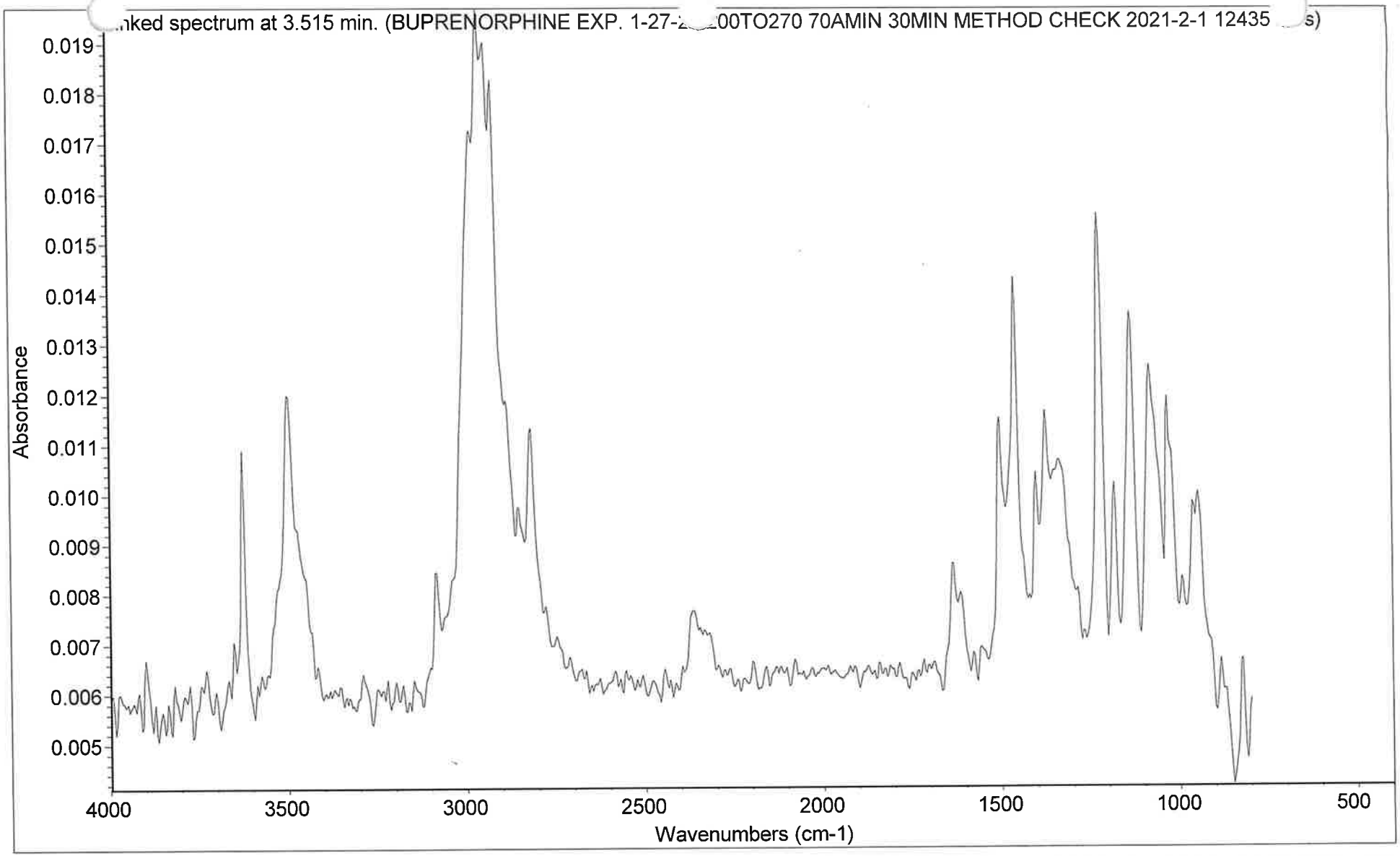
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Mon Feb 01 12:48:32 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 3.515 min. (BUPRENORPHINE EXP. 1-27-22 200TO270 70AMIN 30MIN METHOD CHECK 2021-2-1 124351.srs)

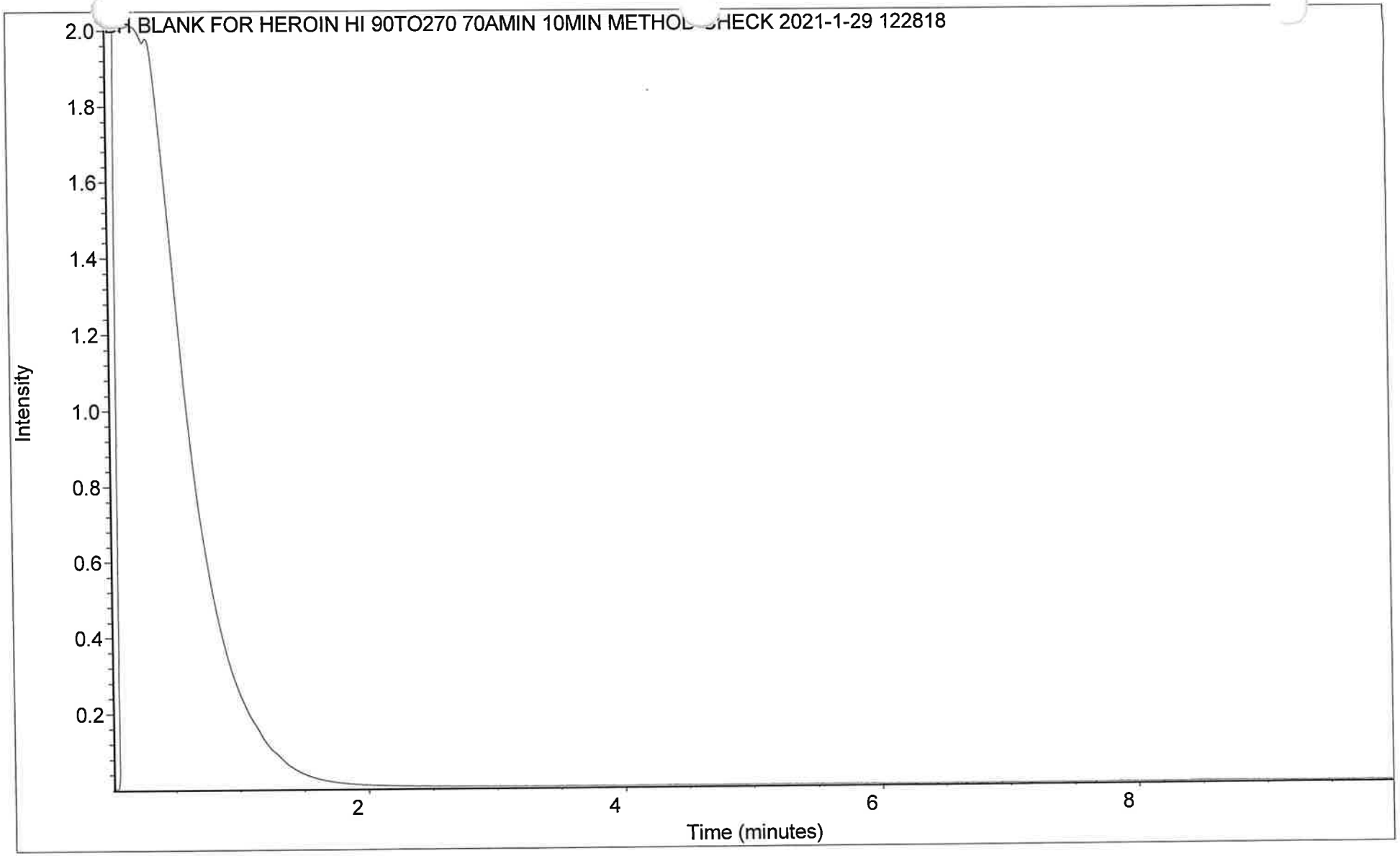
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Mon Feb 01 12:48:32 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

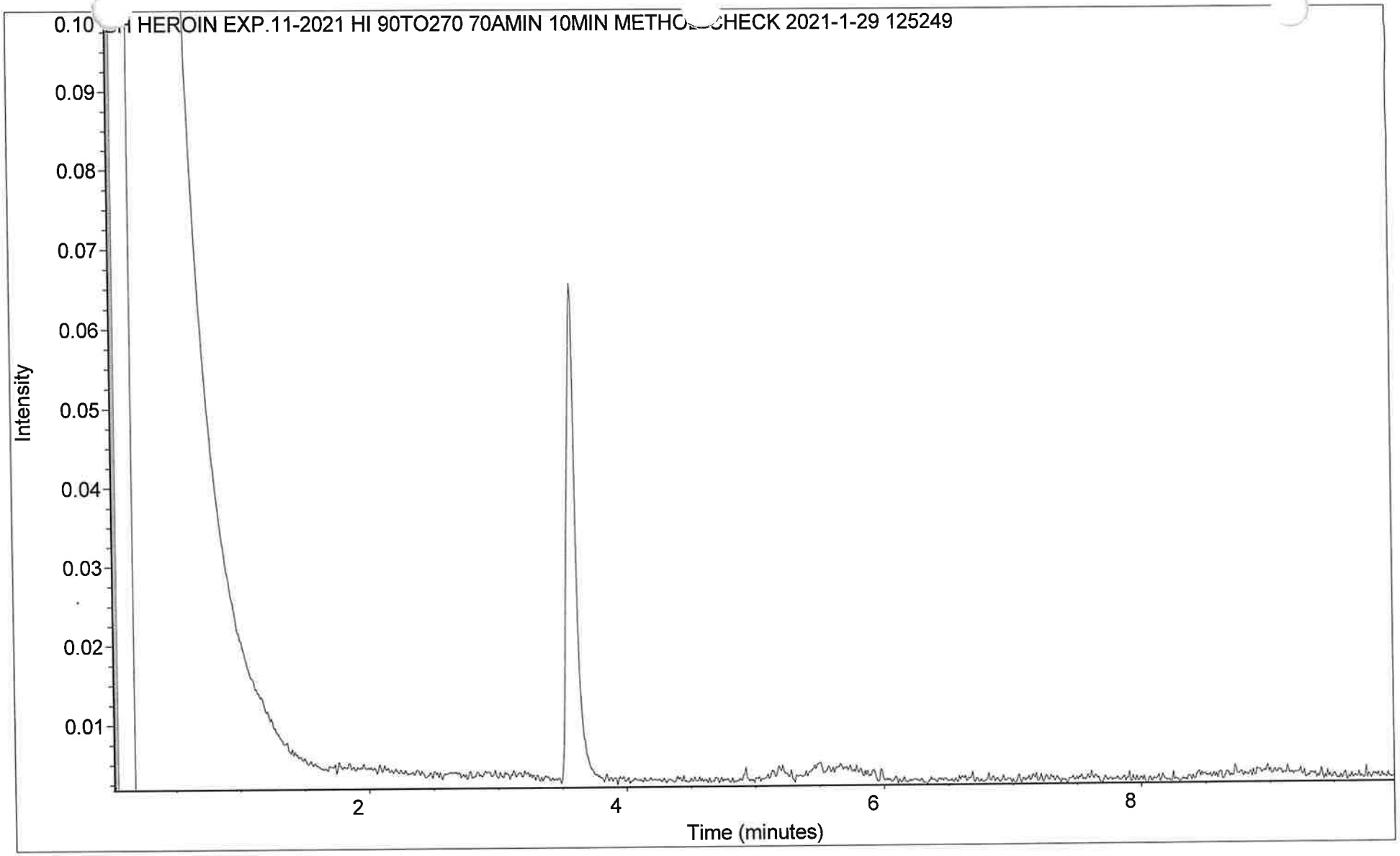
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Fri Jan 29 12:29:20 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 4.676 min.

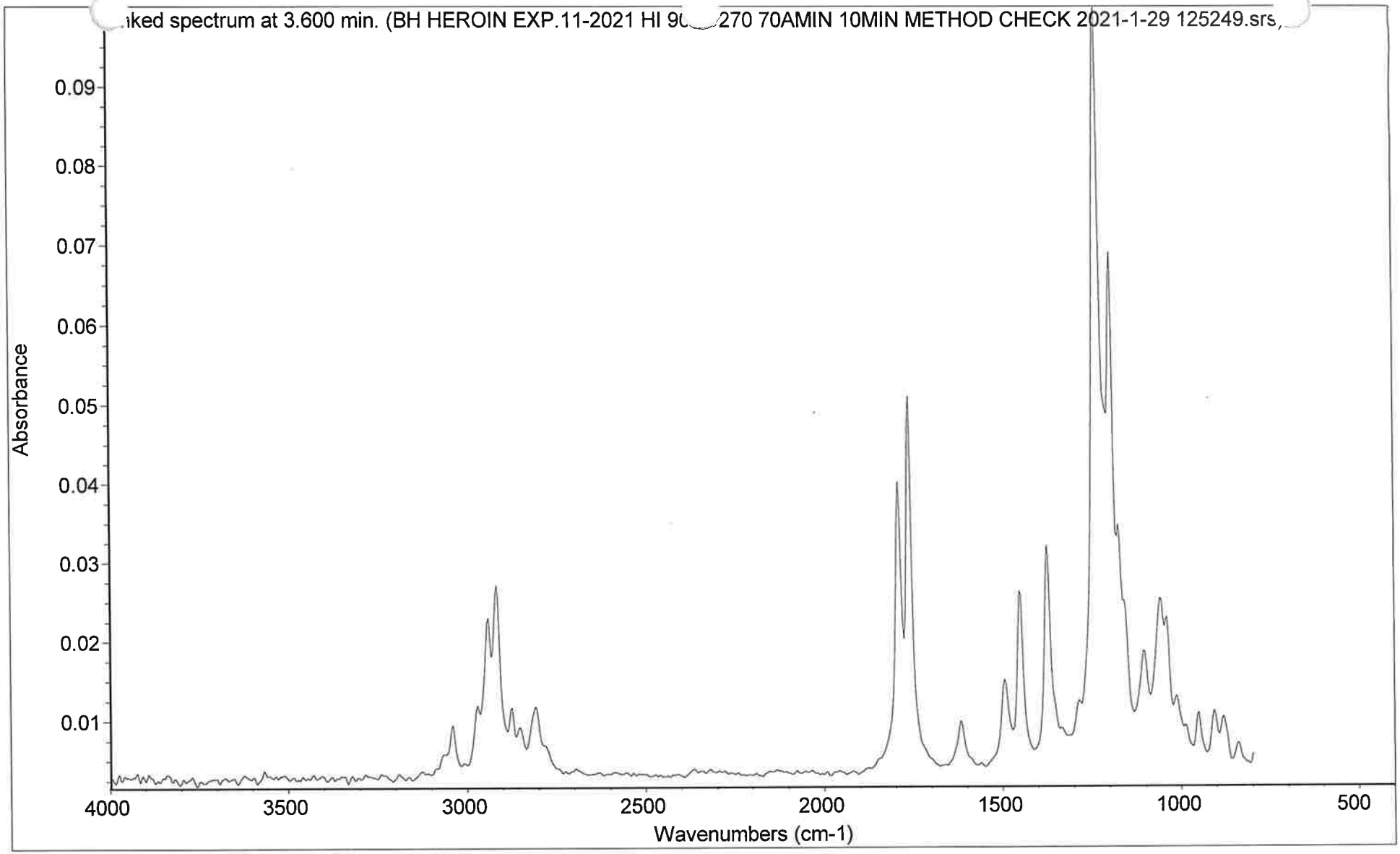
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Fri Jan 29 12:54:56 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 3.600 min. (BH HEROIN EXP.11-2021 HI 90TO270 70AMIN 10MIN METHOD CHECK 2021-1-29 125249.srs)

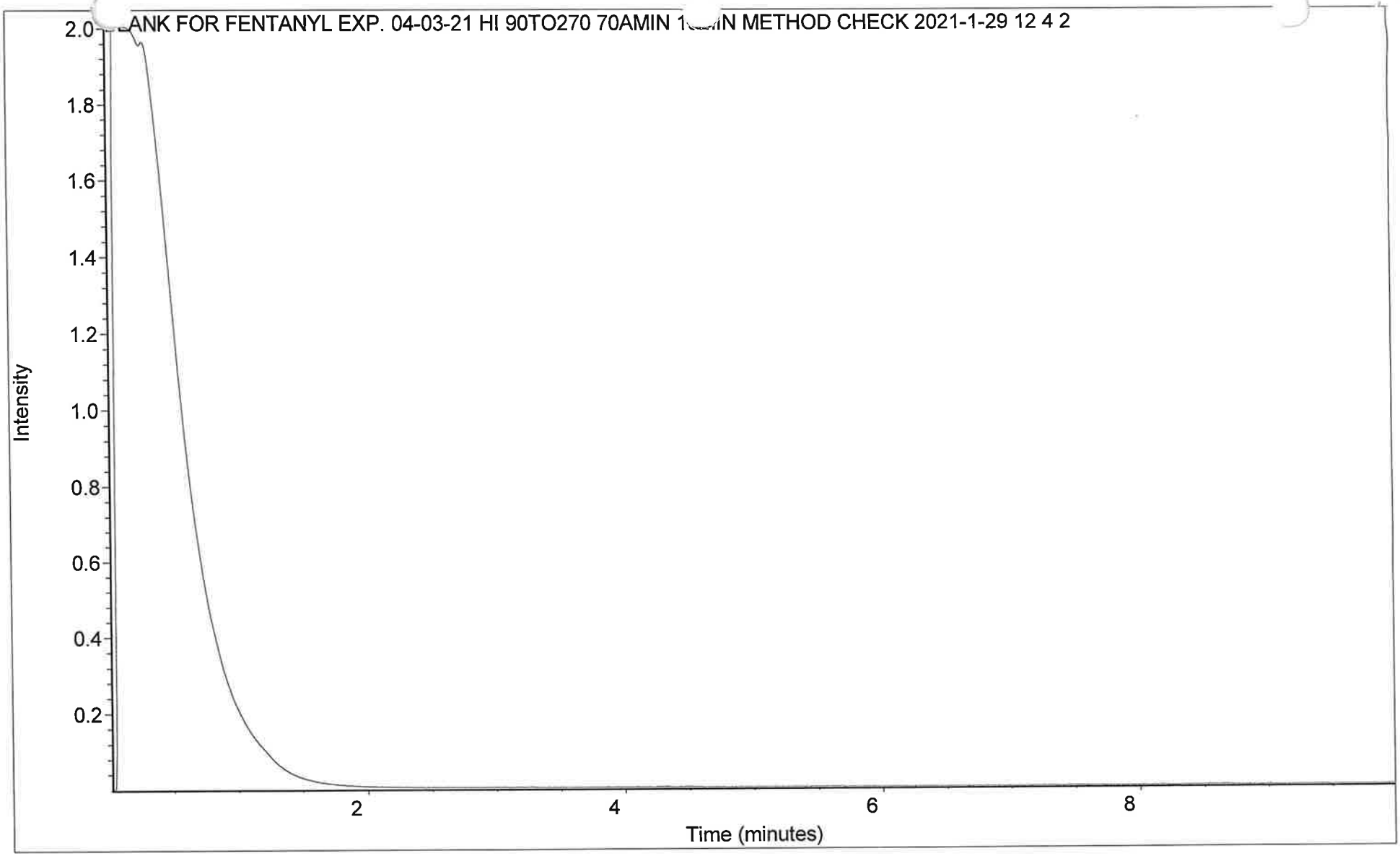
Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Fri Jan 29 12:54:56 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

Column 5 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Fri Jan 29 11:50:56 2021 (GMT-06:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00

TBI-FORENSIC SERVICES DIVISION
PERFORMANCE VERIFICATION FORM

Instrument/Method to Verify:

Thermo Trace 1310 GC Nicolet iS50 FTIR (Hogwarts)

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 Ben Hubert Title SA/FS Initials BH
Completed: Signature [signature] Date 11/6/20

Name NA Title _____ Initials _____
Completed: Signature _____ Date _____

Name NA Title _____ Initials _____
Completed: Signature _____ Date _____

Verification of final review:

Unit Supervisor Allen B. Everett Date 11-6-20

Unit Supervisor NA Date _____

Unit Supervisor NA Date Forensic Chemis

Crime Laboratory Regional Supervisor Jennifer Hall Date 12.2.20

Crime Laboratory Regional Supervisor NA Date Thermo Trace 1

Crime Laboratory Regional Supervisor NA Date _____

Quality Assurance Manager CLD Date 11/09/20

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

Technical Leader Allen B. Everett Date 11-6-20

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.

Hogwarts software familiarization

11-9-20

Andrea King

Brandi Fisher

Brett Trotter

Cassandra Franklin

Ella Carpenter

Glen Glenn

Glenn Everett

Isabella Barnett

Jennifer Sullivan

John Scott

Laura Cole

Laura Newberry

Lela Jackson

Rachel Freeman

Rebecca Hernandez

Rebecca M. Stout

~~Glenn Everett~~

Revalidation and Performance check for Thermo Trace 1310 GC Nicolet iS50 FTIR Hogwarts

Introduction

This validation and performance check is designed to demonstrate the effectiveness of Hogwarts. This instrument will be evaluated on method functionality and previously determined acceptance criteria to determine suitability for the analysis of legally significant compounds.

After an extended period of maintenance and several software updates, Hogwarts required a limited revalidation to demonstrate that it still produces acceptable data for casework. This was done by running specific standards on each approved method. These standards include, fentanyl, methamphetamine, phentermine, amphetamine, pethidine, cocaine, and hydrocodone in order to demonstrate the instrument's effectiveness over a variety of compounds. The data obtained from these runs was then evaluated for instrument response and spectral accuracy. This data can be found attached to this memo.

Materials

Column:

Agilent

J&W GC HP-1 30 meter, 0.32 ID, 0.25 µm

Liner:

Restek Split/ Splitless straight with glass wool liner

Drug Standards

Fentanyl Citrate Standard

(USPC lot # 1275-F) 0.5120 mg/mL

GCMS Standard Mix in MEOH (Fisher lot# 202169) RLF EXP: 04-05-21

Pethidine (S.B. Penick 413 NMN-027) 6.35mg 0.635mg/mL

Cocaine Base (Merck lot # U7472) 2.21mg 0.221 mg/mL

Hydrocodone (Merck lot # V1526) 8.01mg 0.801 mg/mL

GC-IR Standard MIX in 0.5N NaOH -> $CHCl_3$ RH EXP: 05-26-21

D-Amphetamine Sulfate (K&K Labs 83567) 4.98mg 0.996 mg/mL

Phentermine (Sigma 47H0208) 5.07mg 1.014 mg/mL

A-(D-L) Methamphetamine (K&K Labs 732A) 5.02mg 1.004 mg/mL

Results

Analysis of the standards run on Hogwarts have consistently shown compliance with standard operating procedures 22.3 and 22.6.1. All methods have been utilized in the analysis of known drug standards. The data obtained from these standards is consistent with previously verified standards in the Nashville forensic chemistry standard library. The instrument response was compared to older data taken from before the period of maintenance. The chromatography, peak shape, and separation all appear to be consistent to the data that the instrument was generating prior to the software update.

Conclusions

After monitoring parameters specified in Forensic Chemistry Standard Operating Procedure found in chapter 22 and verifying the functionality of previously utilized methods with known drug standards, it has been demonstrated that Hogwarts produced comparable results to previous instrument response and GC-FTIR libraries.

After performing theses runs, the instrument showed comparable results to its premaintenance and prior software state. Using the instrument will not require new competency training, but I do recommend that scientists in the Forensic Chemistry Unit be familiarized with the updated software and the instrument be returned to service.

Hogwarts

GC-FTIR

Chromeleon®7 Software

Dionex Chromeleon version 7.2.10

Ominc 9.11.745 software

Ominc Series 9.11.727

Driver version 9.11.709

Nicolet iS50

Firmware version 1.11

Thermo Scientific Hogwarts GC-FTIR Operating Procedures

Each GC-FTIR system will be identified from all other GC-FTIR systems by use of a unique identifier. This identifier could be a reference to a particular number, model number, serial number, name, etc. All GC-FTIR systems employ OMNIC software. The Hogwart's GC-FTIR additionally employs Chromeleon 7 GC software. See the instrument's maintenance logbook for the specific OMNIC and Chromeleon 7 software version.

General Operations:

1. Ensure that the power is on to all components
2. Open the Chromeleon 7 application by double clicking the icon on the computer desktop (This may take a few moments)
3. Once the Chromeleon 7 application has successfully opened, open the OMNIC application by double clicking the icon on the computer desktop

NOTE: IT IS IMPORTANT THAT YOU FIRST OPEN CHROMELEON AND THEN OMNIC. OMNIC WILL NOT COLLECT DATA IF YOU DO NOT OPEN CHROMELEON FIRST.

To Set Up for Analysis:

Make sure that the **Default iS50 GC-IR** experiment is selected on the OMNIC **Experiment** tool bar and that the blue button is lit up on the iS50 GC-IR accessory.

This should be selected automatically by the instrument. The instrument should be set to a Gain of 1, Resolution of 8 cm-1, 4 Scans, 64 Scans for the background and a spectral range of 4000 to 800 cm-1.

Data Acquisition:

1. All parameters for analysis on the Hogwart's GC-FTIR are electronically stored in the Chromeleon 7 software under the **Data** tab within the folder name **Chromeleon Local.** The method parameters for an analysis run will be noted in the analyst's case file.

NOTE: Remember that the column on the Hogwart's GC-FTIR has a longer column and thinner film thickness than GC/IR #1 and #2. This should be taken into consideration for certain analytes, using the necessary methods as needed.

2. A sample blank must be run each day per each case file, method, and extraction prior to running a case sample.
3. If the reservoir on the GC-FTIR is not cold, fill the reservoir with liquid nitrogen.
4. In the **OMNIC** application window select the **Series** tab and select **Heater Status…**

5. Make sure the heaters are turned on (checked box) and set the **Flow cell setpoint (deg. C):** and **Transfer line setpoint (deg. C):** to **280°C** in the white box and select the **Update Heaters** button.
6. To the right of the white box where the temperature values are set it will show the actual temperature of the flow cell and transfer line. When the values have not reached the desired set temperature, the filament background picture will become yellow. Once the values of the set temperatures have been reached the filament background will turn green.
7. Exit the **Heater Status…** window once the set temperatures have been reached.

Creating a Sequence:

8. Select the **Data** tab within the **Chromeleon Console** window.
9. Find the file titled **_Series Template_ (COPY AND PASTE)** and copy and paste it to your personal Chromeleon sequence folder.
10. Once the file has been pasted to your folder rename it with the date and your initials.
11. Fill out and select the **Name, Position, Volume, Instrument Meth, and Comment** boxes for the samples on the displayed sequence. The **Instrument Meth** boxes will have drop down arrows to select each method.
12. It is the analyst's discretion as to which method to use.
13. Make sure that in the **Name** box provides detailed sample information and the user's initials (This is how the file information will be saved in **OMNIC**)
14. **Click here to add a new injection** to add more samples to the sequence.
15. Once all of the samples have been added and the sequence is ready to run select the **OMNIC** application window.
16. Select the "Collect Ser" button on the **OMNIC** taskbar.

NOTE: IT WILL TAKE A FEW MOMENTS FOR OMNIC TO LOAD THE COLLECT SERIES IF THE SOFTWARE HAS NOT ALREADY BEEN IN USE.

17. The background will collect once the **OMNIC** software has finished loading and an **External Trigger** window will pop open stating "Ready to start data collection at external trigger.".
18. Select the **Chromeleon Console** window and highlight the beginning of the sequence run (or the sample you wish to run).
19. Click the "Start" button at the top of the sequence.
20. After a few moments the sequence toolbar should load from yellow to green (New→Running) and where the "Start" button appeared it will now state "Stop".

Auto-sampler Injection:

The auto-sampler will automatically inject your sample once the run has been started in the **Chromeleon Console** and the TRACE 1310 instrument is at ready status.

OMNIC will be triggered to start collecting data once the auto-sampler has injected the sample.

Analyzing data in OMNIC:

21. Open the **OMNIC** application window and select "File" and then "Open…" in the toolbar.
22. An "Open" window will appear and in the "Files of type:" box, click the down arrow and select the "Series Files (*.SRS)" option.
23. Select the data file you wish to open and click the "Open" button.
24. Data file will display in **OMNIC**.
25. Use the bottom tools or taskbar to analyze the spectra.
26. To add a spectra region to a new window, right mouse click the bottom screen (spectra) and select "Copy To > New Window" and then click the "OK" button
27. To view a window, select the "Window" tab in the toolbar and click on the window you wish to display.

To Set Up for iS50 ATR Analysis:

Make sure that **iS50 ATR** experiment is selected on the OMNIC **Experiment** tool bar and that the blue button is lit up on the iS50 ATR accessory.

The parameters for using the iS50 ATR accessory should be set to Autogain, Resolution of 4 cm^{-1}, 16 Scans, and a spectral range of 4000 to 600.

iS50 ATR Operating Instructions:

1. At **Experiment** on the tool bar, load the **iS50 ATR** parameter file.
2. Select **Report** on the menu bar and select "Template…".
3. Select the ATRTEMPLATE.RPT at the very top of the scrolled window and click the "Select" button below.
4. Clean ATR stage and underneath ATR accessory.
5. Collect background and add to window.
6. Add sample and turn down ATR accessory.
7. Collect sample, add to window, select stack spectra, fill out sample information in text box, and select print option on taskbar.
8. Clean ATR stage and underneath ATR accessory.
9. Select **Report** on menu bar and select "Template…".
10. Select WILLIENEWGCFTIR.RPT template at very bottom of scrolled window and click the "Select" button below to switch template back.

11. Make sure **Default iS50 GC-IR** parameter file is switched back and loaded in **Experiment** tool bar.

MONTHLY MAINTENANCE

Alignment:

1. At **Experiment** on the tool bar, load the **Transmission E.S.P.** parameter file.
2. Select **Collect** from the menu bar and select **Experiment Setup…**
3. After the window loads go to the **Bench** tab and make sure that the Gain is set to 1.0.
4. Then select the **Diagnostic** tab and select the "Align…" button. When the alignment is complete record the number in the appropriate GC/IR maintenance log.
5. Click "OK" button to exit out.
6. Next, check and make sure the desiccant on the instrument is blue (If pink, moisture is present).

Report & Main, ATR, GC iS50 Performance Tests (KBr)

1. Make sure that the main sample compartment is empty.
2. From the menu bar select **Collect** then select **Advanced Diagnostics….**
3. After "Nicolet iS50 Diagnostics" window opens, select **Performance Test.**
4. Check all the boxes for the **Main, ATR, GC iS50 Tests (KBr).**
5. Select the "Run Selected Test" button.
6. Fill out OMNIC with performance test values for each spectra (**Main, ATR, GC**) and print and place spectra in the appropriate GC/IR maintenance log book.

   Example:

   PERFORMANCE TEST (MAIN) 2200-2100 = 0.004 PASS RMH
   PERFORMANCE TEST (ATR) 2800-2700 = 0.024 PASS RMH
   PERFORMANCE TEST (GC) 2200-2100 = 0.012 PASS RMH

7. After tests are complete, select each spectra (**Main, ATR, GC**) and individually save by setting the filename to title under the "Monthly Performance Tests" folder under the "Spectra/Groups (*.SPA, *.SPG)" file type.
8. Select the back arrow button and select Report, Print, and then the back arrow button again. Place the print out in the GC/IR maintenance log book.
9. Exit out of "Nicolet iS50 Diagnostics" window.

ValPro Qualification:

1. Check to ensure the **Transmission E.S.P.** parameter file is loaded under **Experiment** from the tool bar.
2. Select **Analyze** on the menu bar and then **ValPro Qualification….**
3. Once the "ValPro Qualification" window appears use the drop down box under "Qualification test:" and select the "Nicolet iS50 system with DTGS in built-in position KBr-EP".
4. Select the "Qualify" button once the test has been loaded.
5. When the ValPro Qualification has completed, highlight the test that just completed in the "Energy ratio" tab and click the "Report…" button.
6. A window will pop up with the report. Select the "Print" button and fill out ValPro Qualification Report and initial and place in the GC/IR maintenance log book.
7. Select the "Close" button.

For iS50 ATR Accessory

1. In the "Qualification test:" drop down box select the "Nicolet iS50 system with integrated diamond ATR and built-in DTGS-EP" option.
2. Select the "Qualify" button once the test has been loaded and click "OK" when the confirmation window pops up for the background.
3. Retrieve the SMART iTR polystyrene standard "lollipop" from the second drawer near the IR #7.
4. When a window pops up stating "Place the polystyrene in the accessory and apply pressure. Choose OK when you are ready to collect the sample data", place the polystyrene standard "lollipop" on the sample compartment area with the "ATR STD 269-173000" words facing upwards and apply pressure.

   NOTE: Be sure to place the iS50 ATR accessory on the "lollipop" polystyrene standard window in different locations when performing monthly maintenance so as to not place the iS50 ATR accessory on the same location on the "lollipop" window.

5. Select the "OK" button once the "lollipop" polystyrene standard is in place.
6. When the ValPro Qualification has completed, highlight the test that just completed in the "Wavenumber accuracy" tab and click the "Report…" button.
7. A window will pop up with the report. Select the "Print" button and place in the GC/IR maintenance log book.
8. Select the "Close" and then "Exit" button to close out of the ValPro Qualification.
9. Select and load the **Default iS50 GC-IR** parameter file under **Experiment** from the tool bar
10. Remove "lollipop" from iS50 ATR sample area and place back in Thermo box and return it to the second drawer near the IR #7.

11. Fill out ValPro Qualification Report and initial and place in the GC/IR maintenance log book.

To Run the Monthly Standard Check:

1. Check to ensure the **Default iS50 GC-IR** parameter file is loaded under **Experiment** from the tool bar.
2. Make sure the reservoir for the MCT detector is filled with liquid nitrogen.
3. Make sure that the **transfer line** and **flow cell** heaters are at 280°C.
4. Analyze the Monthly QC test standard (Amphetamine, Phentermine, Methamphetamine) that is kept refrigerated.
5. Check its expiration date. If it is past its expiration date, make up a new QC test standard following the correct procedure to ensure the proper concentrations.
6. Make sure that the **60@20AMIN** is loaded and used to run the Monthly QC standard.
7. Run this sample following the procedures for analyzing data from the GC/FTIR and place in the GC/IR maintenance log book.

This is not meant to be all-inclusive. There may be other ways to accomplish the same task.

Addendum

S/SL Injection Port with HP-1MS 30 meter column, 0.32 column ID, and 0.25 um film thickness:

*Stored Methods for **AUTOSAMPLE SPLIT INJECTION***

120TO270 Initial 120C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 10.00 minutes.

120TO270(30MIN) Initial 120C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 30.00 minutes.

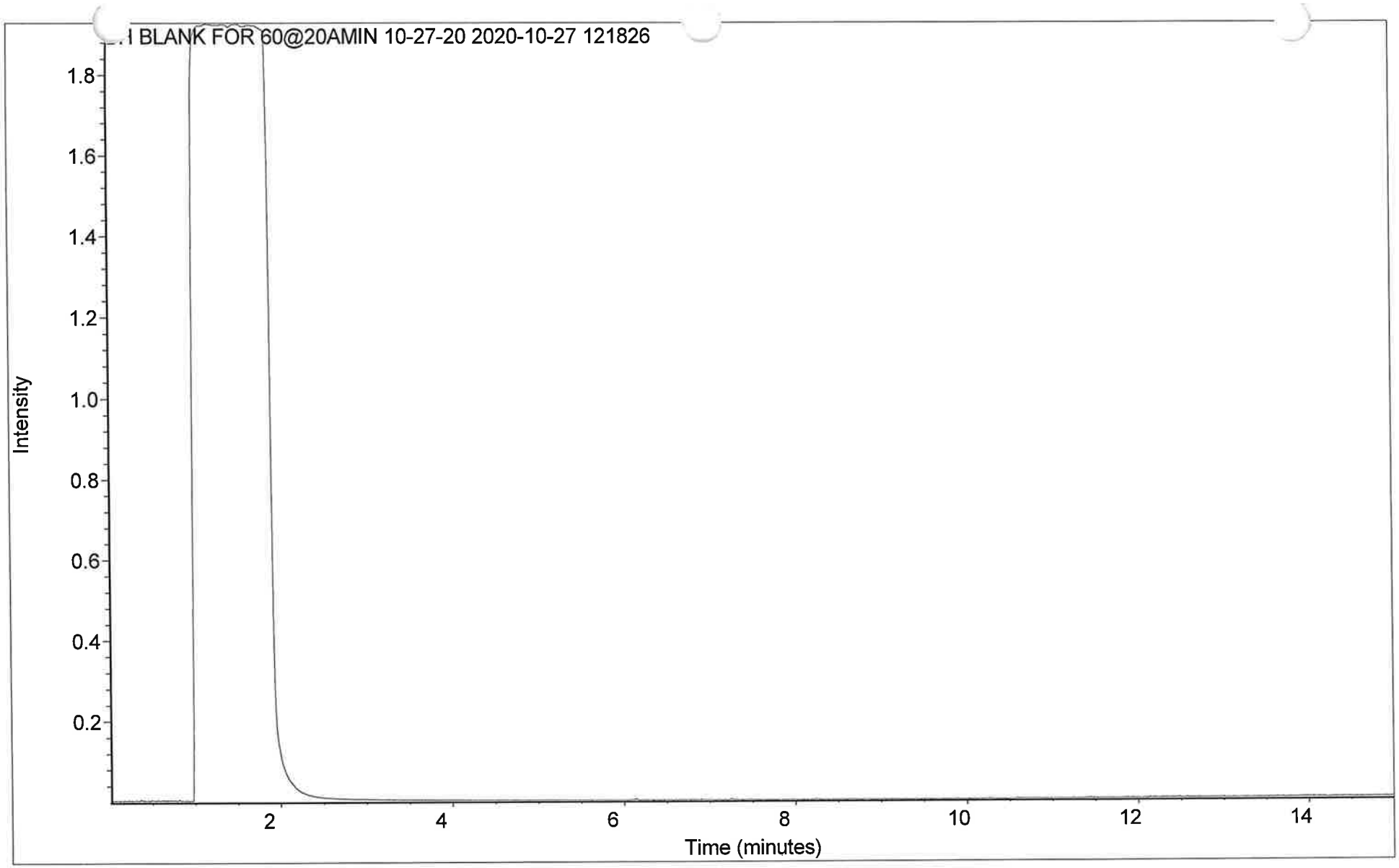
200TO270 Initial 200C degrees hold for 1 minutes ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 15.00 minutes.

ISO270 270C degrees isothermal. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 20.00 minutes.

60@20AMIN Initial 60C degrees hold for 1 minute ramped to 270C degrees at 20C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 15.00 minutes.

200TO270@20AMIN Initial 200C degrees hold for 1 minute ramped to 270C degrees at 20C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 10.00 minutes.

Always verify that the temperature for the GC interface is at least 10 degrees higher than the maximum temperature of the GC oven.



Linked spectrum at 0.010 min.

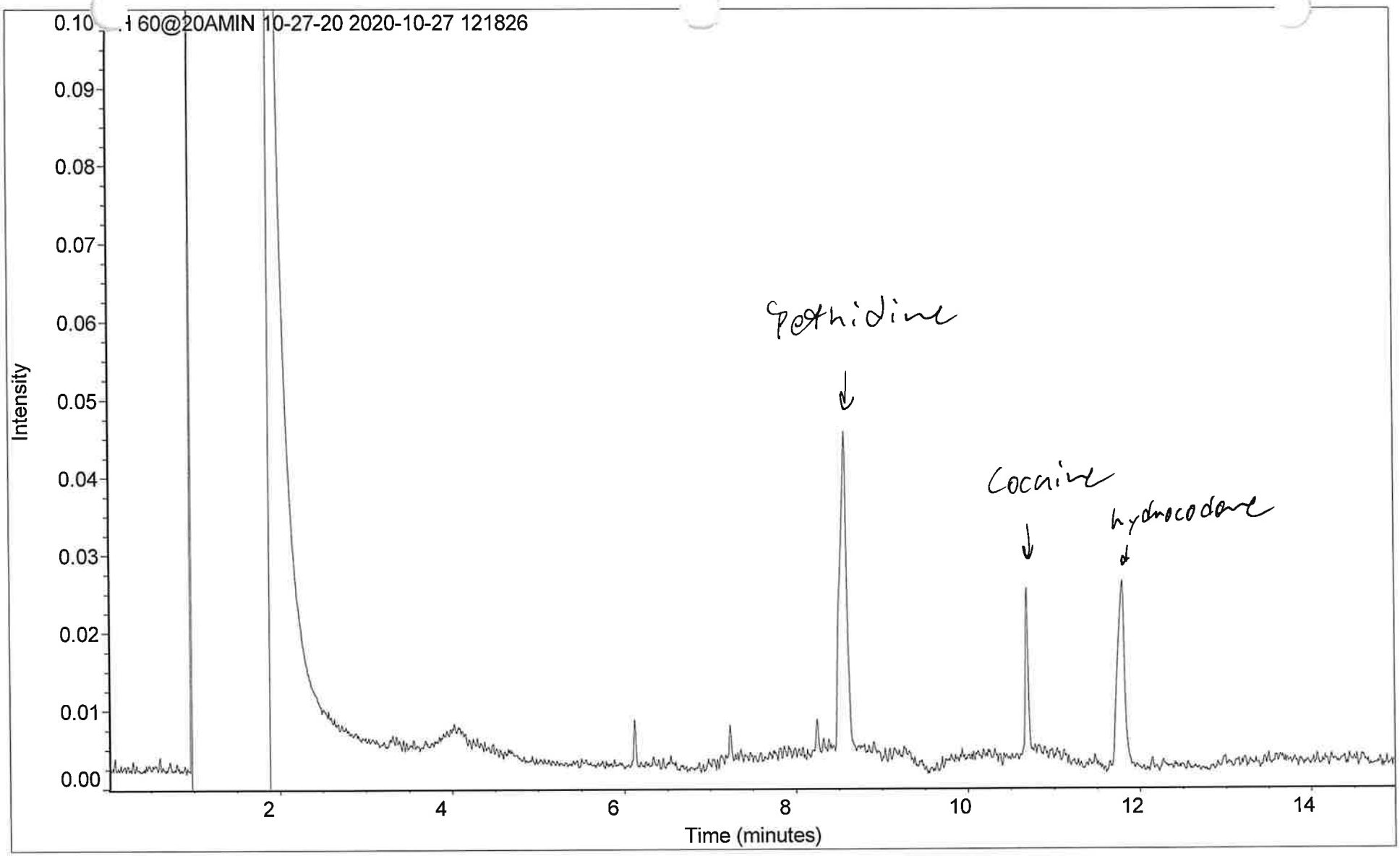
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 12:21:04 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 8.583 min.

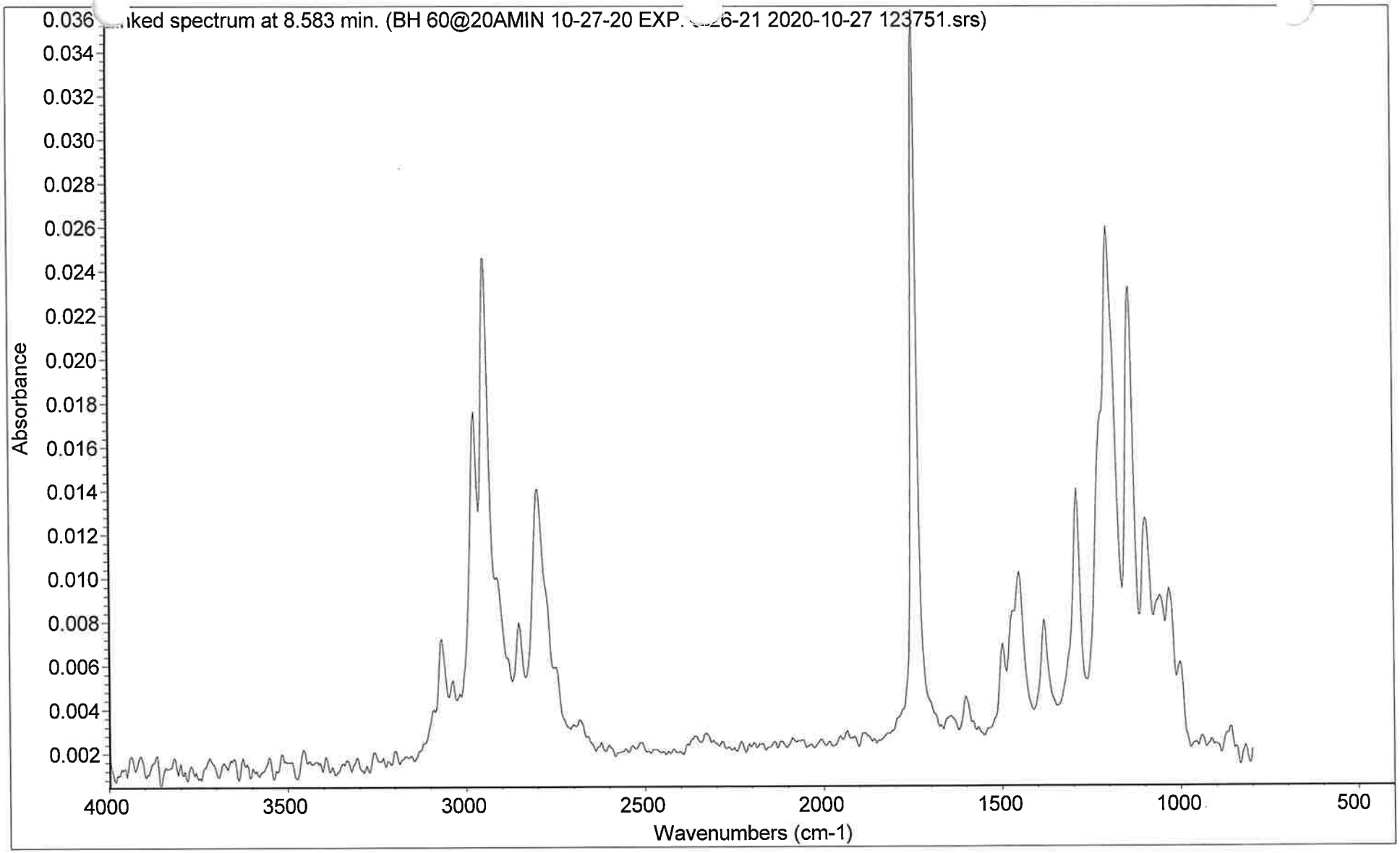
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 12:42:24 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 8.583 min. (BH 60@20AMIN 10-27-20 EXP. 5-26-21 2020-10-27 123751.srs)

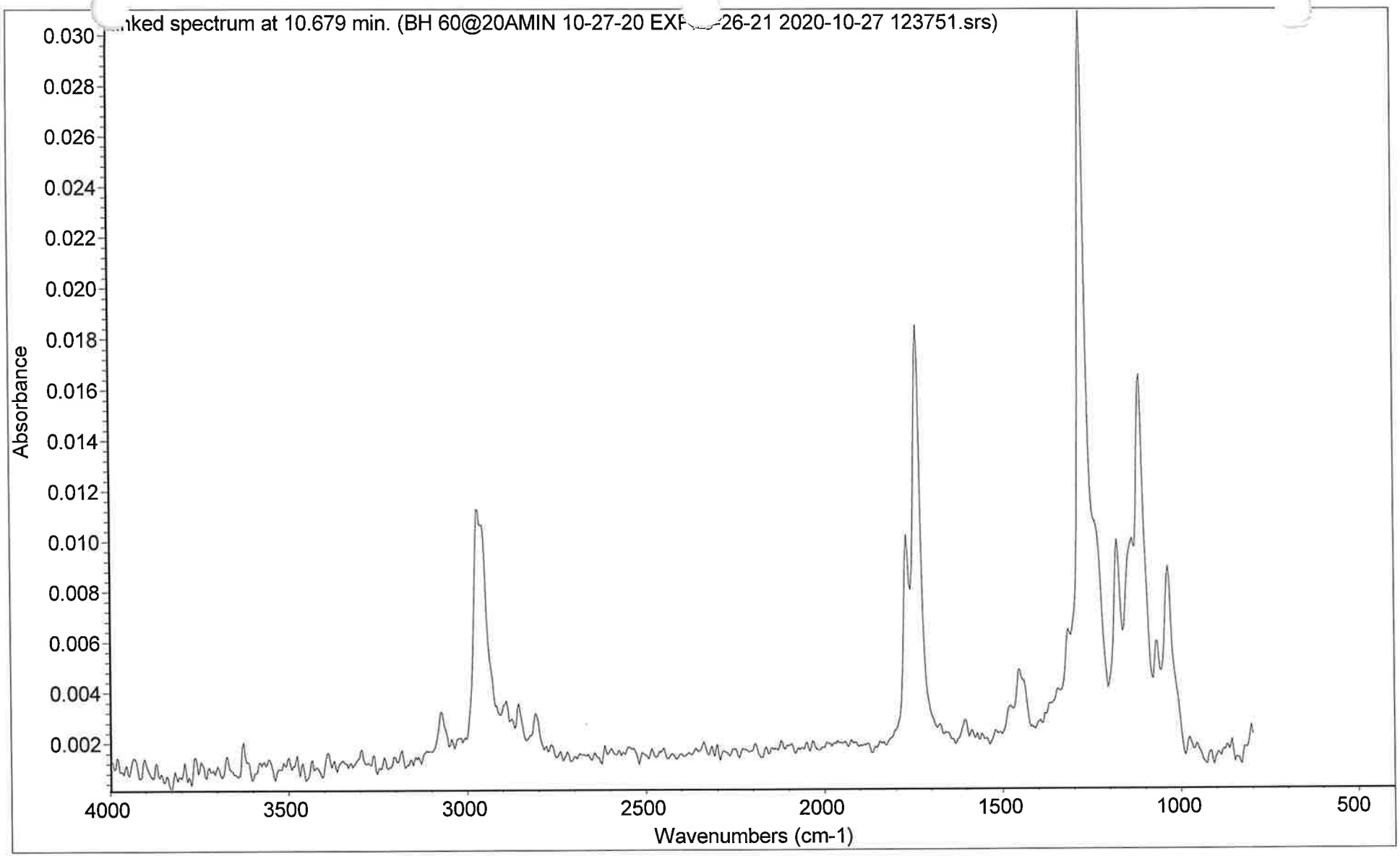
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 12:42:24 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 10.679 min. (BH 60@20AMIN 10-27-20 EXP. 5-26-21 2020-10-27 123751.srs)

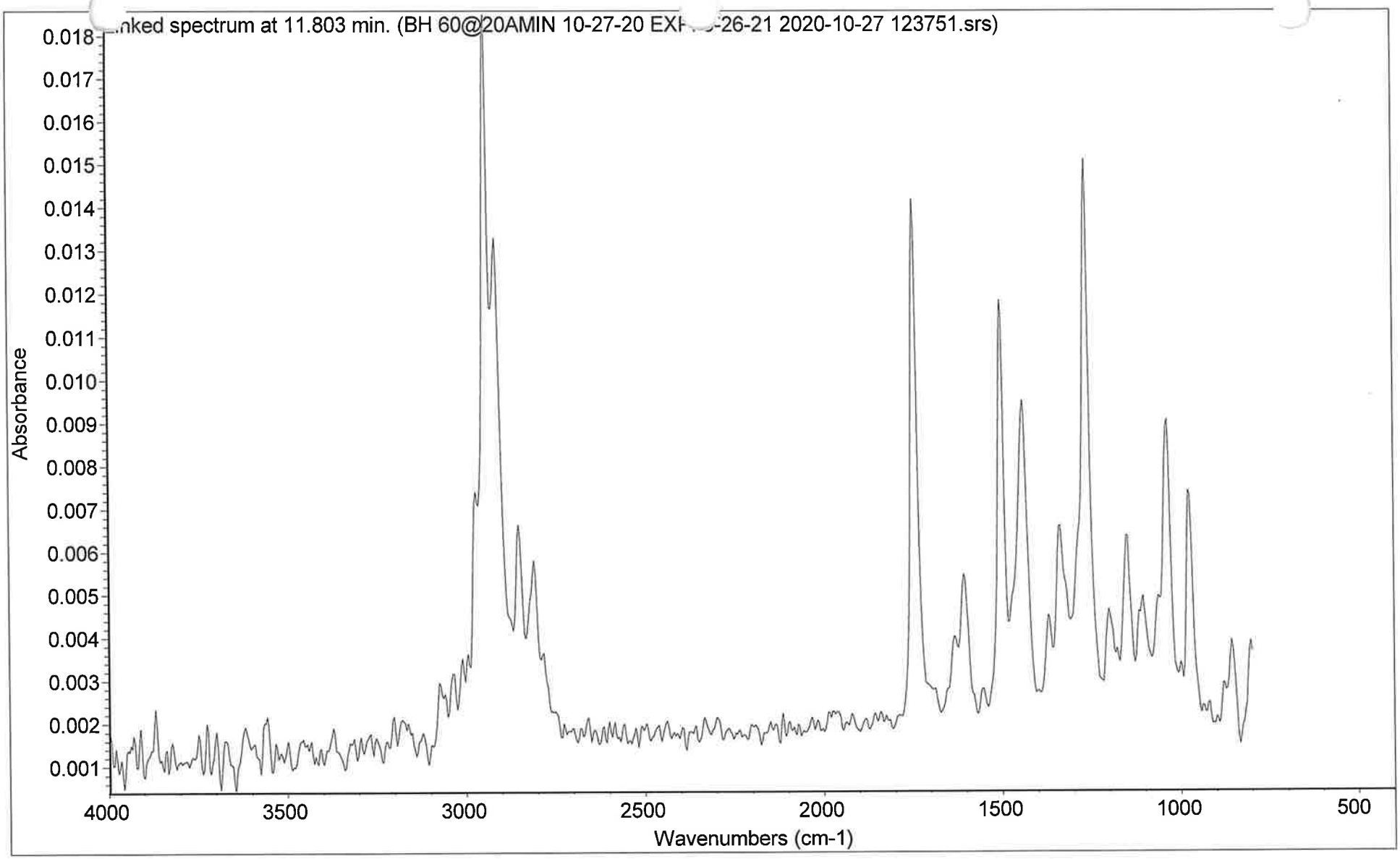
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 12:42:24 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 11.803 min. (BH 60@20AMIN 10-27-20 EXP. 5-26-21 2020-10-27 123751.srs)

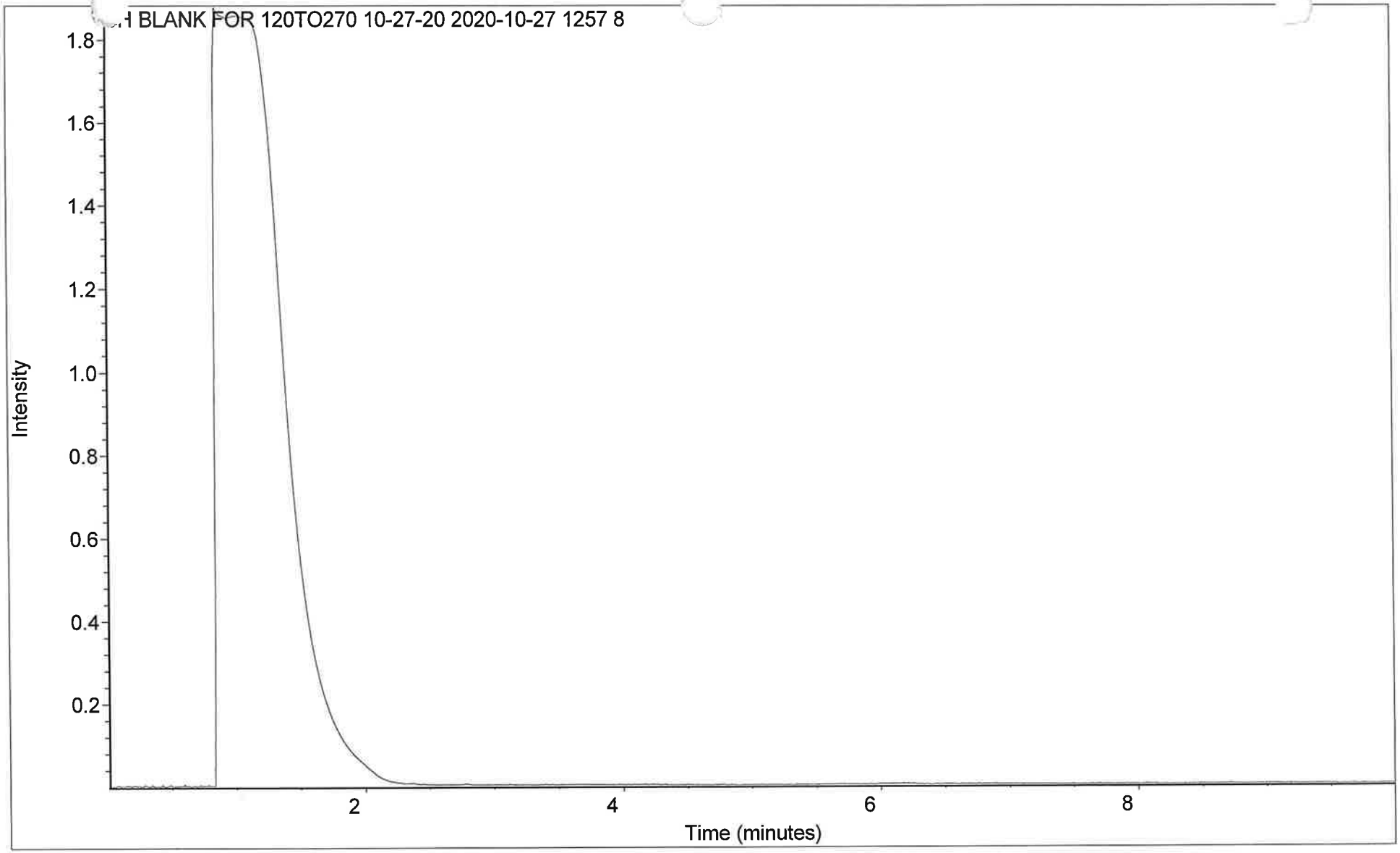
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 12:42:24 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

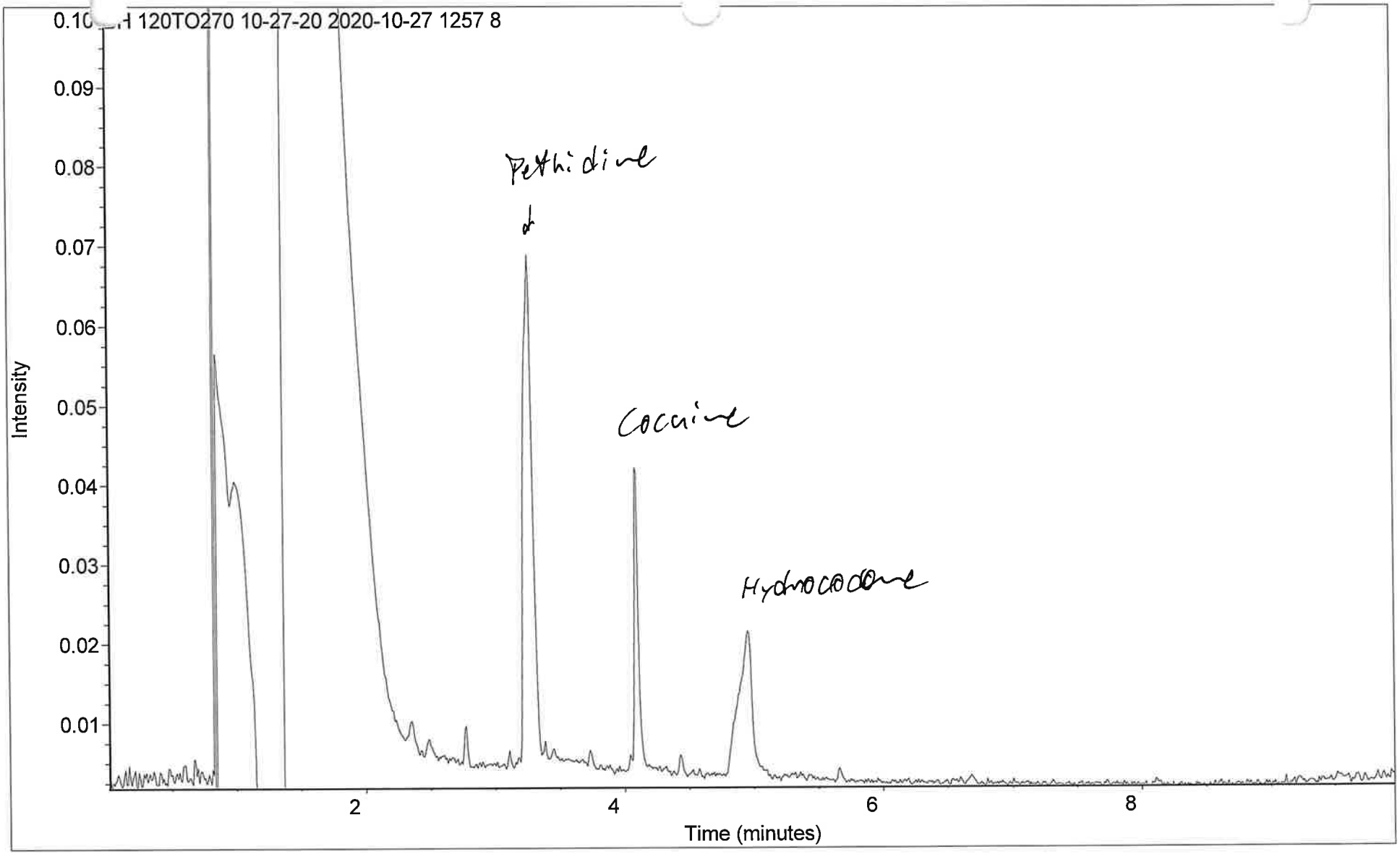
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 12:59:28 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 3.306 min.

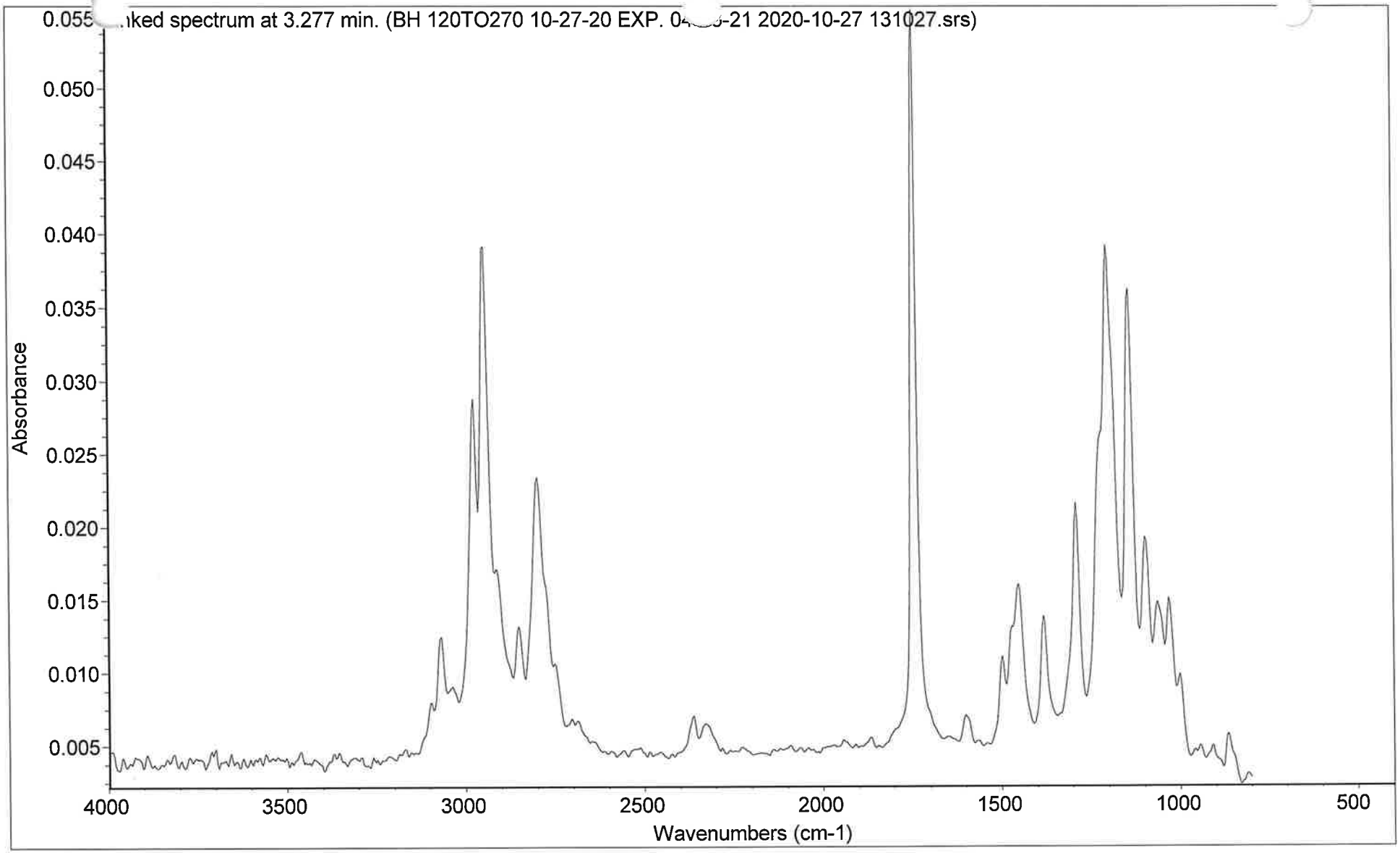
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 13:12:16 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 3.277 min. (BH 120TO270 10-27-20 EXP. 04-05-21 2020-10-27 131027.srs)

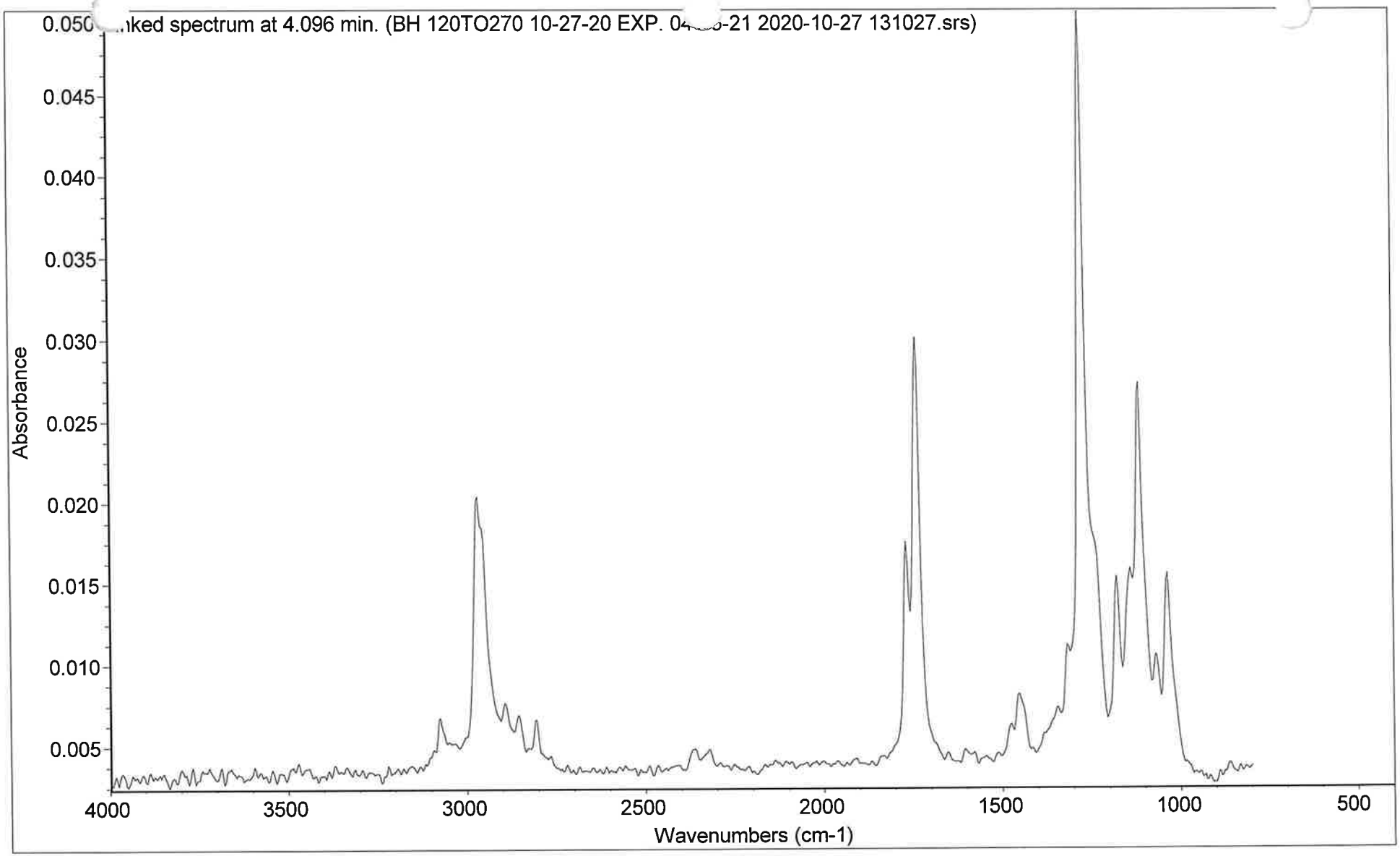
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 13:12:16 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 4.096 min. (BH 120TO270 10-27-20 EXP. 04-05-21 2020-10-27 131027.srs)

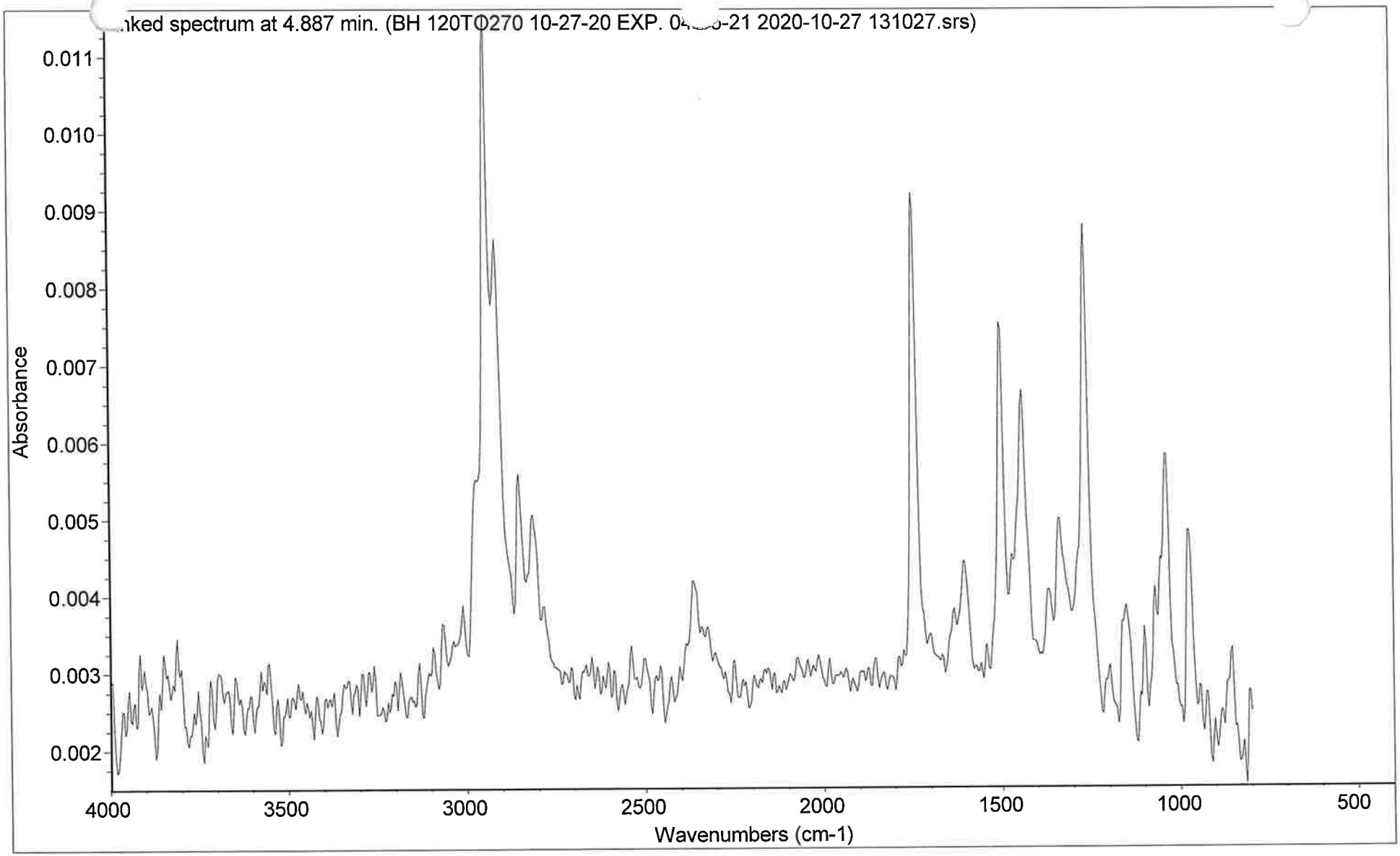
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 13:12:16 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 4.887 min. (BH 120TO270 10-27-20 EXP. 04-05-21 2020-10-27 131027.srs)

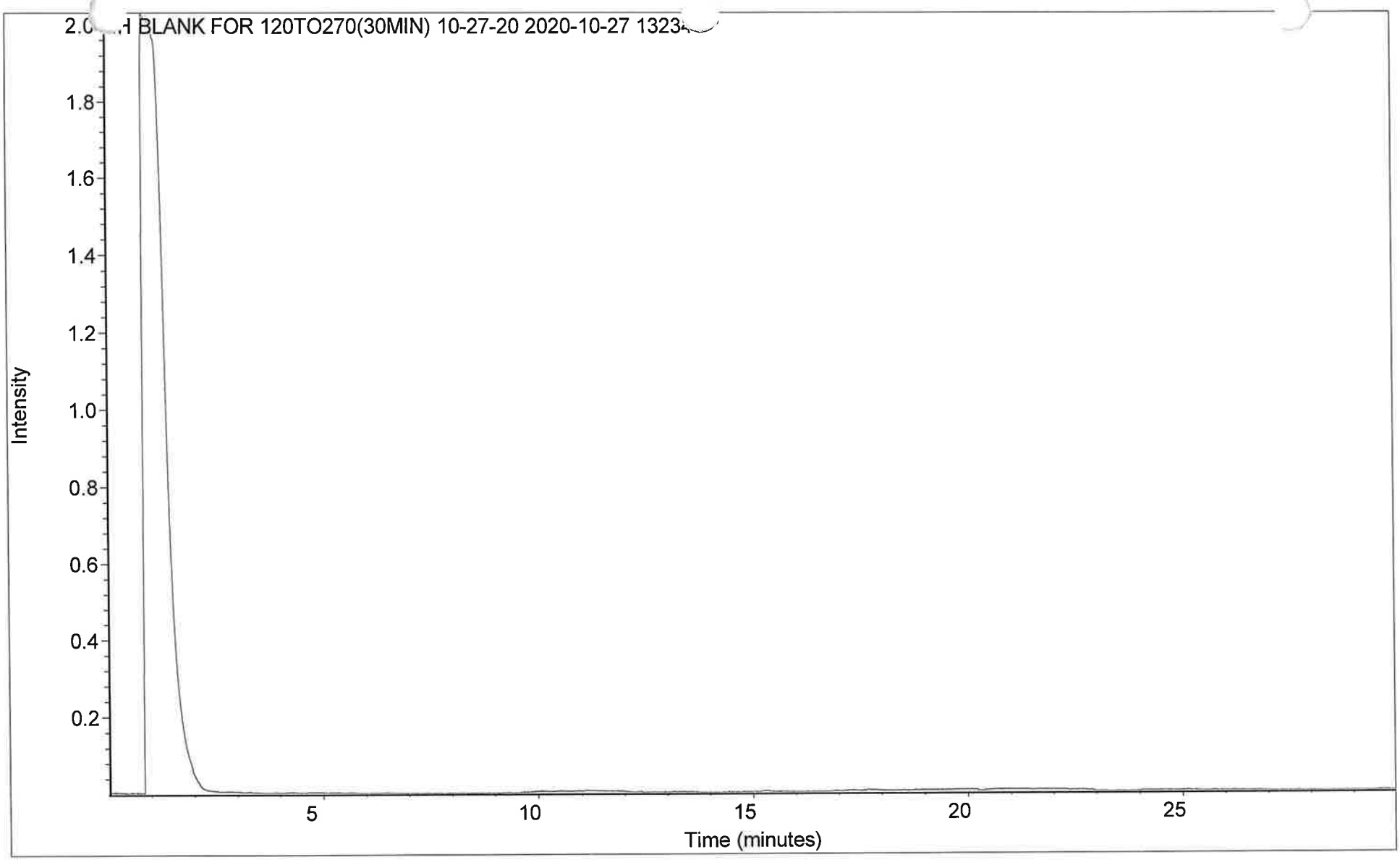
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 13:12:16 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

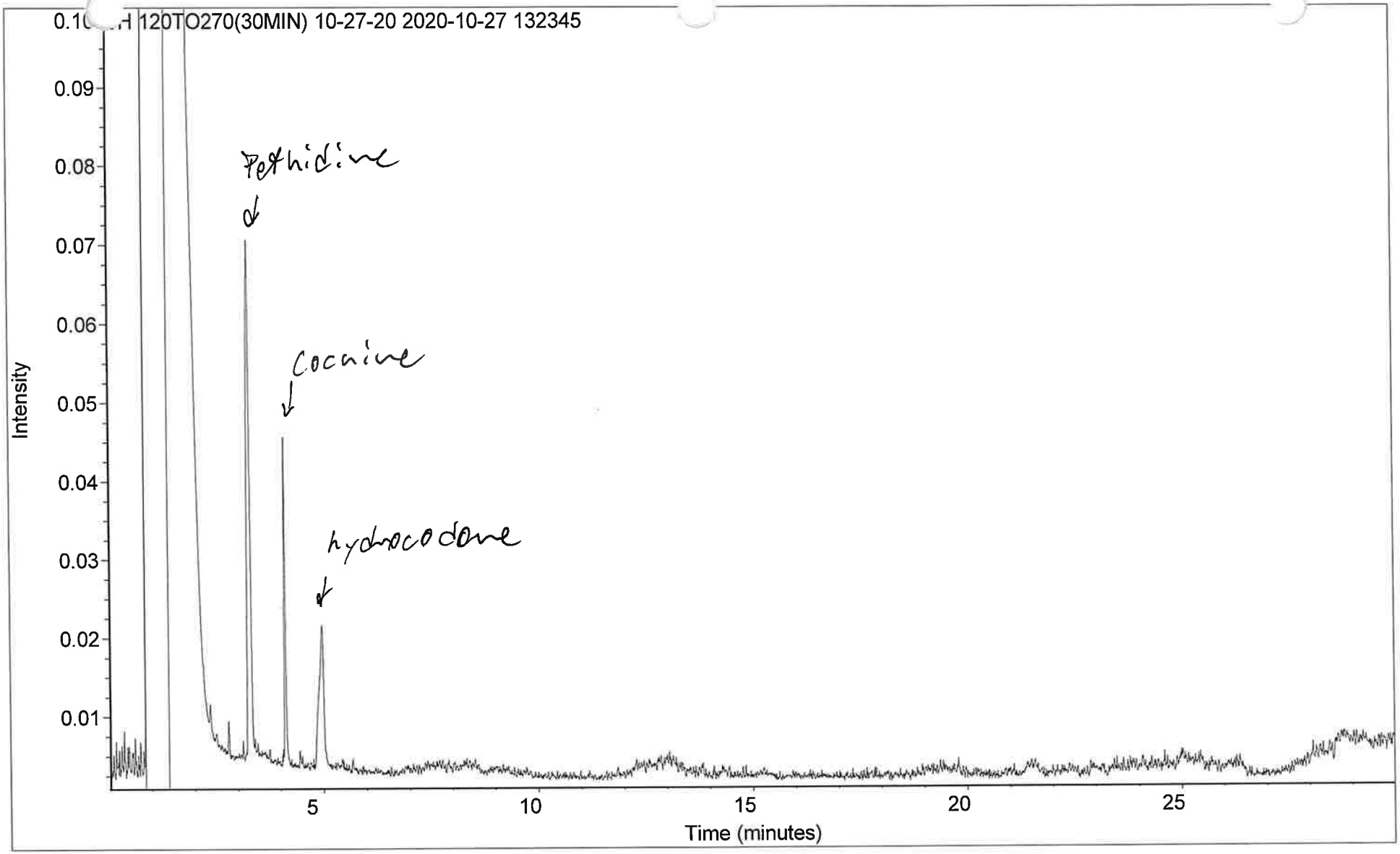
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 13:25:04 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

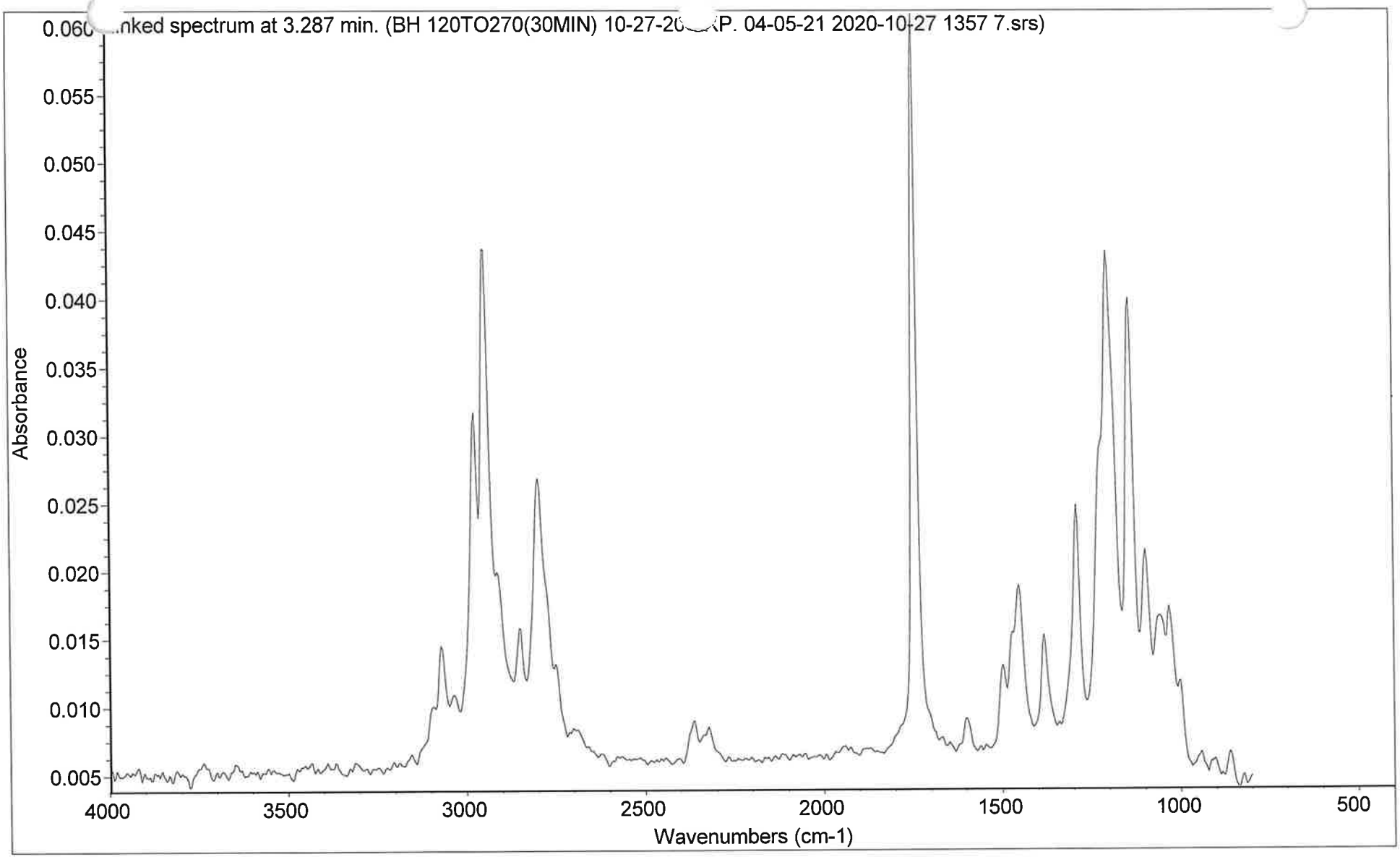
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 13:59:12 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 3.287 min. (BH 120TO270(30MIN) 10-27-20 EXP. 04-05-21 2020-10-27 1357 7.srs)

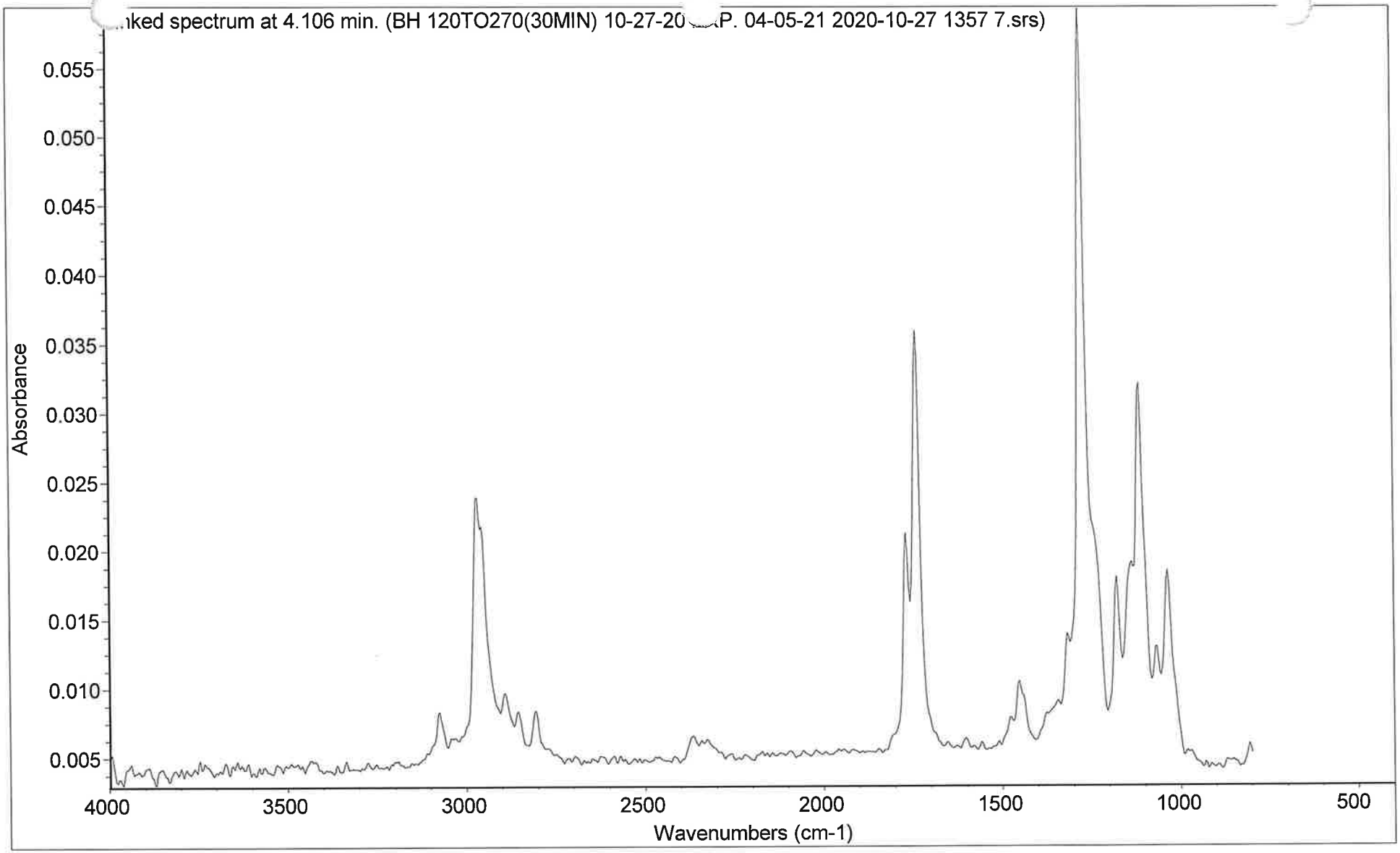
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 13:59:12 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 4.106 min. (BH 120TO270(30MIN) 10-27-20 EXP. 04-05-21 2020-10-27 1357 7.srs)

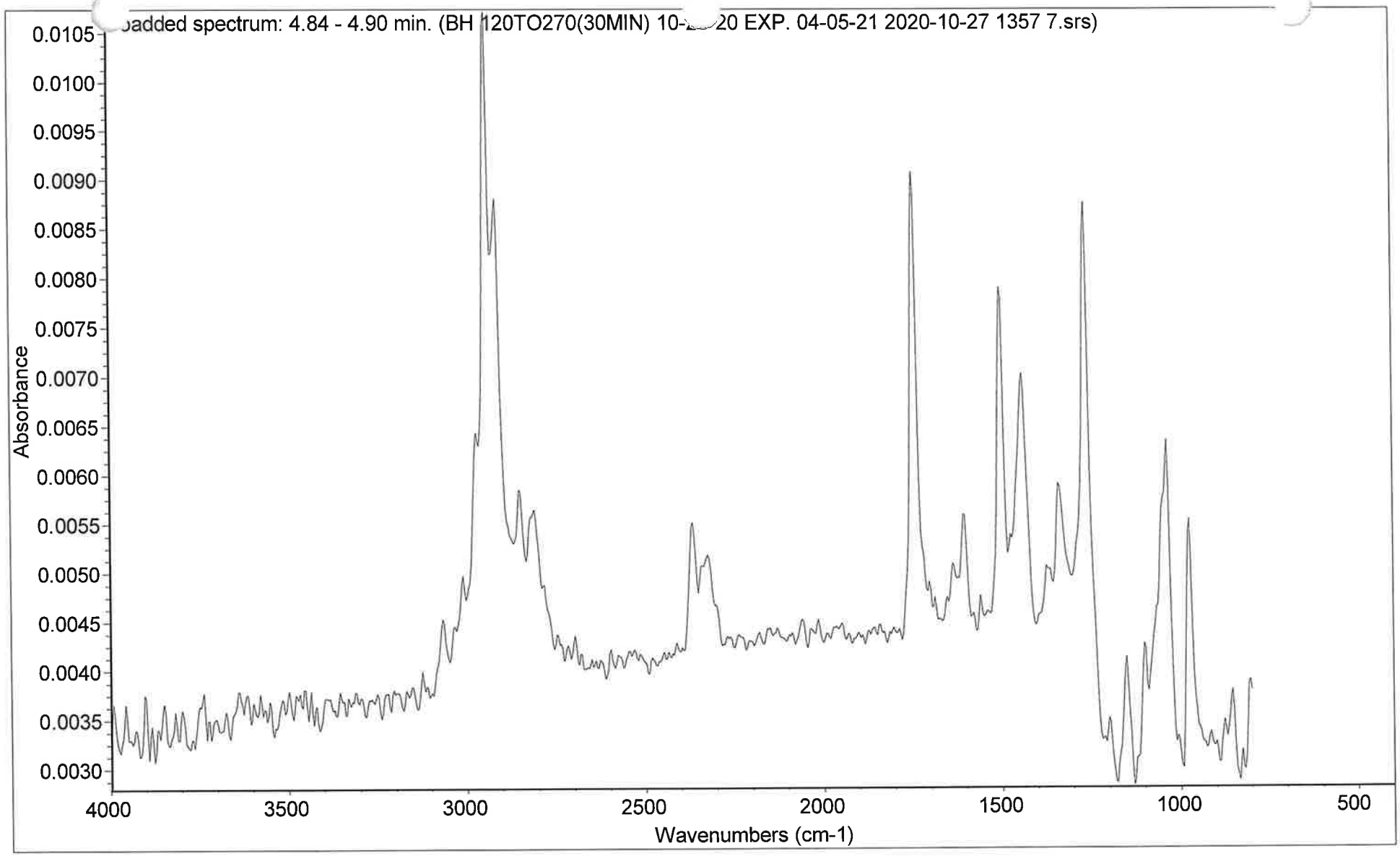
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 13:59:12 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Coadded spectrum: 4.84 - 4.90 min. (BH 120TO270(30MIN) 10-27-20 EXP. 04-05-21 2020-10-27 1357 7.srs)

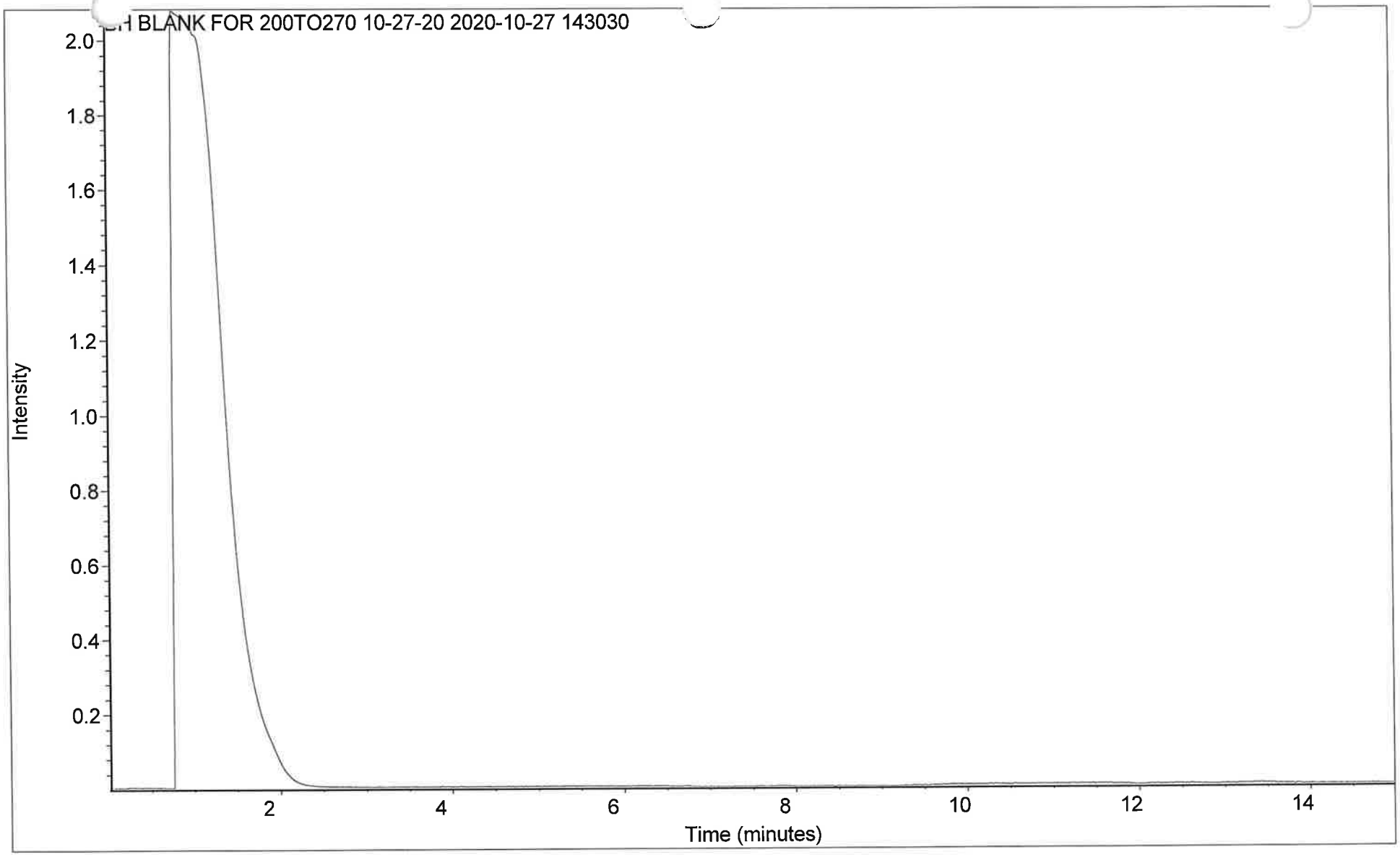
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 14:00:27 2020 (GMT-05:00)

Number of sample scans: 24
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

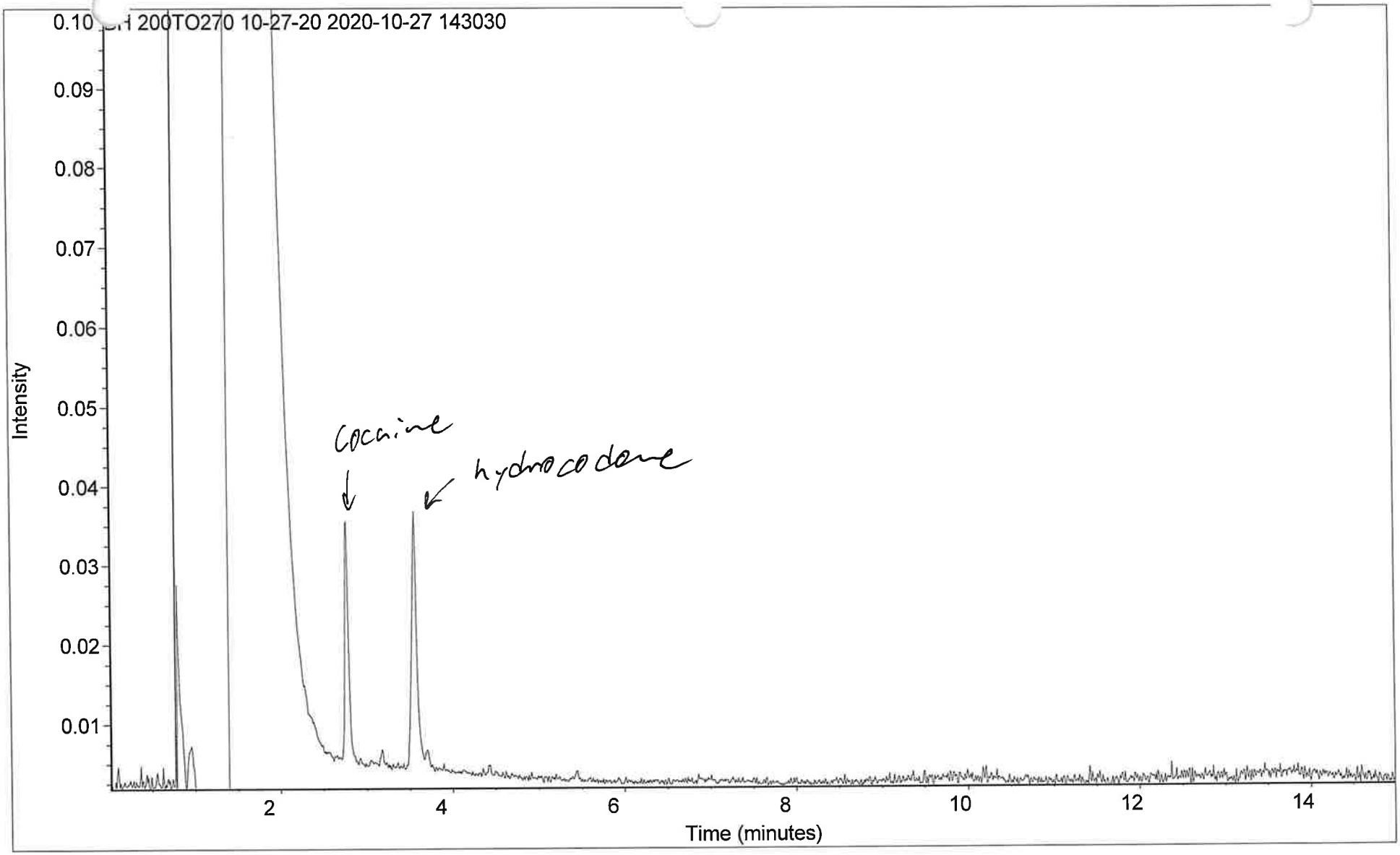
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 14:33:20 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 2.773 min.

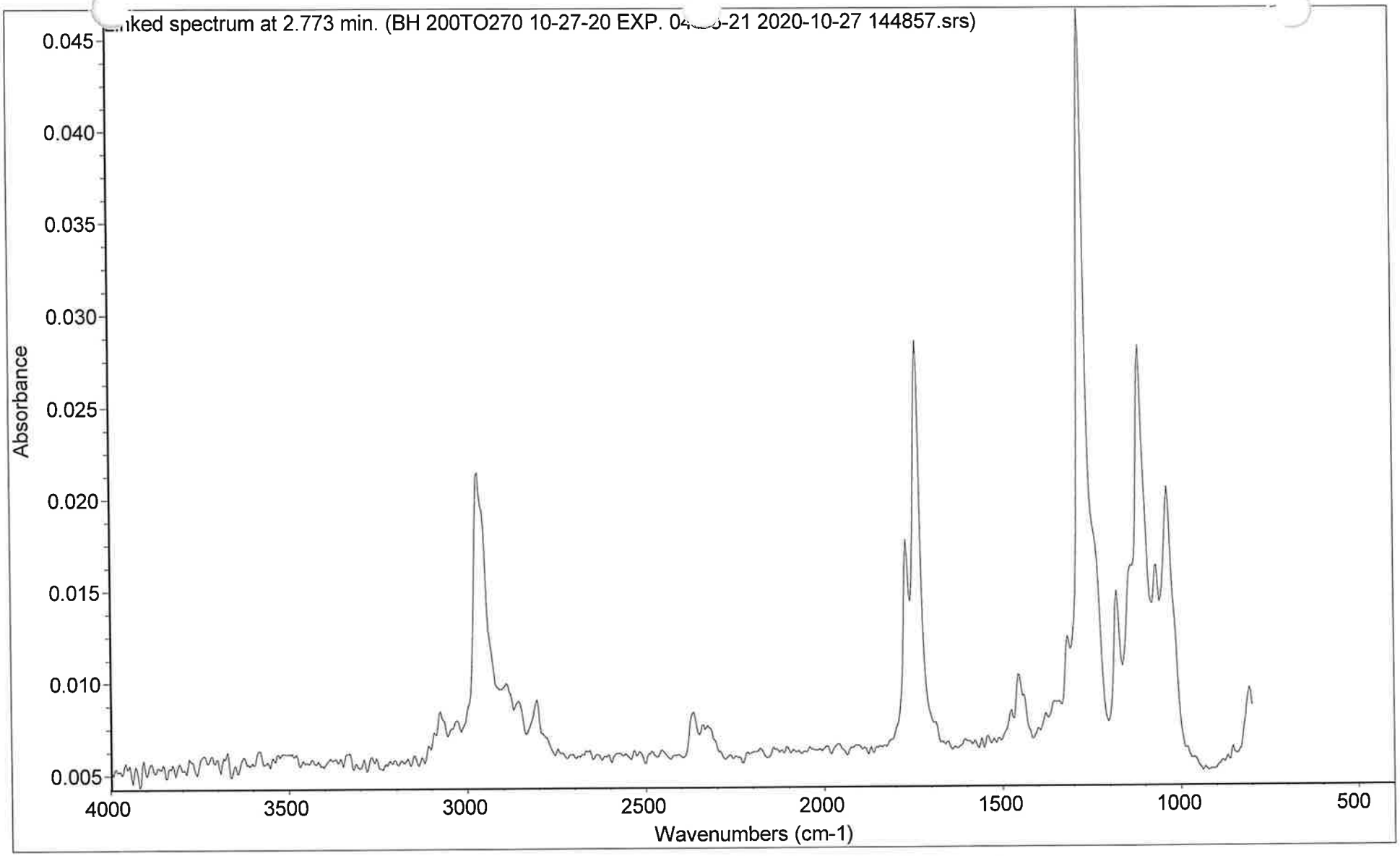
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 14:50:24 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 2.773 min. (BH 200TO270 10-27-20 EXP. 04-05-21 2020-10-27 144857.srs)

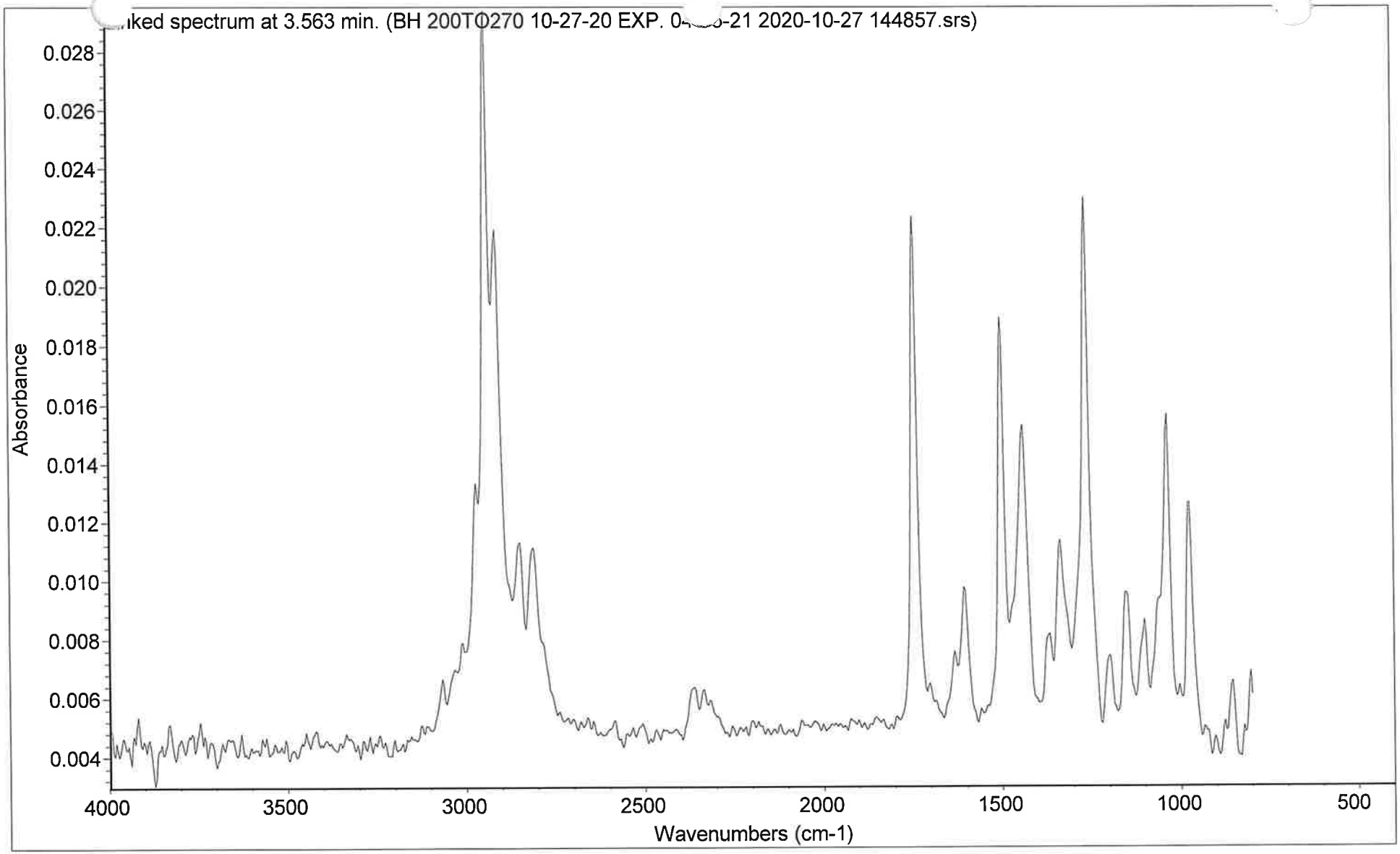
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 14:50:24 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 3.563 min. (BH 200TO270 10-27-20 EXP. 04-05-21 2020-10-27 144857.srs)

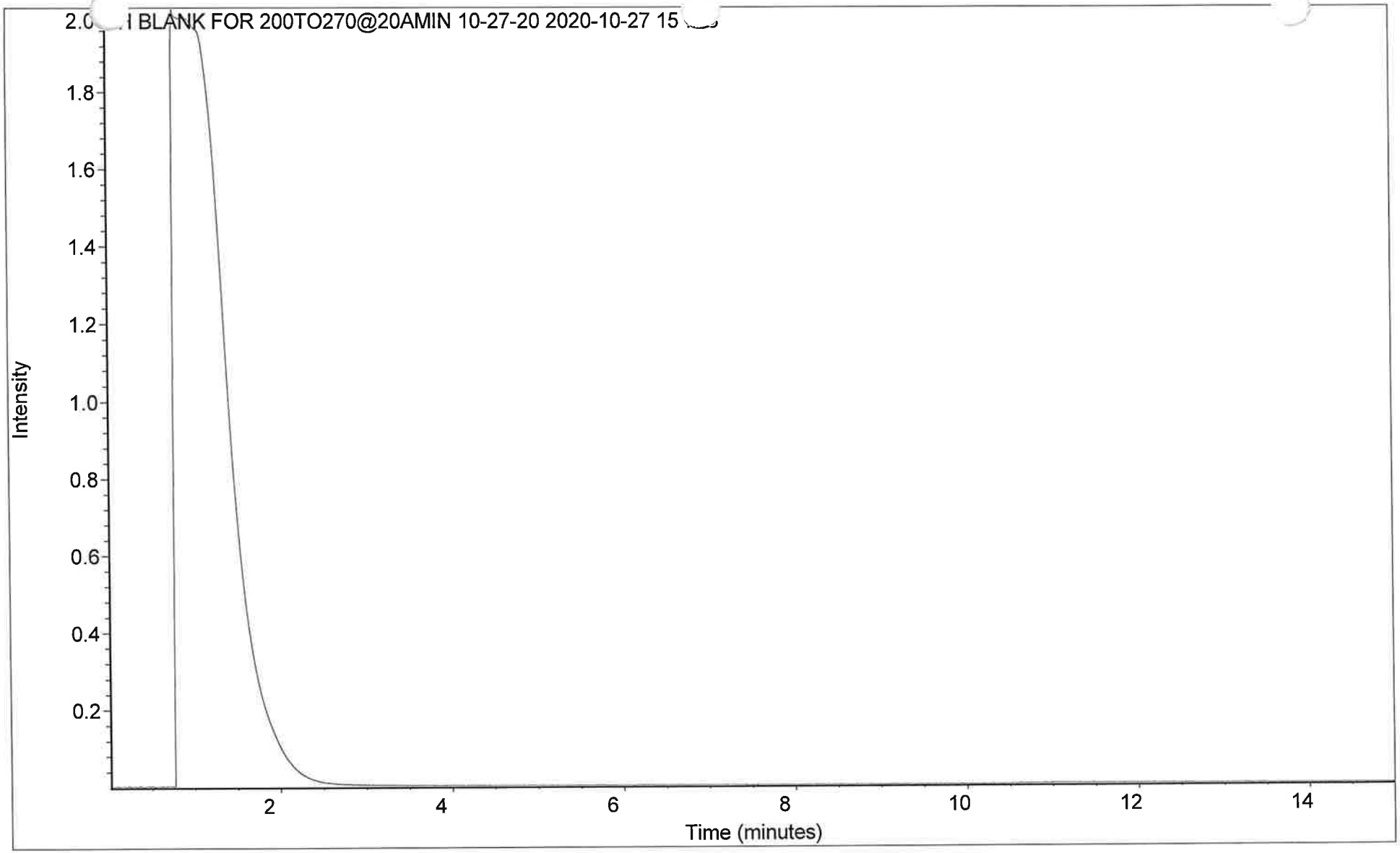
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 14:50:24 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

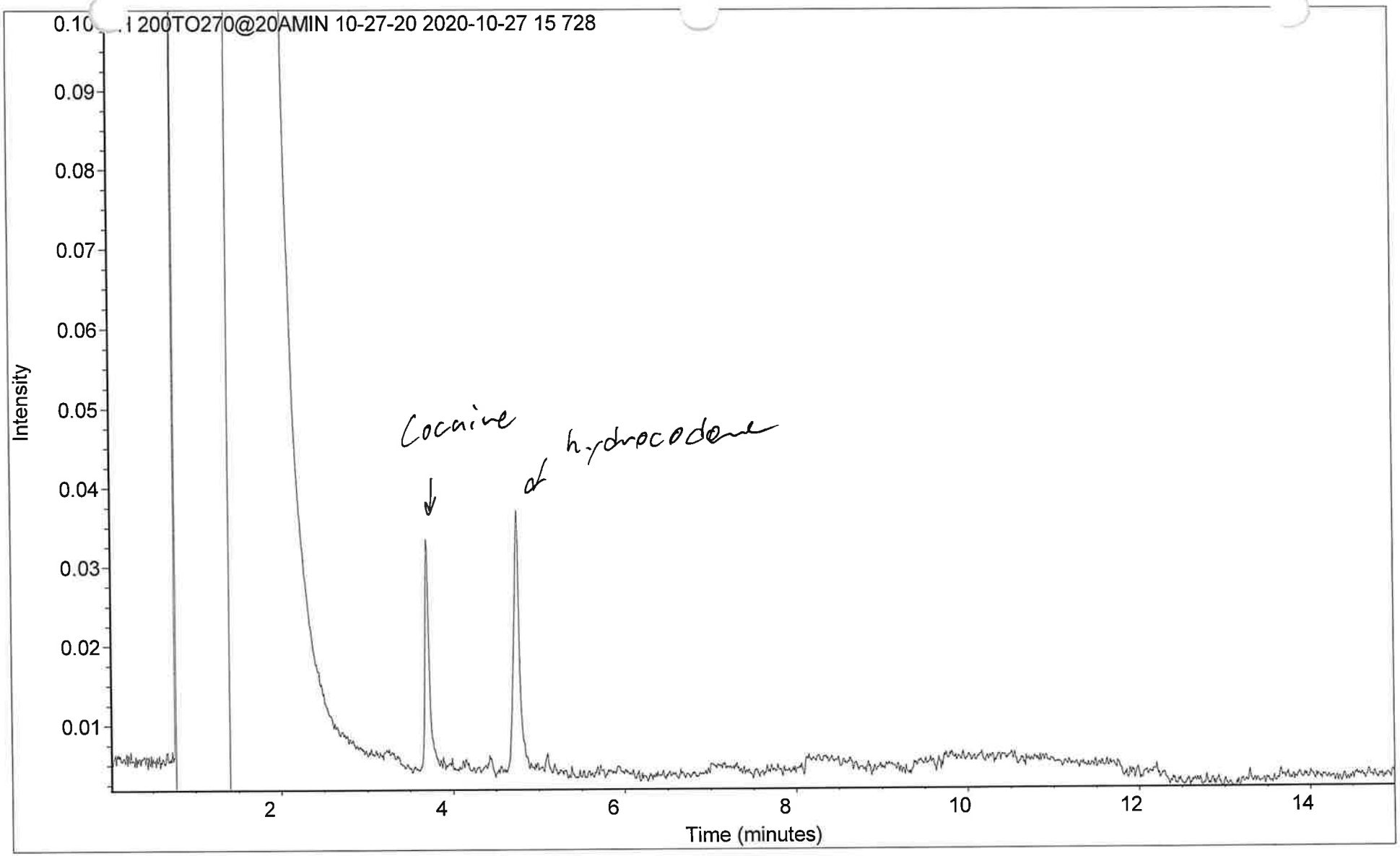
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 15:11:44 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



BH 200TO270@20AMIN 10-27-20 2020-10-27 15 728

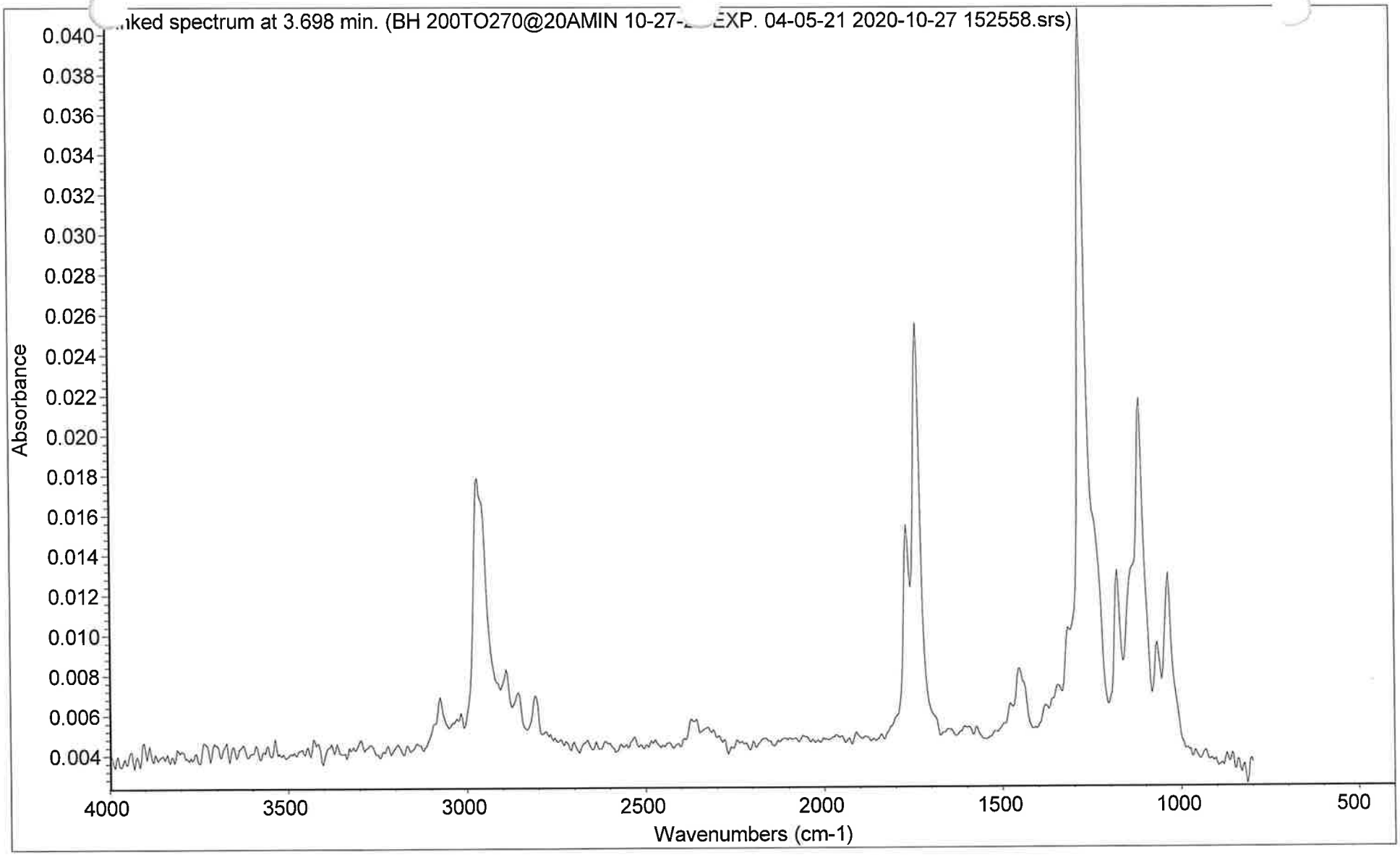
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

HOGWARTS

Collection time: Unknown

Detector: MCT/A
Beamsplitter: KBr
Source: Off

Number of sample scans: 1
Number of background scans: 0
Resolution: Unknown
Sample gain: 0.0
Optical velocity: 0.0000
Aperture: 0.00



Linked spectrum at 3.698 min. (BH 200TO270@20AMIN 10-27-20 EXP. 04-05-21 2020-10-27 152558.srs)

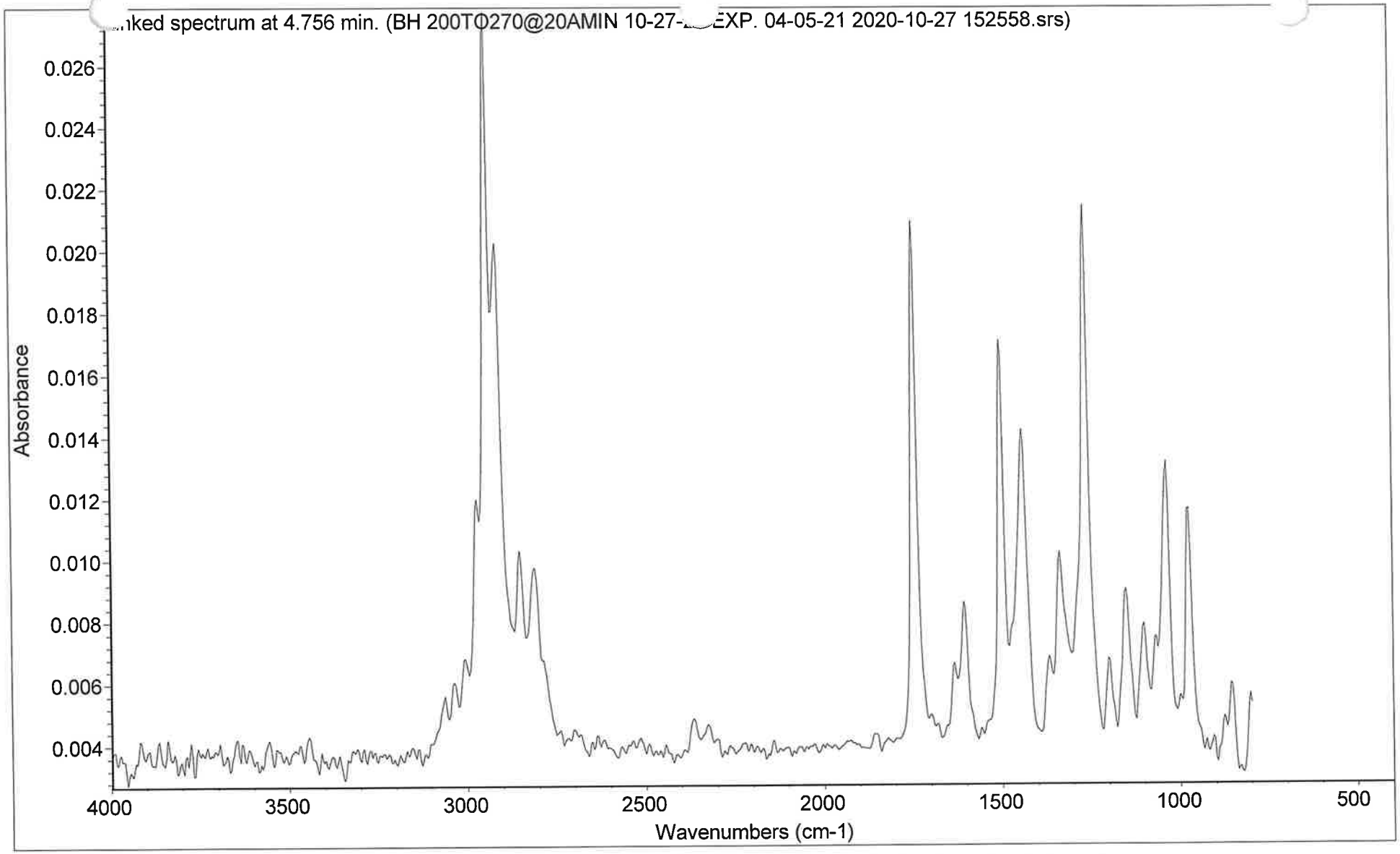
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 15:28:48 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 4.756 min. (BH 200TO270@20AMIN 10-27-20 EXP. 04-05-21 2020-10-27 152558.srs)

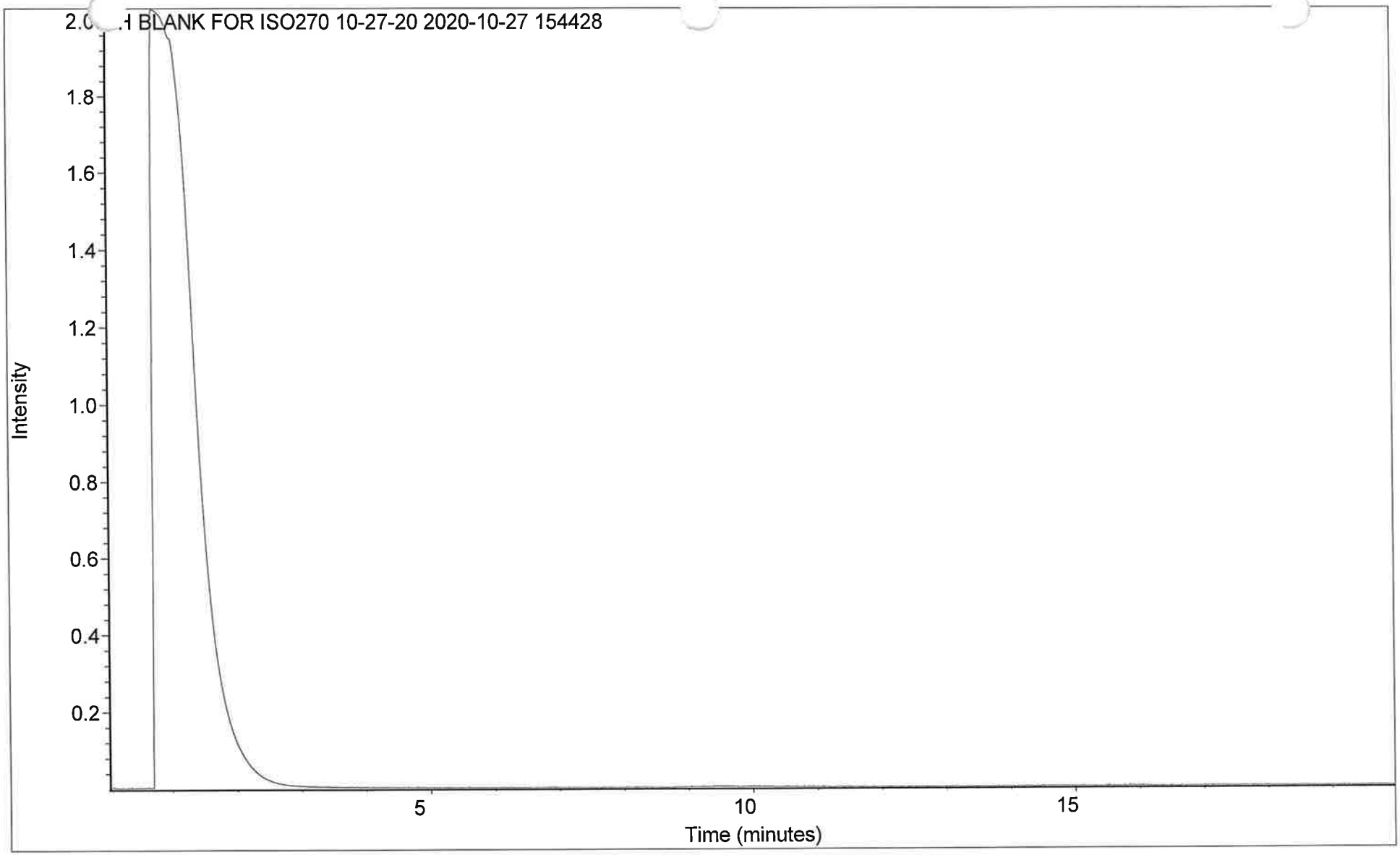
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 15:28:48 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

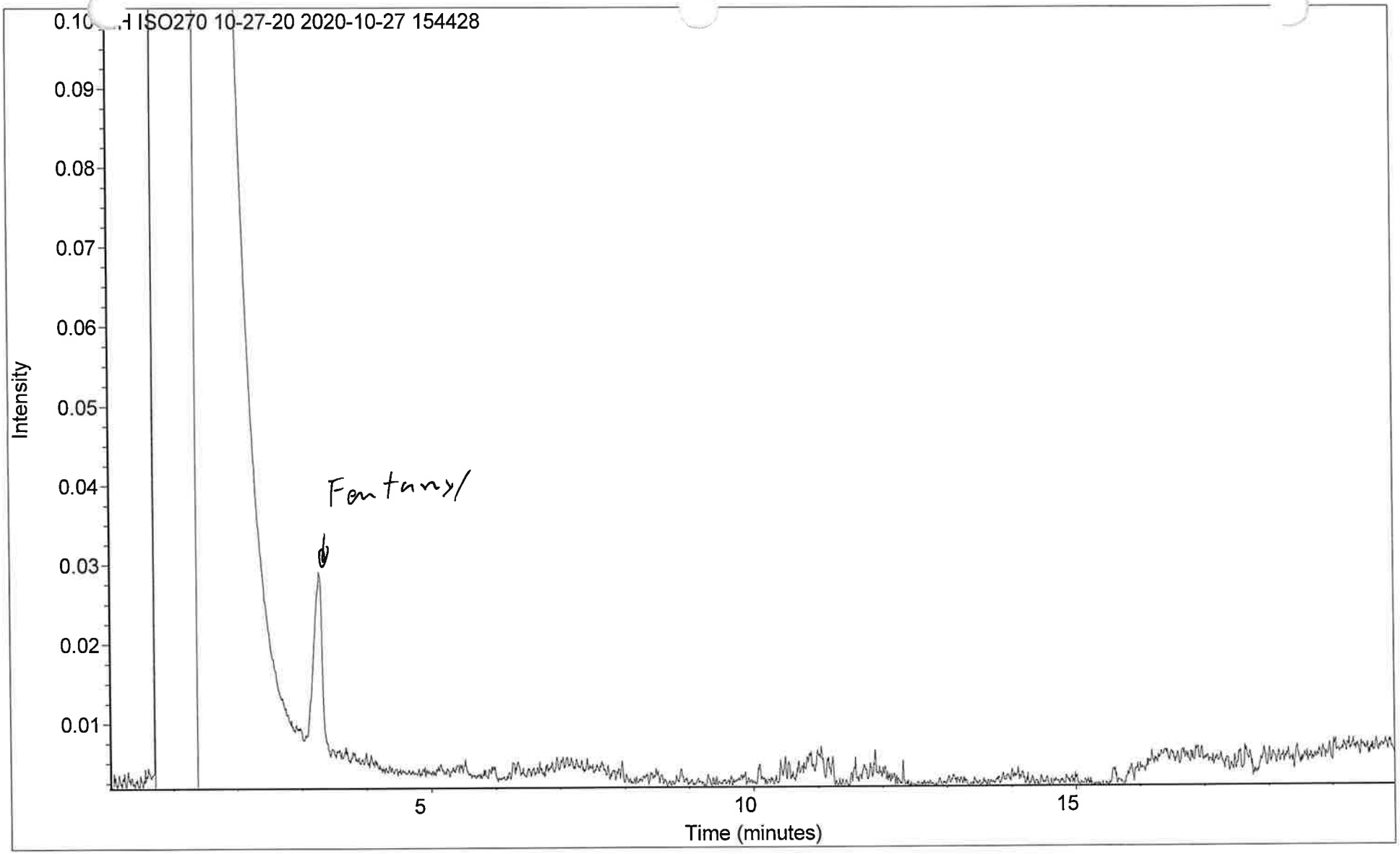
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 15:45:52 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Coadded spectrum: 3.22 - 3.33 min.

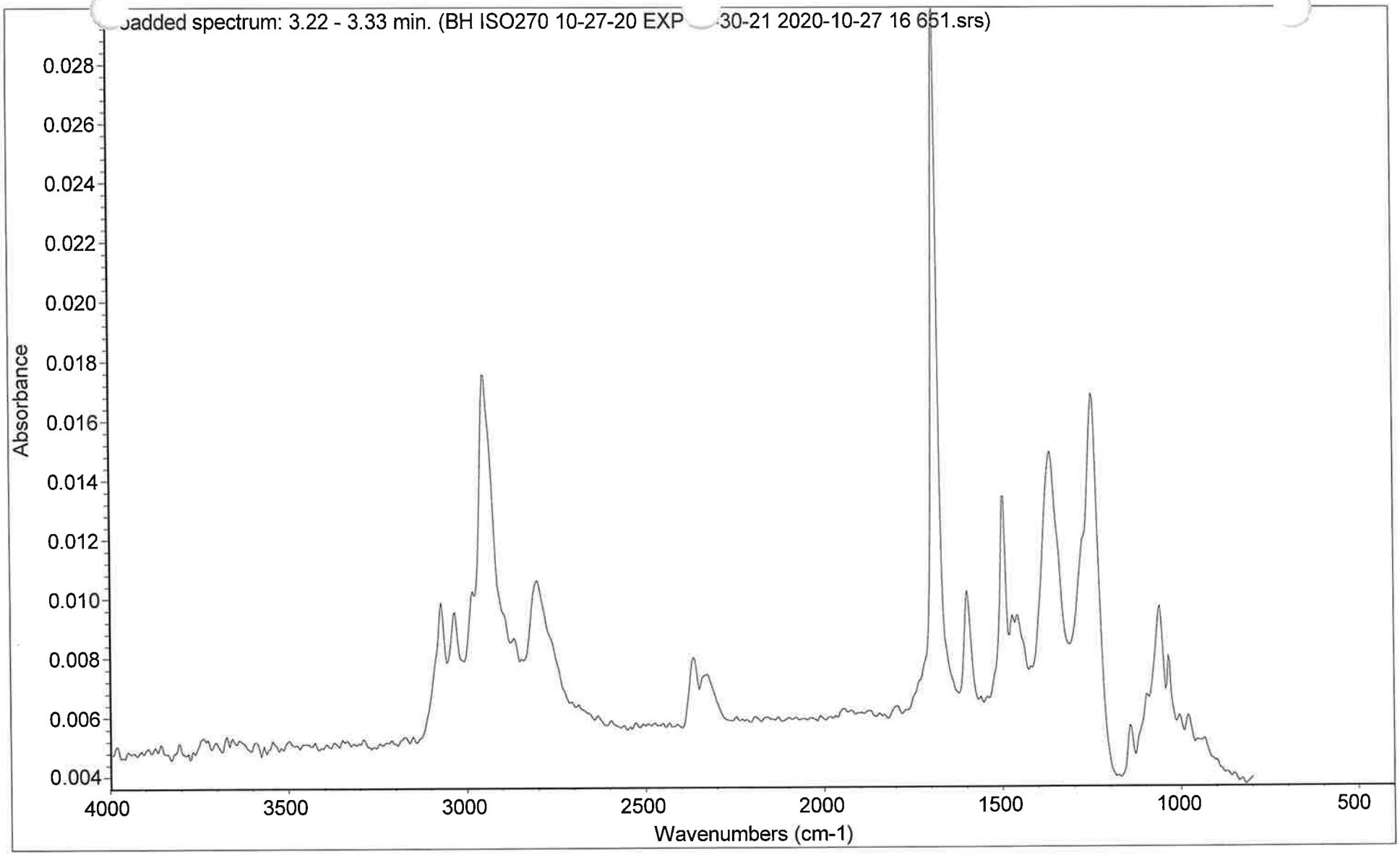
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 16:08:59 2020 (GMT-05:00)

Number of sample scans: 48
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Coadded spectrum: 3.22 - 3.33 min. (BH ISO270 10-27-20 EXP 04-30-21 2020-10-27 16 651.srs)

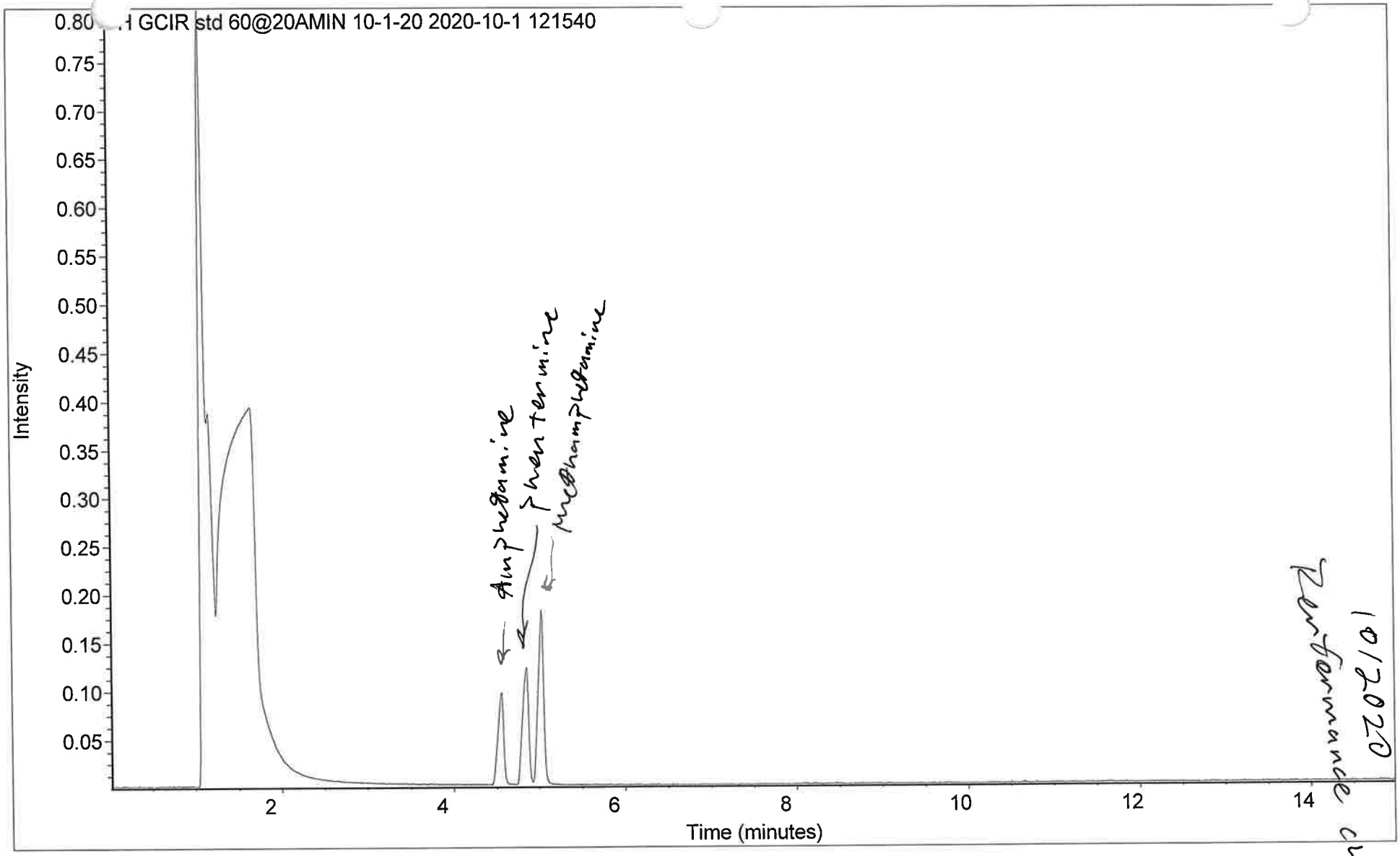
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue Oct 27 16:08:59 2020 (GMT-05:00)

Number of sample scans: 48
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

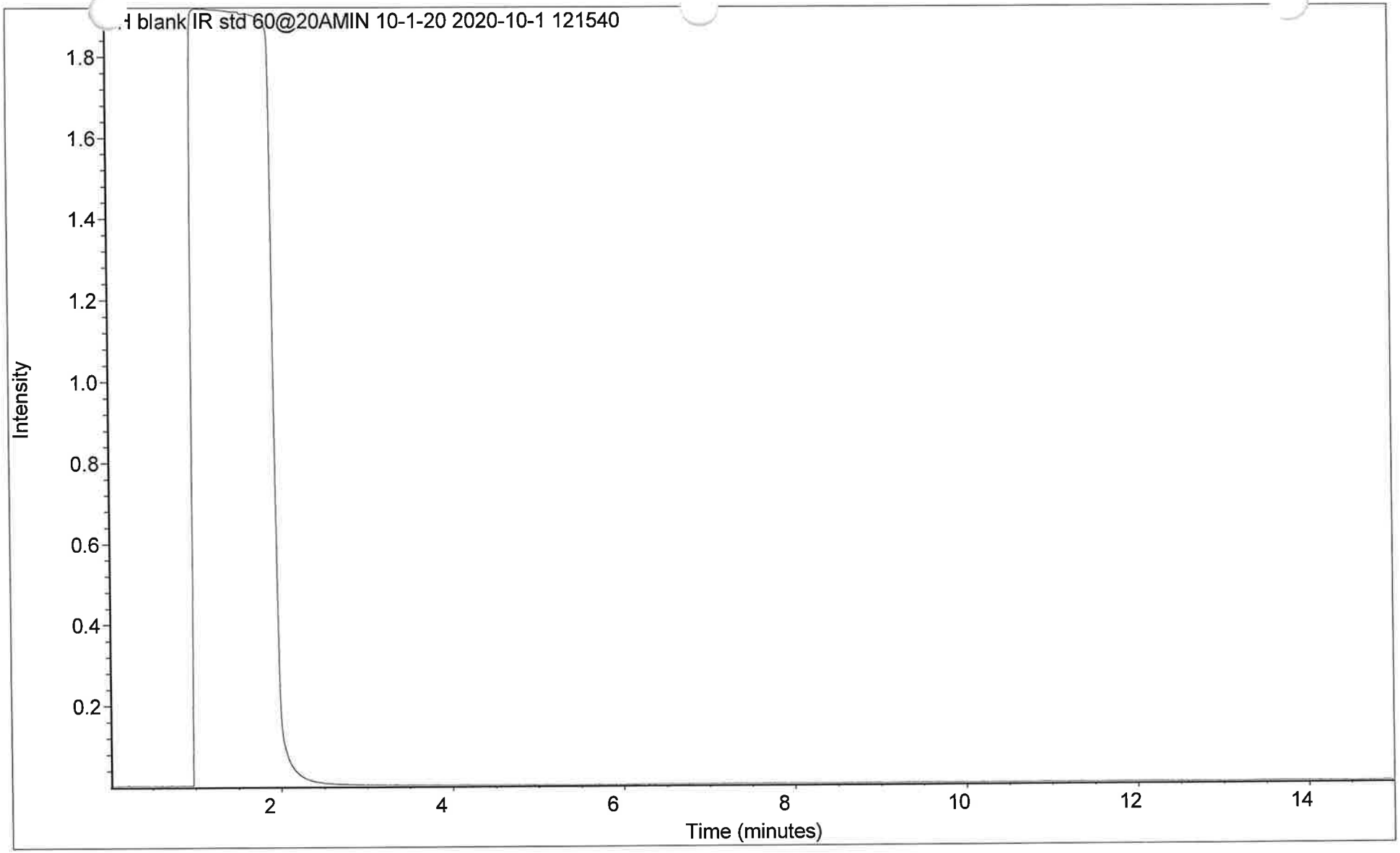
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Oct 01 12:38:08 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 256
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 0.010 min.

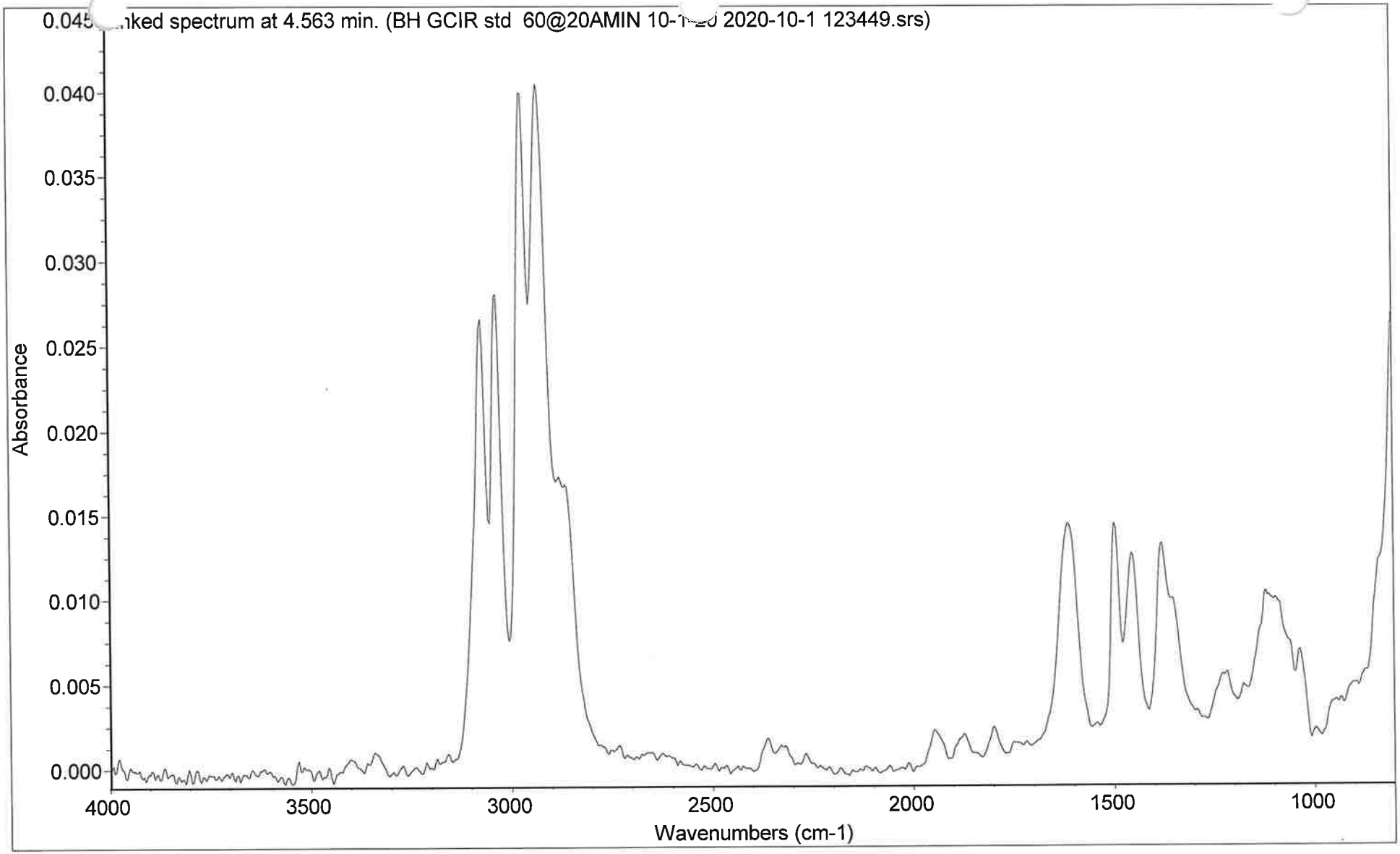
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Oct 01 12:21:04 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 256
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 4.563 min. (BH GCIR std 60@20AMIN 10-1-20 2020-10-1 123449.srs)

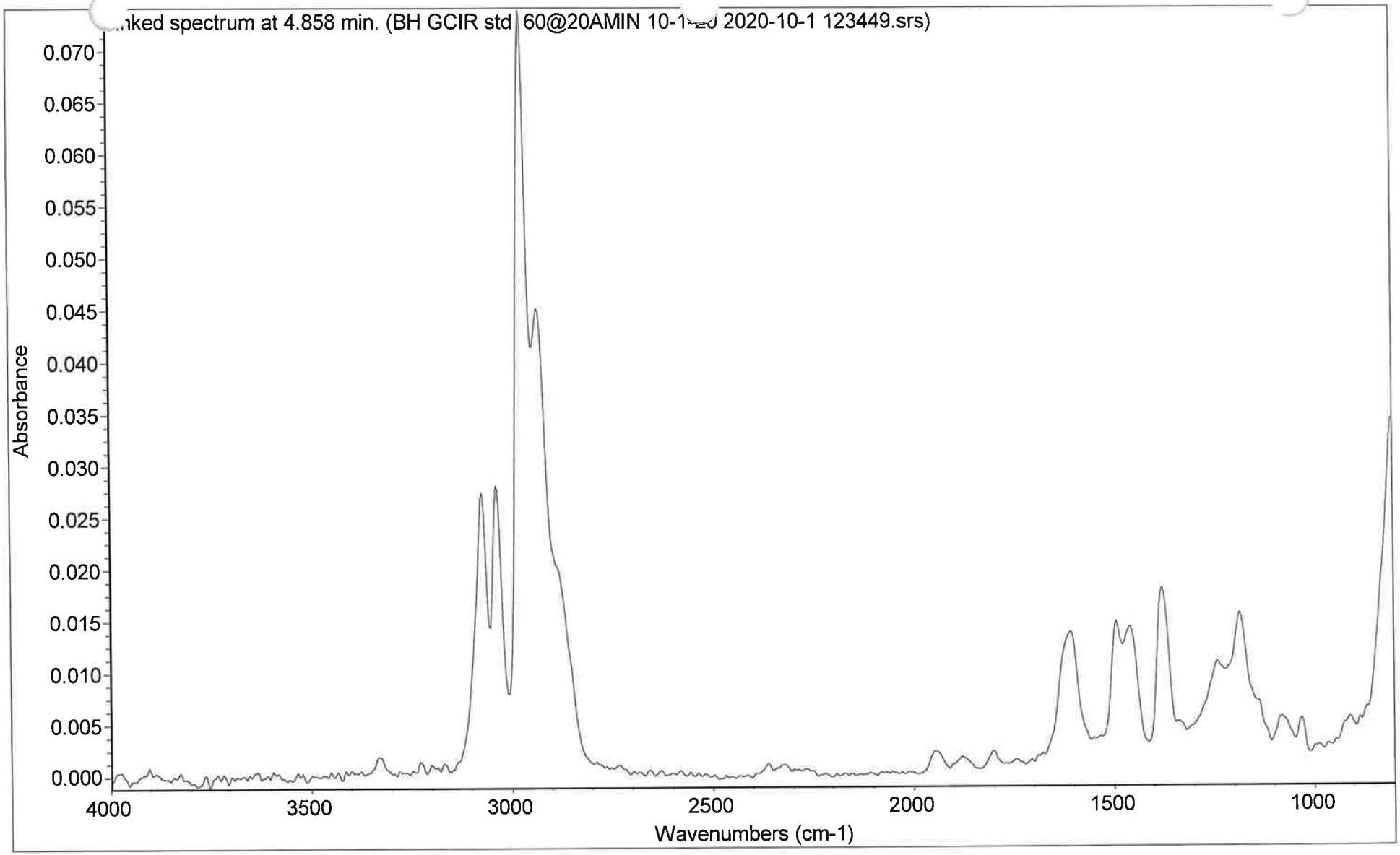
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Oct 01 12:38:08 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 256
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 4.858 min. (BH GCIR std 60@20AMIN 10-1-20 2020-10-1 123449.srs)

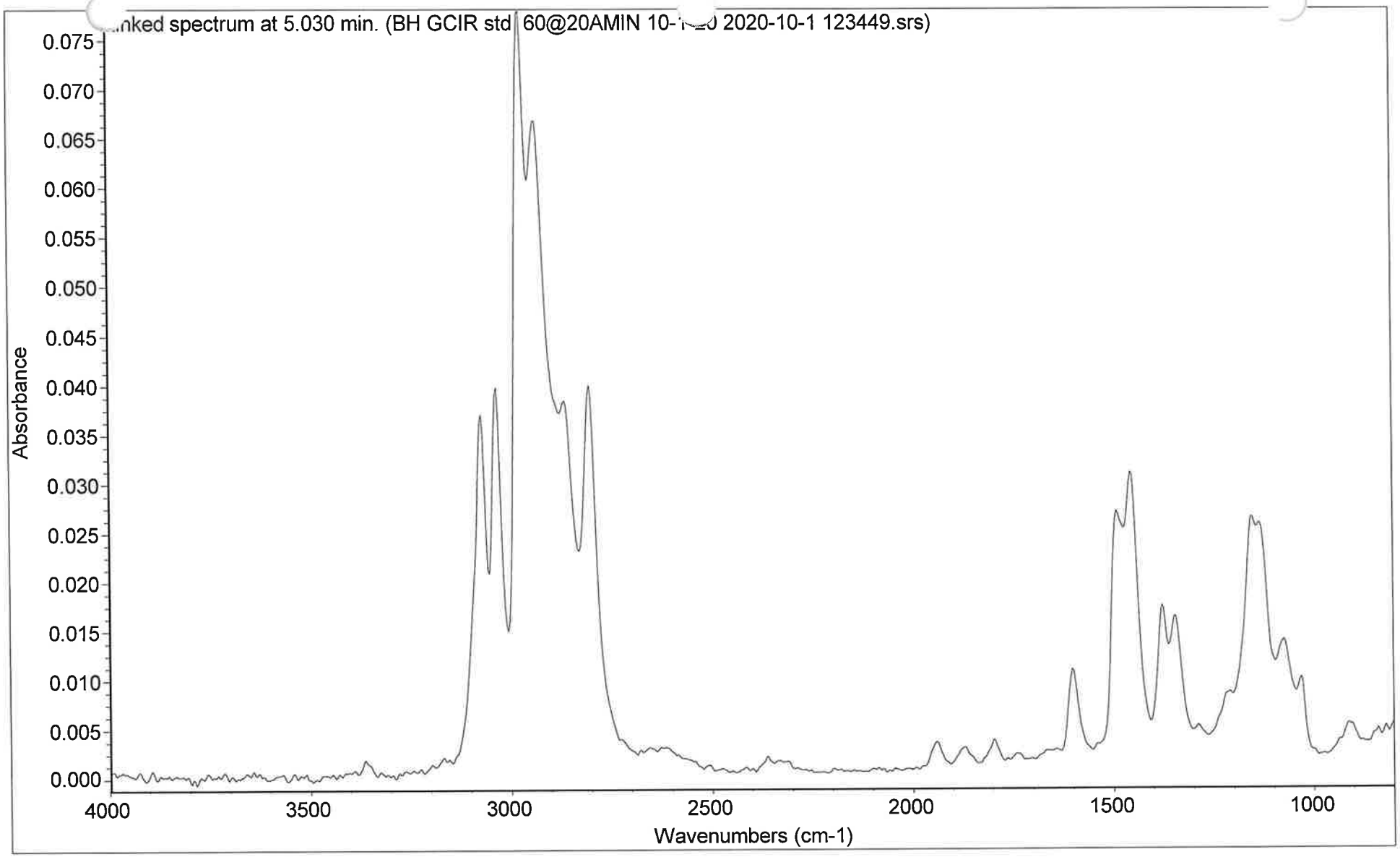
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Oct 01 12:38:08 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 256
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00



Linked spectrum at 5.030 min. (BH GCIR std 60@20AMIN 10-1-20 2020-10-1 123449.srs)

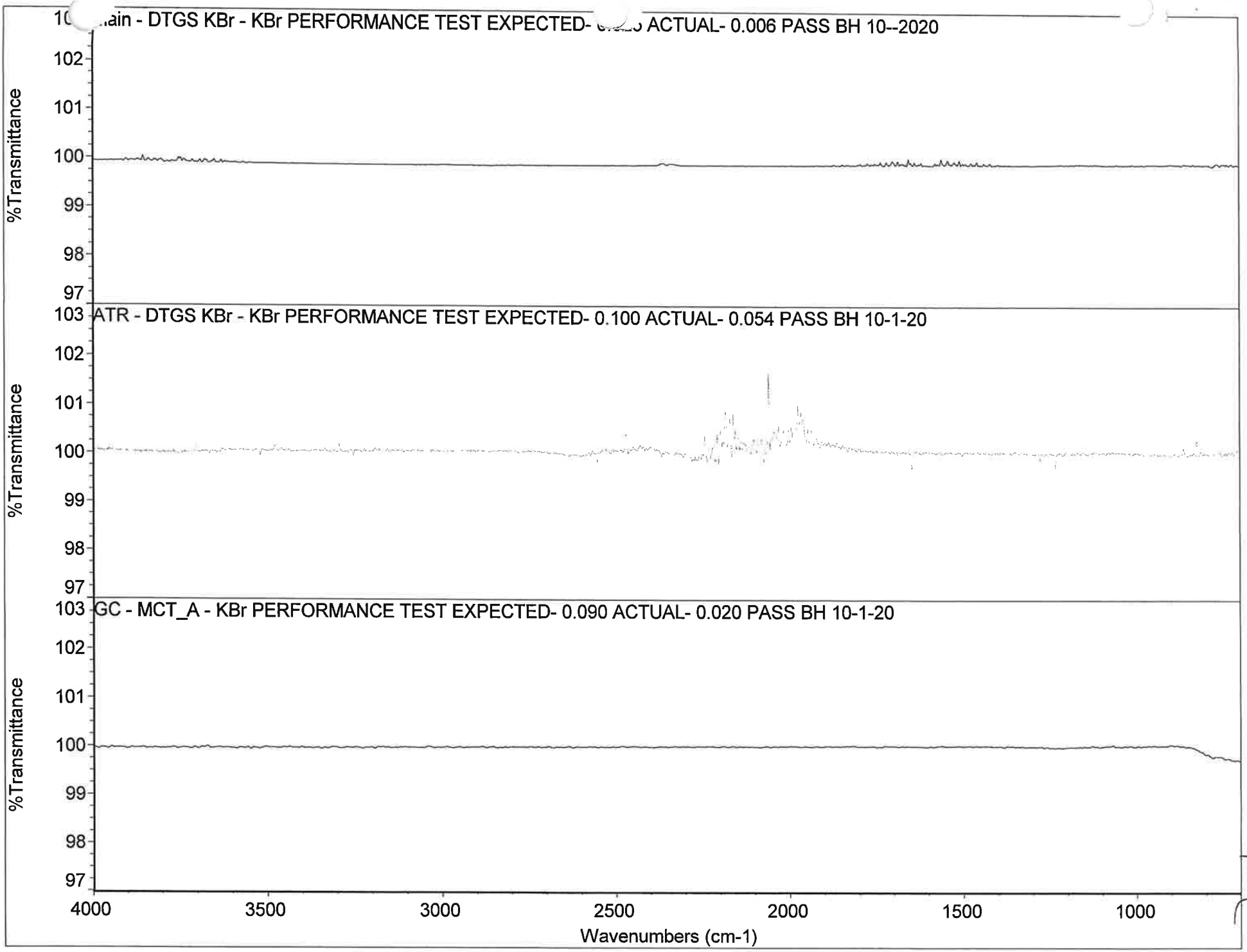
Column 149117H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Thu Oct 01 12:38:08 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 256
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.7974
Aperture: 100.00


ain - DTGS KBr - KBr PERFORMANCE TEST EXPECTED- ACTUAL- 0.006 PASS BH 10--2020
ATR - DTGS KBr - KBr PERFORMANCE TEST EXPECTED- 0.100 ACTUAL- 0.054 PASS BH 10-1-20
GC - MCT_A - KBr PERFORMANCE TEST EXPECTED- 0.090 ACTUAL- 0.020 PASS BH 10-1-20
%Transmittance
Wavenumbers (cm-1)
4000
3500
3000
2500
2000
1500
1000

Firmware version: 1.11
Serial number: AUP1400276
Date/Time: Thursday, October 1, 2020, 01:13 PM

Bench Status Readings

Parameter	Status	Current	Acceptable Range
+5 Volt	Pass	5.07V	4.50V to 5.50V
+12 Volt	Pass	11.99V	10.80V to 13.20V
-12 Volt	Pass	-11.87V	-13.20V to -10.80V
+3.3 Volt	Pass	3.32V	3.00V to 3.60V
Laser Current	Pass	0.65mA	0.20mA to 1.30mA
Laser Frequency	Pass	15798.26	
Source Voltage	Pass	8.90V	8.00V to 10.00V
Source Current	Pass	2.05A	1.50A to 2.50A
Source Power	Pass	18.21W	
Modulator Temperature	Pass	31.90°C	0.00°C to 100.00°C
Board Temperature	Pass	39.66°C	0.50°C to 70.00°C
Detector	Pass	DTGS KBr	
Beamsplitter	Pass	KBr	

Installations

Component	Serial Number	Installation Date
Spectrometer	Nicolet iS50	Apr 22, 2014*
Interferometer	ATL1400157	Apr 22, 2014
Electronics	AUT1400184	Apr 22, 2014
Source, IR	AUG1400799	Apr 07, 2014
Source, Whitelight Laser	ATQ1400155	Apr 22, 2014
Desiccant	N.A.	
Power Supply	AUS1400196	Apr 22, 2014

Performance Test Result

Test Item	Region (cm-1)	Expected	Actual	Status
Main - DTGS KBr - KBr	2200 - 2100	0.025	0.006	Pass
ATR - DTGS KBr - KBr	2800 - 2700	0.100	0.054	Pass
GC - MCT/A - KBr	2200 - 2100	0.090	0.020	Pass

ValPro Qualification Report

Qualification test: Nicolet iS50 system with DTGS in built-in position KBr-EP
Operator: Chemistry
Date: Tuesday, October 20, 2020 12:40:47 PM (GMT-05:00)
Instrument: Nicolet iS50 Serial number: AUP1400276
Validation wheel serial number: AYC4899
Filename: Nicolet iS50 system with DTGS in built-in position KBr-EP_20201020_124047.spg

Test description	High limit	Low limit	Measured	Result
Energy ratio				
Energy ratio 4000 / 2000	1.00	0.20	0.37	Pass
Energy ratio 2000 / 1000	4.00	0.80	1.66	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	0.003	Pass
P-P noise 1050 - 950 (%T)	0.10	0.00	0.03	Pass
P-P noise 550 - 450 (%T)	1.50	0.00	0.12	Pass
RMS noise 4050 - 3950	0.05	0.00	0.00	Pass
RMS noise 2050 - 1950	0.039	0.00	0.001	Pass
RMS noise 1050 - 950	0.014	0.00	0.005	Pass
RMS noise 550 - 450	0.30	0.00	0.03	Pass
Wavenumber accuracy				
Peak at 3060.0 (cm-1)	3061.0	3059.0	3059.8	Pass
Peak at 2849.5 (cm-1)	2850.5	2848.5	2849.3	Pass
Peak at 1942.9 (cm-1)	1943.9	1941.9	1942.7	Pass
Peak at 1601.2 (cm-1)	1602.2	1600.2	1601.2	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
Optical resolution				
Resolution 2870 - 2849.5 (Abs)	10.00	0.33	0.43	Pass
Resolution 1589 - 1583 (Abs)	10.00	0.08	0.12	Pass
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	0.00	Pass
Intensity at 1028.3 (%T)	0.50	-0.50	0.02	Pass
Detector linearity				
Slope	1.10	0.90	1.01	Pass
Intercept (%T)	1.00	-1.00	0.09	Pass

Performed by: _____ Title: _____ Date: 10/20/20

Approved by: _____ Title: _____ Date: _____

Comments: _____

Digital comment(s):

No digital comments found.

ValPro Qualification Report

Qualification test: Nicolet iS50 system with integrated diamond ATR and built-in DTGS-EP
Operator: Chemistry
Date: Tuesday, October 20, 2020 1:04:25 PM (GMT-05:00)
Instrument: Nicolet iS50 Serial number: AUP1400276
Validation wheel serial number: AYC4899
ATR accessory serial number: AVM1400384
Filename: Nicolet iS50 system with integrated diamond ATR and built-in DTGS-EP_20201020_130425.spg

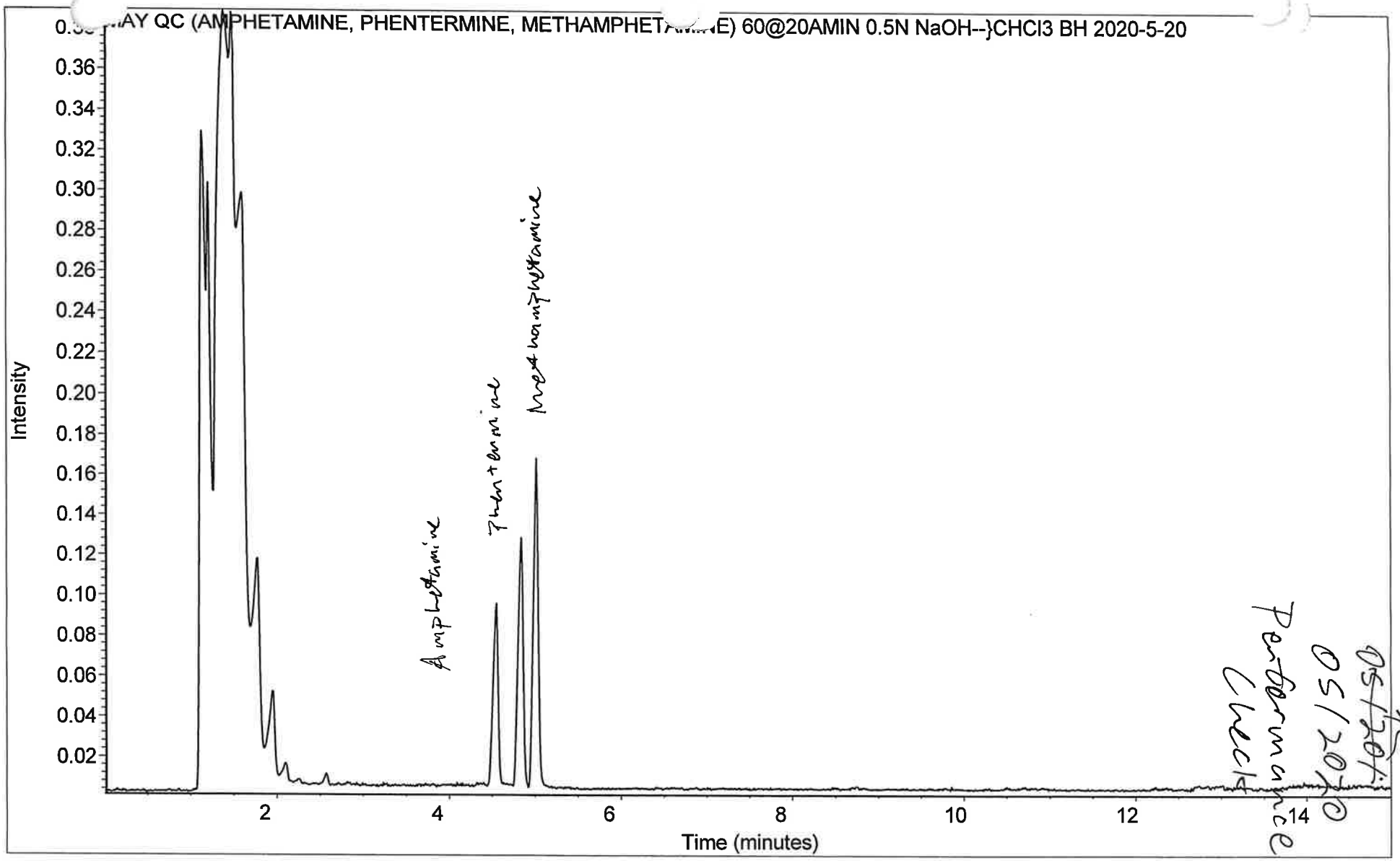
Test description	High limit	Low limit	Measured	Result
Wavenumber accuracy				
Peak at 2849.5 (cm-1)	2850.5	2848.5	2849.9	Pass
Peak at 1601.2 (cm-1)	1602.2	1600.2	1601.2	Pass
Peak at 1583.0 (cm-1)	1584.0	1582.0	1582.9	Pass
Peak at 1154.5 (cm-1)	1155.5	1153.5	1154.6	Pass
Peak at 1028.3 (cm-1)	1029.3	1027.3	1028.3	Pass
Optical Resolution				
FWHH at 1154 (cm-1)	10.00	5.00	8.12	Pass
FWHH at 907 (cm-1)	14.00	5.00	12.73	Pass

Performed by: _____ Title: _____ Date: 10/20/20

Approved by: _____ Title: _____ Date: _____

Comments: _____

Digital comment(s):
No digital comments found.



Linked spectrum at 0.010 min.

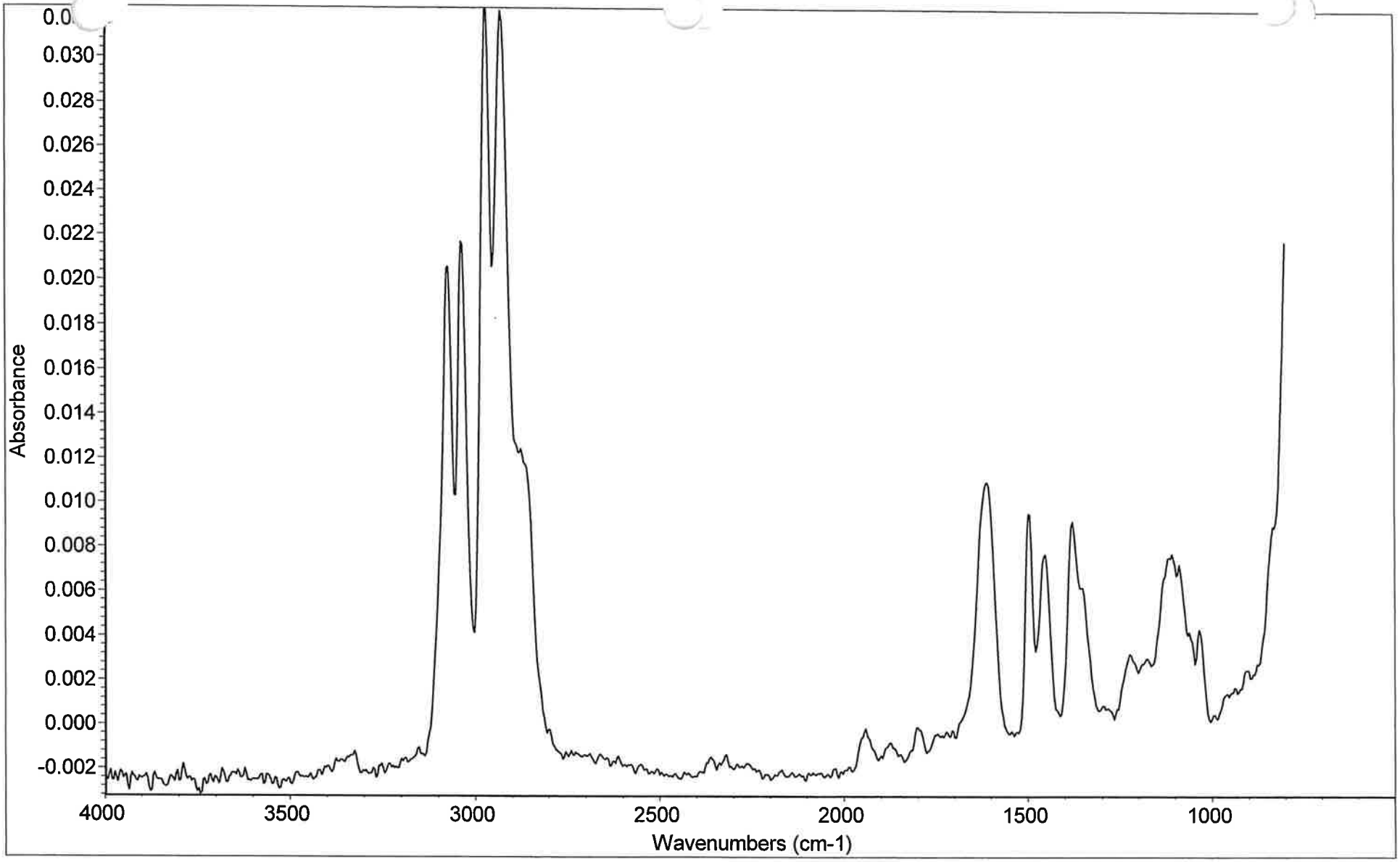
Column UST408011H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue May 19 11:28:53 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.1647
Aperture: 100.00



MAY QC AMPHETAMINE 60@20AMIN 0.5N NaOH--}CHCl3 BH 2020-5-20 Linked spectrum at 4.551 min.

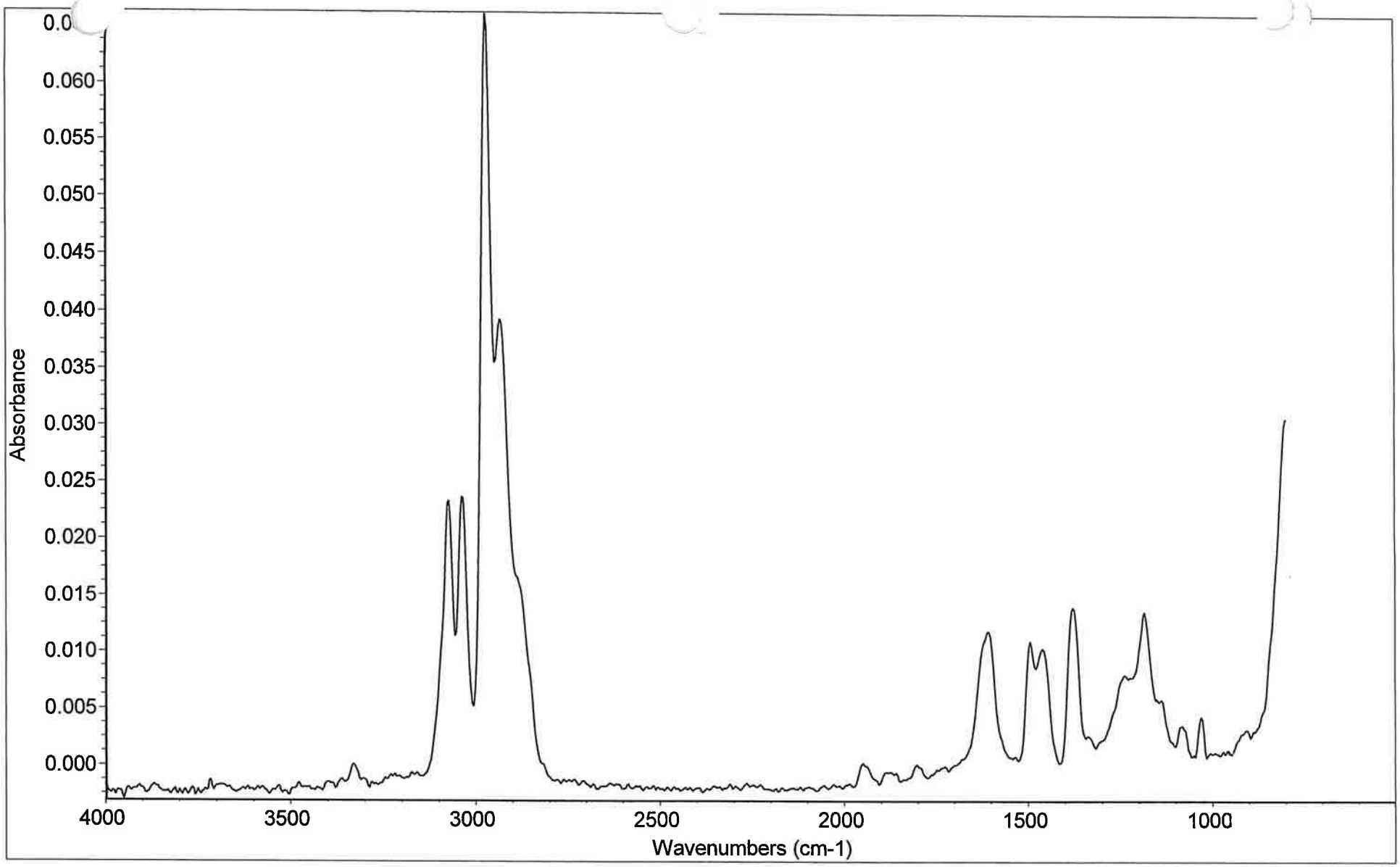
Column UST408011H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue May 19 11:28:57 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.1647
Aperture: 100.00



MAY QC PHENTERMINE 60@20AMIN 0.5N NaOH--}CHCl3 BH 2020-5-20

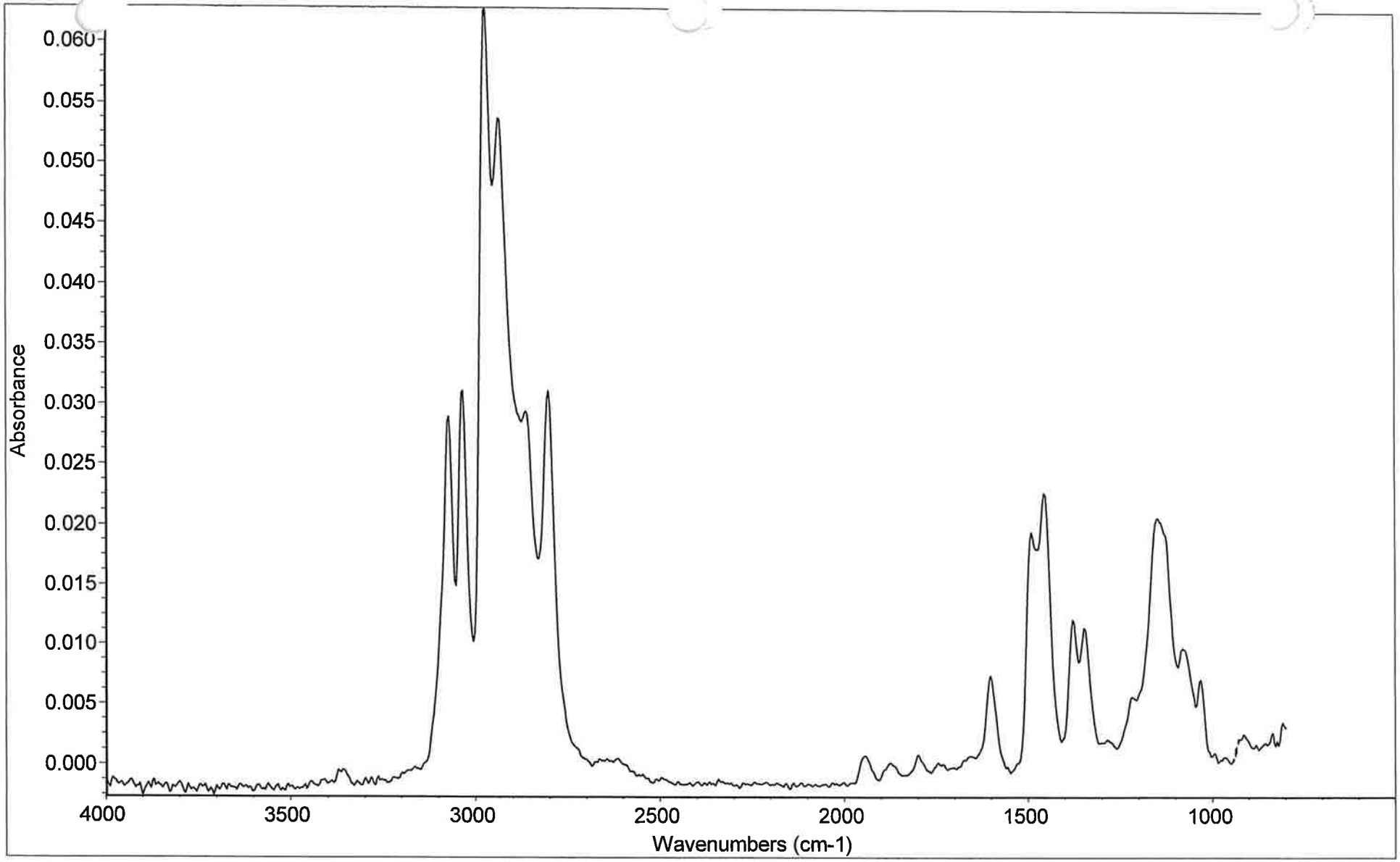
Column UST408011H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue May 19 11:28:57 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.1647
Aperture: 100.00



MAY QC METHAMPHETAMINE 60@20AMIN 0.5N NaOH--}CHCl3 BH 2020-5-20 Linked spectrum at 5.019 min.

Column UST408011H 30 Meters
Column flow 3.0
Split ratio 2.0
Transfer Line 280 degrees C
Light Pipe 280 degrees C

Detector: MCT/A
Beamsplitter: KBr
Source: IR

HOGWARTS

Collection time: Tue May 19 11:28:58 2020 (GMT-05:00)

Number of sample scans: 4
Number of background scans: 64
Resolution: 8.000
Sample gain: 1.0
Optical velocity: 3.1647
Aperture: 100.00

ValPro Qualification Report

Qualification test: Nicolet iS50 system with integrated diamond ATR and built-in DTGS-EP
Operator: OMNICAdmin
Date: Tuesday, May 19, 2020 10:41:43 AM (GMT-05:00)
Instrument: Nicolet iS50 Serial number: AUP1400276
Validation wheel serial number: AYC4899
ATR accessory serial number: AVM1400384
Filename: Nicolet iS50 system with integrated diamond ATR and built-in DTGS-EP_20200519_104143.spg

Test description	High limit	Low limit	Measured	Result
Wavenumber accuracy				
Peak at 2849.5 (cm-1)	2850.5	2848.5	2849.9	Pass
Peak at 1601.2 (cm-1)	1602.2	1600.2	1601.2	Pass
Peak at 1583.0 (cm-1)	1584.0	1582.0	1583.0	Pass
Peak at 1154.5 (cm-1)	1155.5	1153.5	1154.7	Pass
Peak at 1028.3 (cm-1)	1029.3	1027.3	1028.3	Pass
Optical Resolution				
FWHH at 1154 (cm-1)	10.00	5.00	8.11	Pass
FWHH at 907 (cm-1)	14.00	5.00	12.77	Pass

Performed by: Ben Hubert Title: SA/FS Date: 5/19/20

Approved by: _____ Title: _____ Date: _____

Comments: _____

Digital comment(s):
No digital comments found.

ValPro Qualification Report

Qualification test: Nicolet iS50 system with DTGS in built-in position KBr-EP
Operator: OMNICAdmin
Date: Tuesday, May 19, 2020 10:21:58 AM (GMT-05:00)
Instrument: Nicolet iS50 Serial number: AUP1400276
Validation wheel serial number: AYC4899
Filename: Nicolet iS50 system with DTGS in built-in position KBr-EP_20200519_102158.spg

Test description	High limit	Low limit	Measured	Result
Energy ratio				
Energy ratio 4000 / 2000	1.00	0.20	0.37	Pass
Energy ratio 2000 / 1000	4.00	0.80	1.66	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	0.004	Pass
P-P noise 1050 - 950 (%T)	0.10	0.00	0.02	Pass
P-P noise 550 - 450 (%T)	1.50	0.00	0.21	Pass
RMS noise 4050 - 3950	0.05	0.00	0.00	Pass
RMS noise 2050 - 1950	0.039	0.00	0.001	Pass
RMS noise 1050 - 950	0.014	0.00	0.005	Pass
RMS noise 550 - 450	0.30	0.00	0.04	Pass
Wavenumber accuracy				
Peak at 3060.0 (cm-1)	3061.0	3059.0	3059.8	Pass
Peak at 2849.5 (cm-1)	2850.5	2848.5	2849.3	Pass
Peak at 1942.9 (cm-1)	1943.9	1941.9	1942.7	Pass
Peak at 1601.2 (cm-1)	1602.2	1600.2	1601.2	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
Optical resolution				
Resolution 2870 - 2849.5 (Abs)	10.00	0.33	0.43	Pass
Resolution 1589 - 1583 (Abs)	10.00	0.08	0.12	Pass
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	0.00	Pass
Intensity at 1028.3 (%T)	0.50	-0.50	0.02	Pass
Detector linearity				
Slope	1.10	0.90	1.01	Pass
Intercept (%T)	1.00	-1.00	0.08	Pass

Performed by: Ben Hubert Title: SA/FS Date: 5/19/20

Approved by: _____ Title: _____ Date: _____

Comments: _____

Digital comment(s):

No digital comments found.

Firmware version: 1.11
Serial number: AUP1400276
Date/Time: Tuesday, May 19, 2020, 10:14 AM

JM
5/19/20

Bench Status Readings

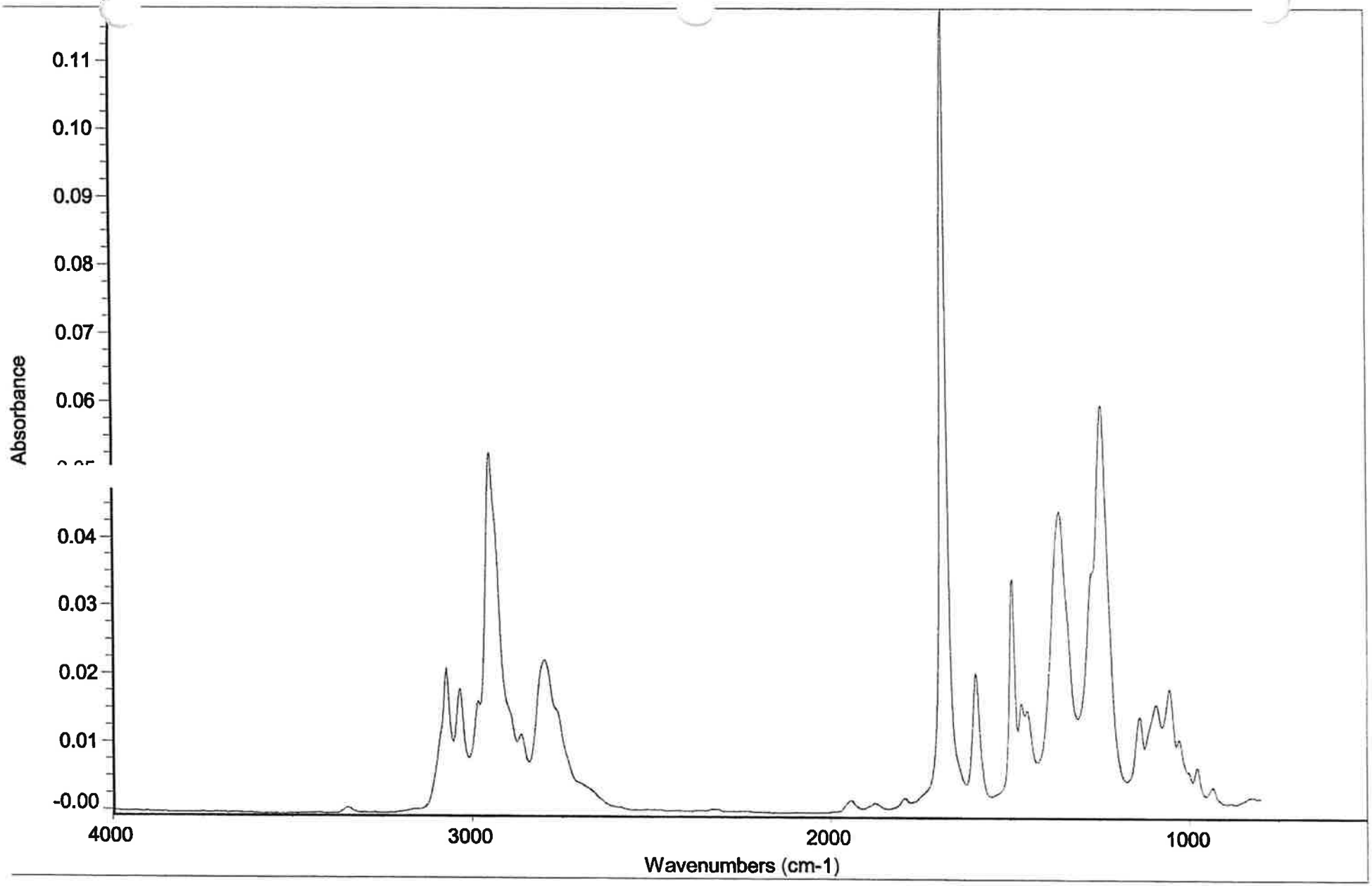
Parameter	Status	Current	Acceptable Range
+5 Volt	Pass	5.07V	4.50V to 5.50V
+12 Volt	Pass	11.98V	10.80V to 13.20V
-12 Volt	Pass	-11.87V	-13.20V to -10.80V
+3.3 Volt	Pass	3.32V	3.00V to 3.60V
Laser Current	Pass	0.65mA	0.20mA to 1.30mA
Laser Frequency	Pass	15798.26	
Source Voltage	Pass	8.87V	8.00V to 10.00V
Source Current	Pass	2.05A	1.50A to 2.50A
Source Power	Pass	18.16W	
Modulator Temperature	Pass	31.30°C	0.00°C to 100.00°C
Board Temperature	Pass	40.13°C	0.50°C to 70.00°C
Detector	Pass	DTGS KBr	
Beamsplitter	Pass	KBr	

Installations

Component	Serial Number	Installation Date
Spectrometer	Nicolet iS50	Apr 22, 2014*
Interferometer	ATL1400157	Apr 22, 2014
Electronics	AUT1400184	Apr 22, 2014
Source, IR	AUG1400799	Apr 07, 2014
Source, Whitelight Laser	ATQ1400155	Apr 22, 2014
Desiccant	N.A.	
Power Supply	AUS1400196	Apr 22, 2014

Performance Test Result

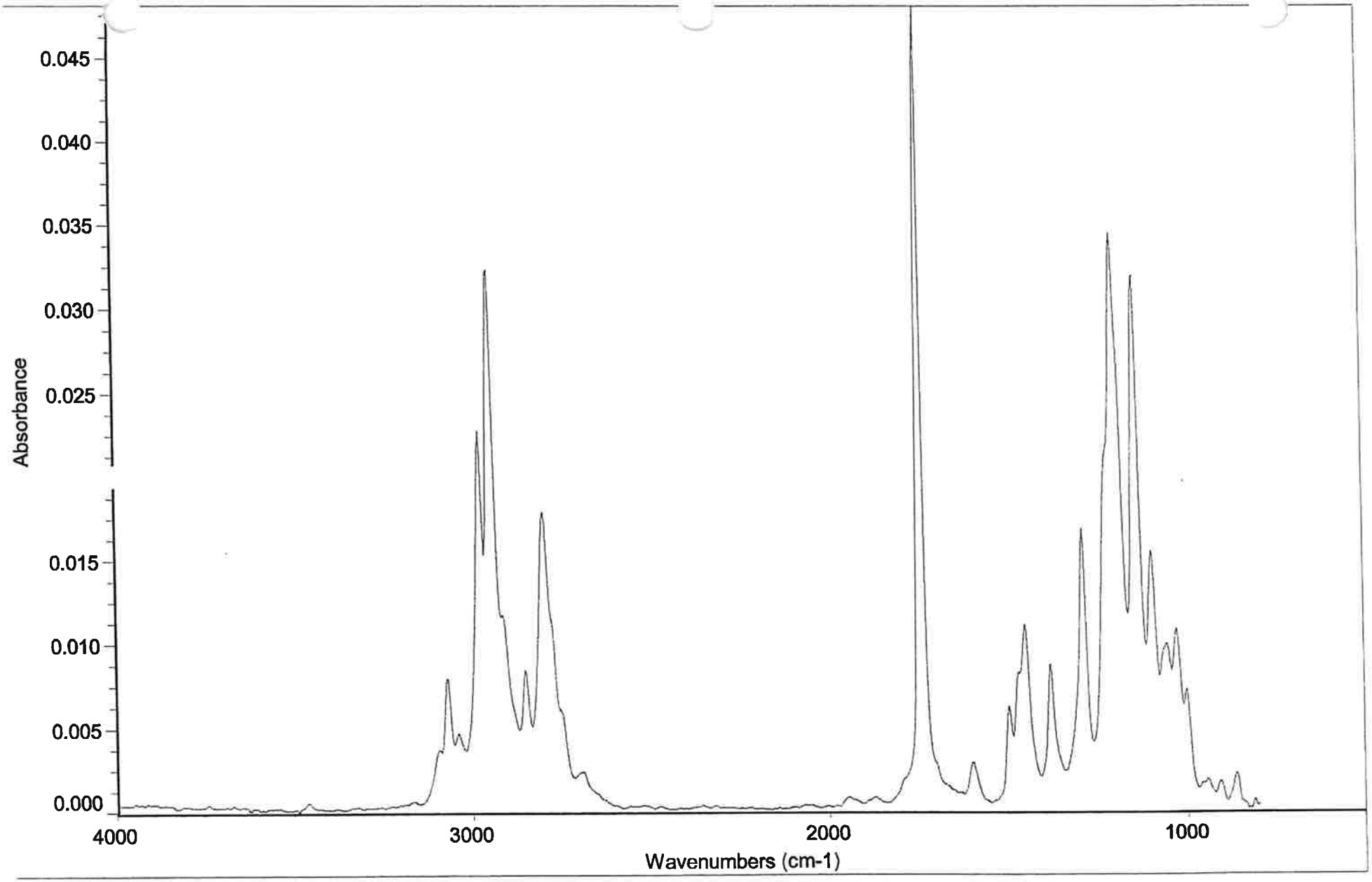
Test Item	Region (cm-1)	Expected	Actual	Status
Main - DTGS KBr - KBr	2200 - 2100	0.025	0.004	Pass
ATR - DTGS KBr - KBr	2800 - 2700	0.100	0.029	Pass
GC - MCT/A - KBr	2200 - 2100	0.090	0.018	Pass



Fentanyl Citrate std. USPC labs lot# 1275-F JDM

GC/FTIR

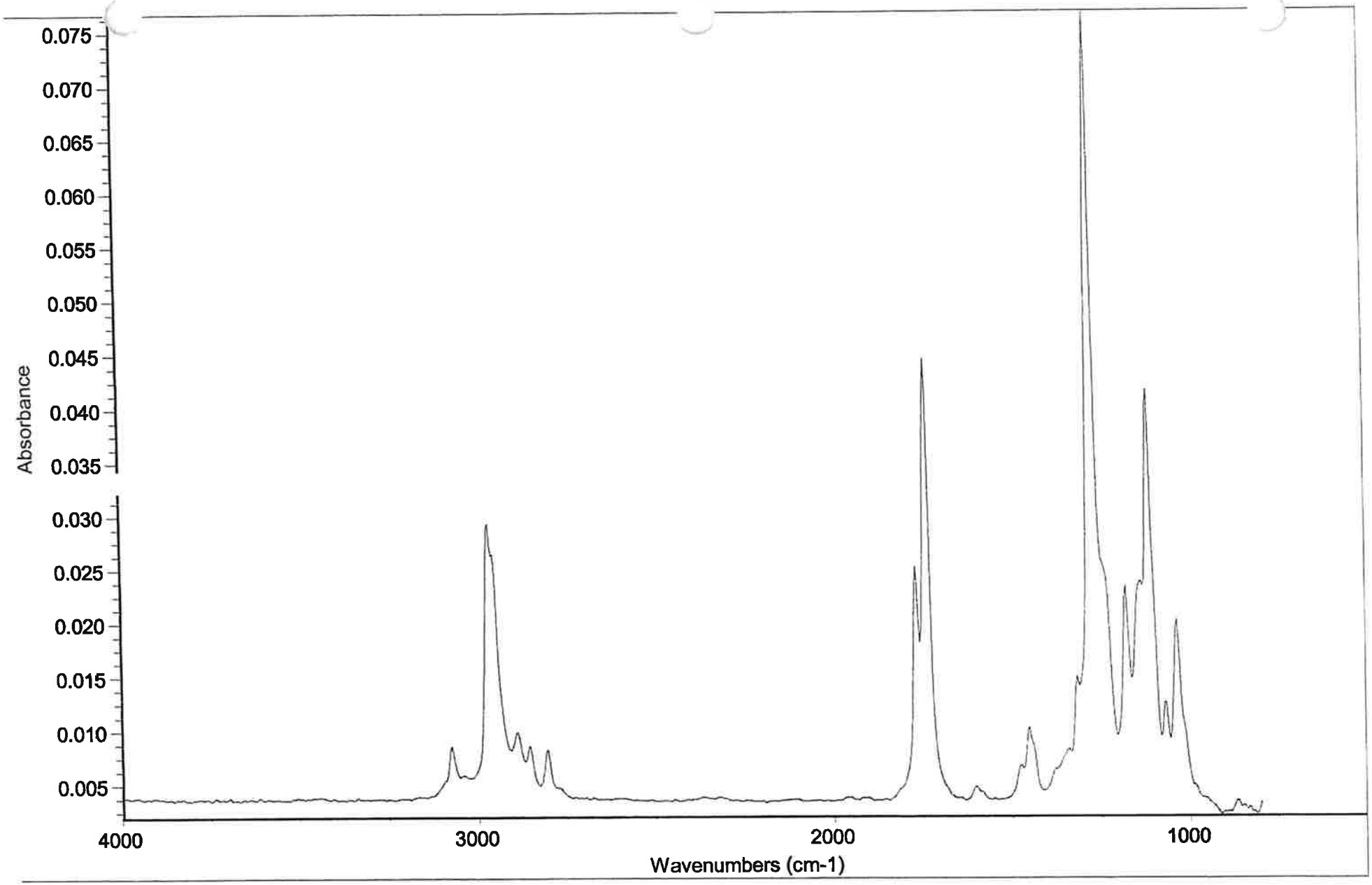
Collection time: Tue Jun 25 09:59:43 2002



Pethidine Std. B>CHCL3 USP Lot#413NMN-027 GBE

IR #1

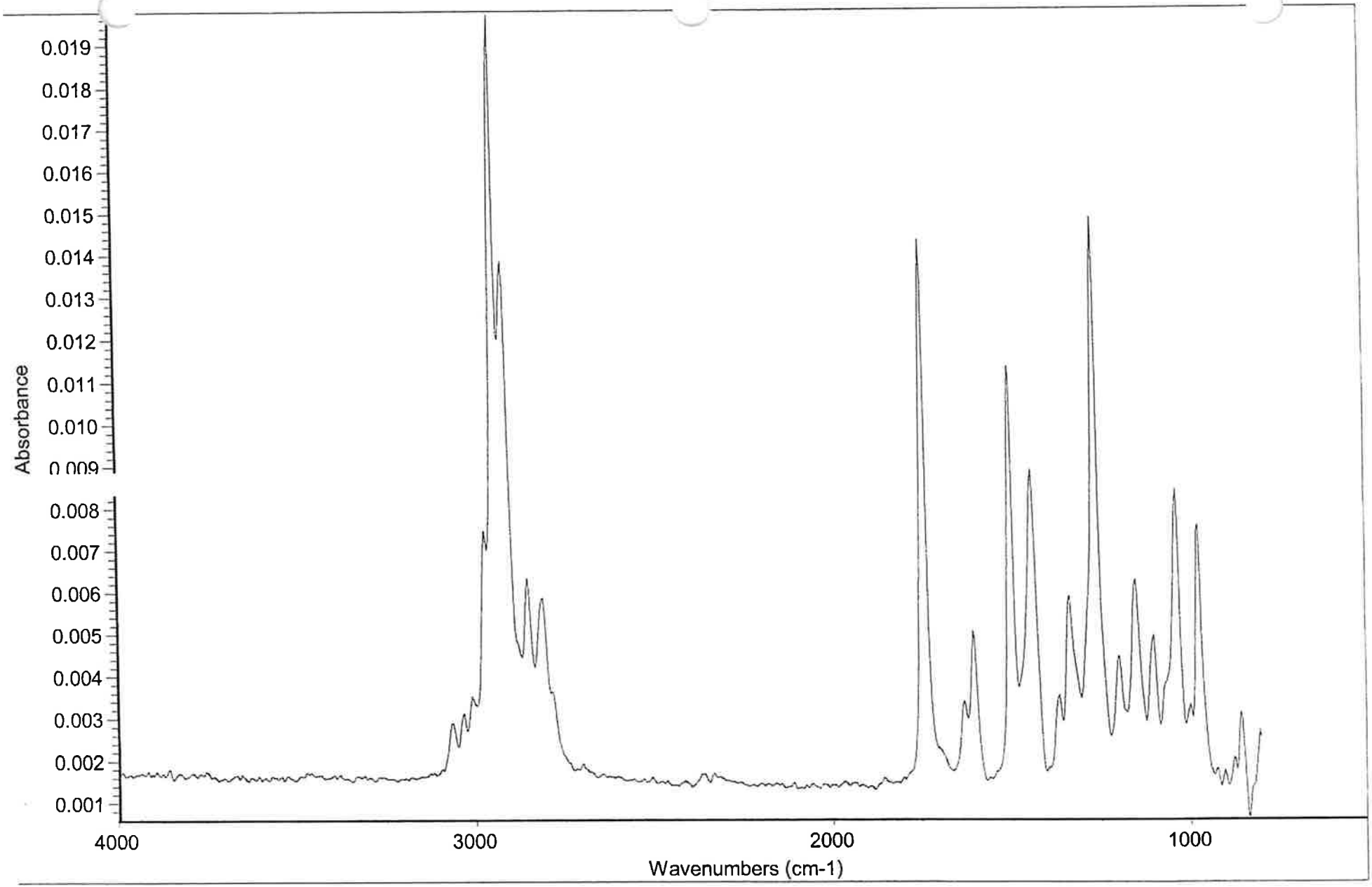
Collection time: Tue Jul 31 13:20:57 2001



Cocaine Standard Sigma Lot 50K1124 WHS

IR #1

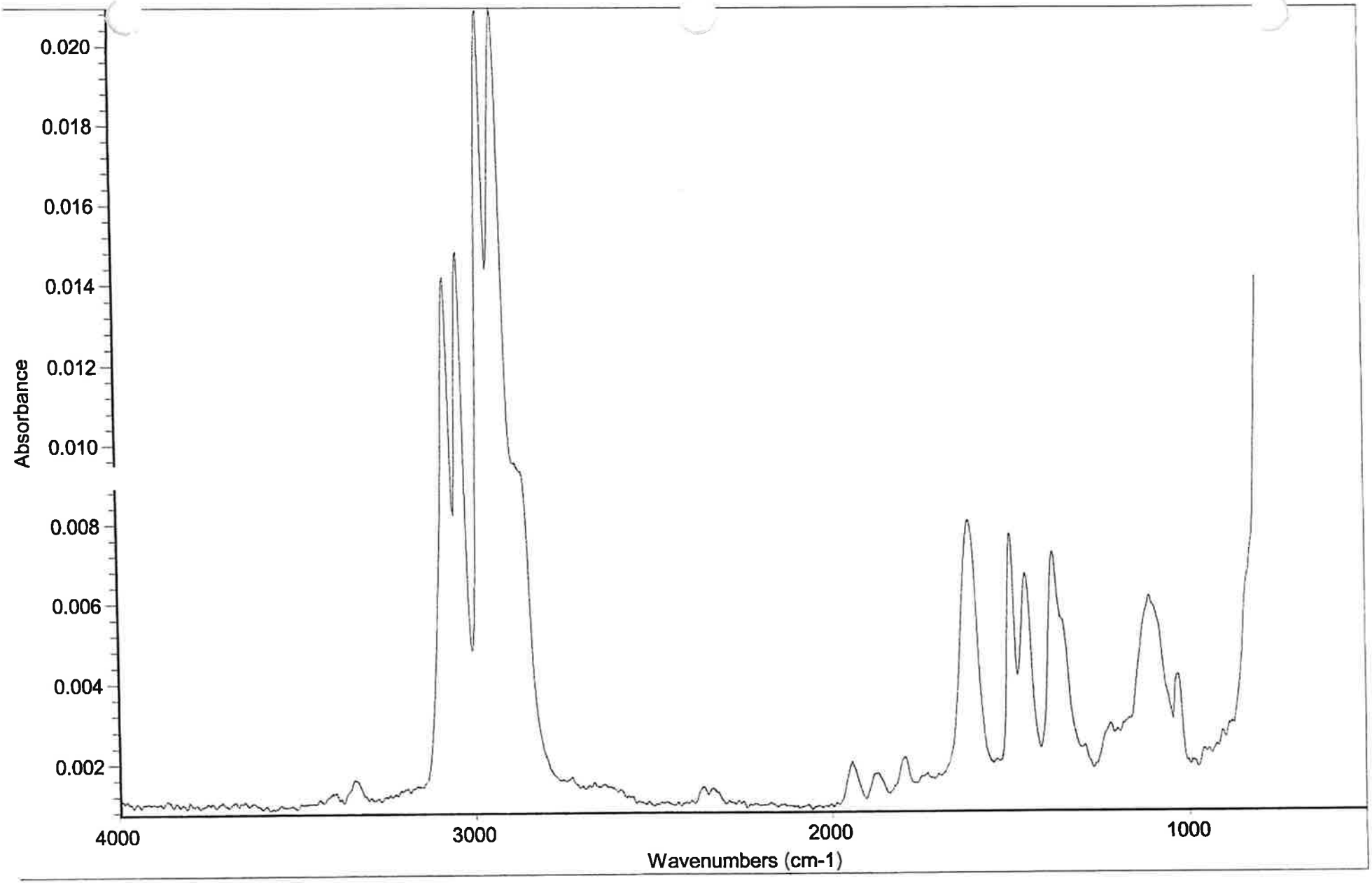
Collection time: Tue Jul 17 16:34:50 2001



Dihydrocodeinone (Hydrocodone) Std. B>CHCL3 Merck Lot#V1526 GBE

IR #1

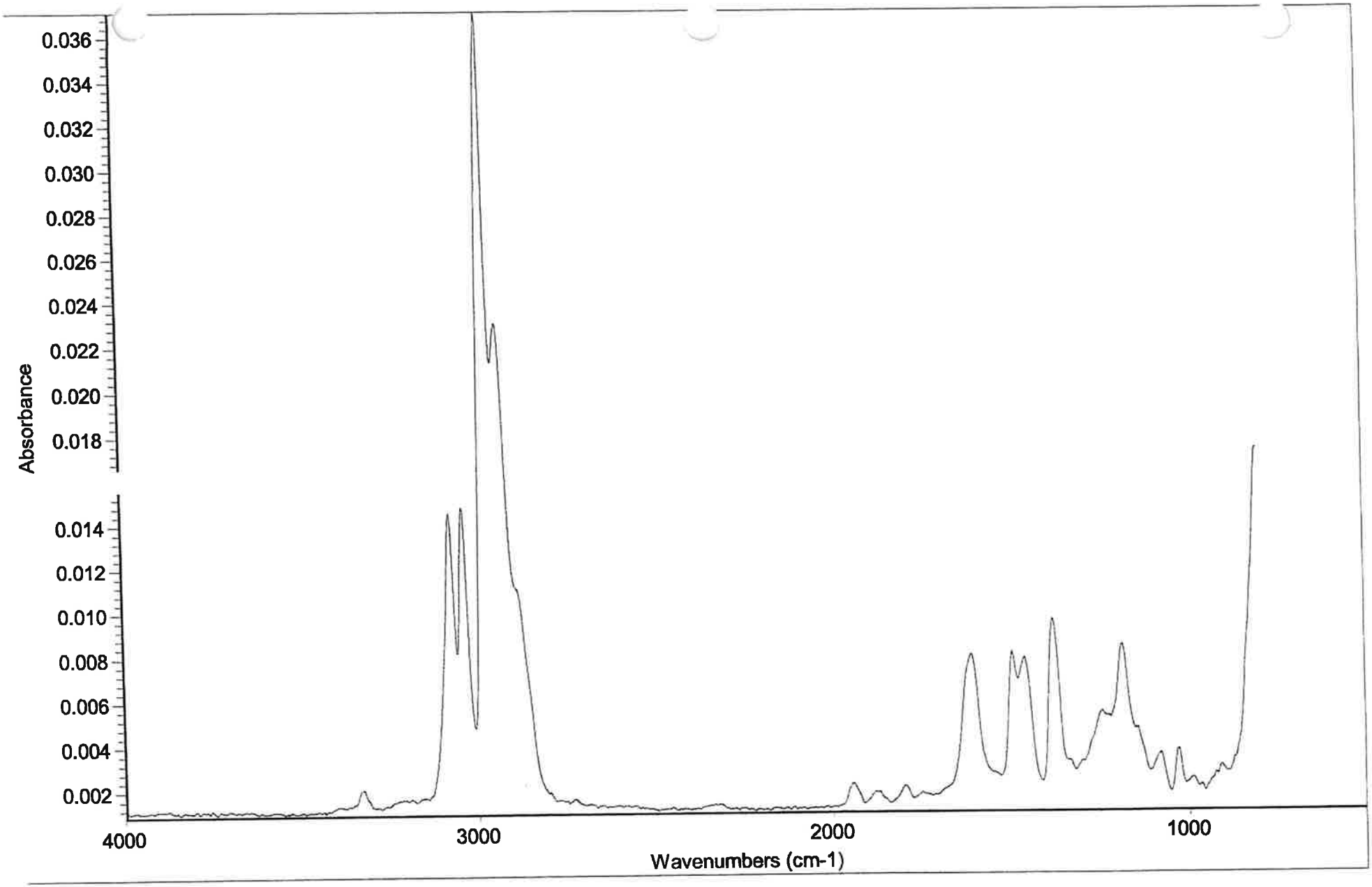
Collection time: Tue Jul 31 13:22:03 2001



D-Amphetamine std. (basic ext. in CHCl3) from D-Amphetamine Sulfate K&K Labs lot# 83567 WHS

IR #1

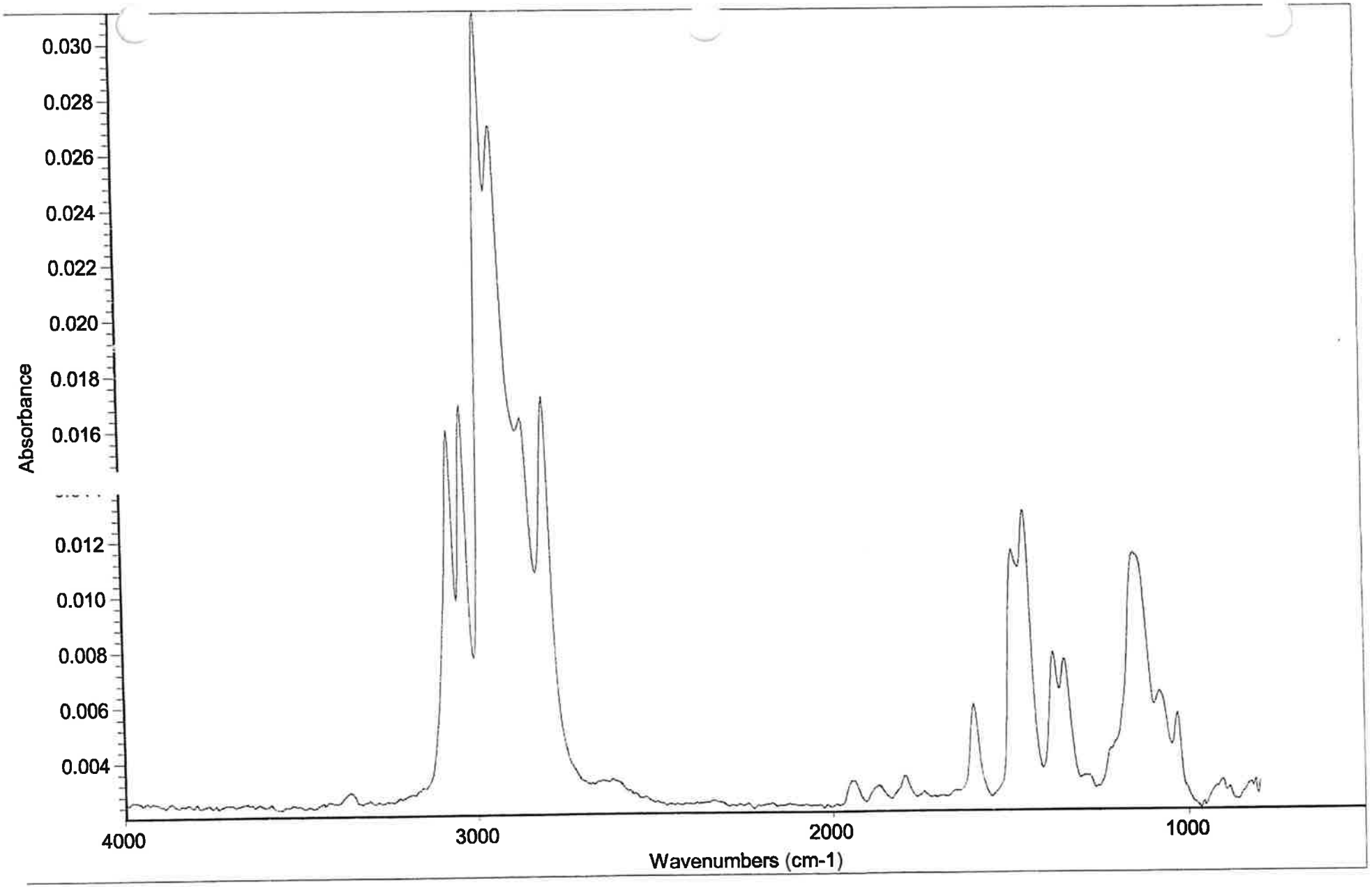
Collection time: Wed Jul 18 10:36:17 2001



Phentermine std. (basic/CHCl3 ext.) Sigma lot# 47H0208 WHS

IR #1

Collection time: Wed Jul 18 13:11:27 2001



Methamphetamine std. (basic/CHCl3 ext.) Sigma lot # 34H0144 WHS

IR #1

Collection time: Wed Jul 18 13:00:47 2001

Hogwarts

GC-FTIR

Chromeleon®7 Software

Dionex Chromeleon version 7.2.10

Ominc 9.11.745 software

Ominc Series 9.11.727

Driver version 9.11.709

Nicolet iS50

Firmware version 1.11

Hogwarts

GC-FTIR

Chromeleon®7 Software

Dionex Chromeleon Version 7.12.1713

OMNIC 9.2.106 Software

OMNIC Series 9.2.41

Driver Version 9.2

Nicolet iS50

Firmware Version 1.11

Thermo Scientific Hogwarts GC-FTIR Operating Procedures

Each GC-FTIR system will be identified from all other GC-FTIR systems by use of a unique identifier. This identifier could be a reference to a particular number, model number, serial number, name, etc. All GC-FTIR systems employ OMNIC software. The Hogwart's GC-FTIR additionally employs Chromeleon 7 GC software. See the instrument's maintenance logbook for the specific OMNIC and Chromeleon 7 software version.

General Operations:

1. Ensure that the power is on to all components
2. Open the Chromeleon 7 application by double clicking the icon on the computer desktop (This may take a few moments)
3. Once the Chromeleon 7 application has successfully opened, open the OMNIC application by double clicking the icon on the computer desktop

NOTE: IT IS IMPORTANT THAT YOU FIRST OPEN CHROMELEON AND THEN OMNIC. OMNIC WILL NOT COLLECT DATA IF YOU DO NOT OPEN CHROMELEON FIRST.

To Set Up for Analysis:

Make sure that the **Default iS50 GC-IR** experiment is selected on the OMNIC **Experiment** tool bar and that the blue button is lit up on the iS50 GC-IR accessory.

This should be selected automatically by the instrument. The instrument should be set to a Gain of 1, Resolution of 8 cm-1, 4 Scans, 64 Scans for the background and a spectral range of 4000 to 800 cm-1.

Data Acquisition:

1. All parameters for analysis on the Hogwart's GC-FTIR are electronically stored in the Chromeleon 7 software under the **Data** tab within the folder name **Chromeleon Local.** The method parameters for an analysis run will be noted in the analyst's case file.

NOTE: Remember that the column on the Hogwart's GC-FTIR has a longer column and thinner film thickness than GC/IR #1 and #2. This should be taken into consideration for certain analytes, using the necessary methods as needed.

2. A sample blank must be run each day per each case file, method, and extraction prior to running a case sample.
3. If the reservoir on the GC-FTIR is not cold, fill the reservoir with liquid nitrogen.
4. In the **OMNIC** application window select the **Series** tab and select **Heater Status…**

Thermo Scientific Hogwarts GC-FTIR Operating Procedures

Each GC-FTIR system will be identified from all other GC-FTIR systems by use of a unique identifier. This identifier could be a reference to a particular number, model number, serial number, name, etc. All GC-FTIR systems employ OMNIC software. The Hogwart's GC-FTIR additionally employs Chromeleon 7 GC software. See the instrument's maintenance logbook for the specific OMNIC and CHromeleon 7 software version.

General Operations:

1. Ensure that the power is on to all components
2. Open the Chromeleon 7 application by double clicking the icon on the computer desktop (This may take a few moments)
3. Once the Chromeleon 7 application has successfully opened, open the OMNIC application by double clicking the icon on the computer desktop

NOTE: IT IS IMPORTANT THAT YOU FIRST OPEN CHROMELEON AND THEN OMNIC. OMNIC WILL NOT COLLECT DATA IF YOU DO NOT OPEN CHROMELEON FIRST.

To Set Up for Analysis:

Make sure that the **Default iS50 GC-IR** experiment is selected on the OMNIC **Experiment** tool bar and that the blue button is lit up on the iS50 GC-IR accessory.

This should be selected automatically by the instrument. The instrument should be set to a Gain of 1, Resolution of 8 cm-1, 4 Scans, 64 Scans for the background and a spectral range of 4000 to 800 cm-1.

Data Acquisition:

1. All parameters for analysis on the Hogwart's GC-FTIR are electronically stored in the Chromeleon 7 software under the **eWorkflows** tab within the instrument name **OMNICADMIN-PC-1.** The method parameters for an analysis run will be noted in the analyst's case file.

NOTE: Remember that the column on the Hogwart's GC-FTIR has a longer column and thinner film thickness than GC/IR #1 and #2. This should be taken into consideration for certain analytes, using the necessary methods as needed.

2. A sample blank must be run each day per each case file, method, and extraction prior to running a case sample.
3. If the reservoir on the GC-FTIR is not cold, fill the reservoir with liquid nitrogen.
4. In the **OMNIC** application window select the **Series** tab and select **Heater Status…**

5. Make sure the heaters are turned on (checked box) and set the **Flow cell setpoint (deg. C):** and **Transfer line setpoint (deg. C):** to **280°C** in the white box and select the **Update Heaters** button.
6. To the right of the white box where the temperature values are set it will show the actual temperature of the flow cell and transfer line. When the values have not reached the desired set temperature, the filament background picture will become yellow. Once the values of the set temperatures have been reached the filament background will turn green.
7. Exit the **Heater Status…** window once the set temperatures have been reached.

Creating a Sequence:

8. Select the **eWorkflows** tab within the **Chromeleon Console** window.
9. Right click the eWorkflow titled **OMNICADMIN-PC_1** and select **Launch…** or **Enter.**
10. A **Select Sampler** window will pop open and select the injection option needed for analysis. **Inject Valve** for manual injection or **Sampler** for auto-sampler injection.
11. Once the injection method has been selected, an **eWorkflow Wizard** window will open with a **Processing Method** box and a flashing cursor. Leave the **Processing method, Report template, and View settings boxes BLANK (For quantitation processes only)** and select the "Next >>" button.
12. After selecting the "Next>>" button, a **Sample** window will appear.
13. Leave the **Number of samples:** box at 1 (Note: Chromeleon will still make you add each new injection for each sample within your sequence no matter how many samples you enter here).
14. Leave the **Sampler start position:** box at 1 and select the "Next>>" button when finished.
15. In the **Sequence** window within the **Sequence name:** type the title for your sequence (Make sure the sequence is titled where it be easily identified…Date, Initials, etc.)
16. Make any additional comments in the **Comment:** box.
17. In the **Sequence location:** box, select the "Browse…" button.
18. A **Select Sequence Location** window should appear and within the **Look in:** box make sure that **Chromeleon Local** is selected. Within the **Chromeleon Local** folder select **Instrument Data>OMNICADMIN-PC_1** and right mouse click and create one's own folder (ex. RMH for Rebecca M Hernandez or the date). Double-click the created/selected folder and click the "Select" button.
19. Once the **Sequence location:** has been established, click the "Finish" button on the **eWorkflow Wizard** window (Leave the **Run sequence after creation** box unchecked).
20. A new sequence will now be created and displayed in the **Chromeleon Console** under the **Data** tab.

5. Make sure the heaters are turned on (checked box) and set the **Flow cell setpoint (deg. C):** and **Transfer line setpoint (deg. C):** to **280°C** in the white box and select the **Update Heaters** button.
6. To the right of the white box where the temperature values are set it will show the actual temperature of the flow cell and transfer line. When the values have not reached the desired set temperature, the filament background picture will become yellow. Once the values of the set temperatures have been reached the filament background will turn green.
7. Exit the **Heater Status…** window once the set temperatures have been reached.

Creating a Sequence:

8. Select the **Data** tab within the **Chromeleon Console** window.
9. Find the file titled **_Series Template_ (COPY AND PASTE)** and copy and paste it to your personal Chromeleon sequence folder.
10. Once the file has been pasted to your folder rename it with the date and your initials.
11. Fill out and select the **Name, Position, Volume, Instrument Meth, and Comment** boxes for the samples on the displayed sequence. The **Instrument Meth** boxes will have drop down arrows to select each method.
12. It is the analyst's discretion as to which method to use.
13. Make sure that in the **Name** box provides detailed sample information and the user's initials (This is how the file information will be saved in **OMNIC**)
14. **Click here to add a new injection** to add more samples to the sequence.
15. Once all of the samples have been added and the sequence is ready to run select the **OMNIC** application window.
16. Select the "Collect Ser" button on the **OMNIC** taskbar.

NOTE: IT WILL TAKE A FEW MOMENTS FOR OMNIC TO LOAD THE COLLECT SERIES IF THE SOFTWARE HAS NOT ALREADY BEEN IN USE.

17. The background will collect once the **OMNIC** software has finished loading and an **External Trigger** window will pop open stating "Ready to start data collection at external trigger.".
18. Select the **Chromeleon Console** window and highlight the beginning of the sequence run (or the sample you wish to run).
19. Click the "Start" button at the top of the sequence.
20. After a few moments the sequence toolbar should load from yellow to green (New→Running) and where the "Start" button appeared it will now state "Stop".

Auto-sampler Injection:

The auto-sampler will automatically inject your sample once the run has been started in the **Chromeleon Console** and the TRACE 1310 instrument is at ready status.

OMNIC will be triggered to start collecting data once the auto-sampler has injected the sample.

Analyzing data in OMNIC:

21. Open the **OMNIC** application window and select "File" and then "Open…" in the toolbar.
22. An "Open" window will appear and in the "Files of type:" box, click the down arrow and select the "Series Files (*.SRS)" option.
23. Select the data file you wish to open and click the "Open" button.
24. Data file will display in **OMNIC**.
25. Use the bottom tools or taskbar to analyze the spectra.
26. To add a spectra region to a new window, right mouse click the bottom screen (spectra) and select "Copy To > New Window" and then click the "OK" button
27. To view a window, select the "Window" tab in the toolbar and click on the window you wish to display.

To Set Up for iS50 ATR Analysis:

Make sure that **iS50 ATR** experiment is selected on the OMNIC **Experiment** tool bar and that the blue button is lit up on the iS50 ATR accessory.

The parameters for using the iS50 ATR accessory should be set to Autogain, Resolution of 4 cm^{-1}, 16 Scans, and a spectral range of 4000 to 600.

iS50 ATR Operating Instructions:

1. At **Experiment** on the tool bar, load the **iS50 ATR** parameter file.
2. Select **Report** on the menu bar and select "Template…".
3. Select the ATRTEMPLATE.RPT at the very top of the scrolled window and click the "Select" button below.
4. Clean ATR stage and underneath ATR accessory.
5. Collect background and add to window.
6. Add sample and turn down ATR accessory.
7. Collect sample, add to window, select stack spectra, fill out sample information in text box, and select print option on taskbar.
8. Clean ATR stage and underneath ATR accessory.
9. Select **Report** on menu bar and select "Template…".
10. Select WILLIENEWGCFTIR.RPT template at very bottom of scrolled window and click the "Select" button below to switch template back.

21. Fill out and select the **Name, Position, Volume, Instrument Meth, Comment, and Type** boxes for the samples on the displayed sequence. The **Instrument Meth** and **Type** boxes with have drop down arrows to select each method/type. (Volume and Position are not applicable if manual injection is selected when creating the sequence, but may provide beneficial information to the user).
22. It is the analyst's discretion as to which method to use.
23. Make sure that in the **Name** box provides detailed sample information and the user's initials (This is how the file information will be saved in **OMNIC**)
24. **Click here to add a new injection** to add more samples to the sequence.
25. Once all of the samples have been added and the sequence is ready to run select the **OMNIC** application window.
26. Select the "Collect Ser" button on the **OMNIC** taskbar.

NOTE: IT WILL TAKE A FEW MOMENTS FOR OMNIC TO LOAD THE COLLECT SERIES IF THE SOFTWARE HAS NOT ALREADY BEEN IN USE.

27. The background will collect once the **OMNIC** software has finished loading and an **External Trigger** window will pop open stating "Ready to start data collection at external trigger.".
28. Select the **Chromeleon Console** window and highlight the beginning of the sequence run (or the sample you wish to run).
29. Click the "Start" button at the top of the sequence.
30. After a few moments the sequence toolbar should load from yellow to green (New→Running) and where the "Start" button appeared it will now state "Stop".

Auto-sampler Injection:

The auto-sampler will automatically inject your sample once the run has been started in the **Chromeleon Console** and the TRACE 1310 instrument is at ready status. **OMNIC** will be triggered to start collecting data once the auto-sampler has injected the sample.

Manual Injection:

The TRACE 1310 instrument has touchscreen capabilities that allow for you to monitor your run, obtain information about the instrument, and manually inject. When manually injecting, the touchscreen will provide the status of the instrument (Not Ready/Ready). When a green play/arrow button pops up on the screen, the instrument is ready for manual injection. Inject your sample and select the green play/arrow button. The **Chromeleon Console** and TRACE 1310 instrument will start collecting, triggering **OMNIC** to start collecting data.

31. Once the sample or sequence has finished, the toolbar in the sequence of the **Chromeleon Console** will state that the "Run Finished".

Analyzing data in OMNIC:

32. Open the **OMNIC** application window and select "File" and then "Open…" in the toolbar.
33. An "Open" window will appear and in the "Files of type:" box, click the down arrow and select the "Series Files (*.SRS)" option.
34. Select the data file you wish to open and click the "Open" button.
35. Data file will display in **OMNIC**.
36. Use the bottom tools or taskbar to analyze the spectra.
37. To add a spectra region to a new window, right mouse click the bottom screen (spectra) and select "Copy To > New Window" and then click the "OK" button
38. To view a window, select the "Window" tab in the toolbar and click on the window you wish to display.

To Set Up for iS50 ATR Analysis:

Make sure that **iS50 ATR** experiment is selected on the OMNIC **Experiment** tool bar and that the blue button is lit up on the iS50 ATR accessory.

The parameters for using the iS50 ATR accessory should be set to Autogain, Resolution of 4 cm^{-1}, 16 Scans, and a spectral range of 4000 to 600.

iS50 ATR Operating Instructions:

1. At **Experiment** on the tool bar, load the **iS50 ATR** parameter file.
2. Select **Report** on the menu bar and select "Template…".
3. Select the ATRTEMPLATE.RPT at the very top of the scrolled window and click the "Select" button below.
4. Clean ATR stage and underneath ATR accessory.
5. Collect background and add to window.
6. Add sample and turn down ATR accessory.
7. Collect sample, add to window, select stack spectra, fill out sample information in text box, and select print option on taskbar.
8. Clean ATR stage and underneath ATR accessory.
9. Select **Report** on menu bar and select "Template…".
10. Select WILLIENEWGCFTIR.RPT template at very bottom of scrolled window and click the "Select" button below to switch template back.

11. Make sure **Default iS50 GC-IR** parameter file is switched back and loaded in **Experiment** tool bar.

MONTHLY MAINTENANCE

Alignment:

1. At **Experiment** on the tool bar, load the **Transmission E.S.P.** parameter file.
2. Select **Collect** from the menu bar and select **Experiment Setup…**
3. After the window loads go to the **Bench** tab and make sure that the Gain is set to 1.0.
4. Then select the **Diagnostic** tab and select the "Align…" button. When the alignment is complete record the number in the appropriate GC/IR maintenance log.
5. Click "OK" button to exit out.
6. Next, check and make sure the desiccant on the instrument is blue (If pink, moisture is present).

Report & Main, ATR, GC iS50 Performance Tests (KBr)

1. Make sure that the main sample compartment is empty.
2. From the menu bar select **Collect** then select **Advanced Diagnostics….**
3. After "Nicolet iS50 Diagnostics" window opens, select **Performance Test.**
4. Check all the boxes for the **Main, ATR, GC iS50 Tests (KBr).**
5. Select the "Run Selected Test" button.
6. Fill out OMNIC with performance test values for each spectra (**Main, ATR, GC**) and print and place spectra in the appropriate GC/IR maintenance log book.

   Example:

   PERFORMANCE TEST (MAIN) 2200-2100 = 0.004 PASS RMH
   PERFORMANCE TEST (ATR) 2800-2700 = 0.024 PASS RMH
   PERFORMANCE TEST (GC) 2200-2100 = 0.012 PASS RMH

7. After tests are complete, select each spectra (**Main, ATR, GC**) and individually save by setting the filename to title under the "Monthly Performance Tests" folder under the "Spectra/Groups (*.SPA, *.SPG)" file type.
8. Select the back arrow button and select Report, Print, and then the back arrow button again. Place the print out in the GC/IR maintenance log book.
9. Exit out of "Nicolet iS50 Diagnostics" window.

ValPro Qualification:

1. Check to ensure the **Transmission E.S.P.** parameter file is loaded under **Experiment** from the tool bar.
2. Select **Analyze** on the menu bar and then **ValPro Qualification….**
3. Once the "ValPro Qualification" window appears use the drop down box under "Qualification test:" and select the "Nicolet iS50 system with DTGS in built-in position KBr-EP".
4. Select the "Qualify" button once the test has been loaded.
5. When the ValPro Qualification has completed, highlight the test that just completed in the "Energy ratio" tab and click the "Report…" button.
6. A window will pop up with the report. Select the "Print" button and fill out ValPro Qualification Report and initial and place in the GC/IR maintenance log book.
7. Select the "Close" button.

For iS50 ATR Accessory

1. In the "Qualification test:" drop down box select the "Nicolet iS50 system with integrated diamond ATR and built-in DTGS-EP" option.
2. Select the "Qualify" button once the test has been loaded and click "OK" when the confirmation window pops up for the background.
3. Retrieve the SMART iTR polystyrene standard "lollipop" from the second drawer near the IR #7.
4. When a window pops up stating "Place the polystyrene in the accessory and apply pressure. Choose OK when you are ready to collect the sample data", place the polystyrene standard "lollipop" on the sample compartment area with the "ATR STD 269-173000" words facing upwards and apply pressure.

   NOTE: Be sure to place the iS50 ATR accessory on the "lollipop" polystyrene standard window in different locations when performing monthly maintenance so as to not place the iS50 ATR accessory on the same location on the "lollipop" window.

5. Select the "OK" button once the "lollipop" polystyrene standard is in place.
6. When the ValPro Qualification has completed, highlight the test that just completed in the "Wavenumber accuracy" tab and click the "Report…" button.
7. A window will pop up with the report. Select the "Print" button and place in the GC/IR maintenance log book.
8. Select the "Close" and then "Exit" button to close out of the ValPro Qualification.
9. Select and load the **Default iS50 GC-IR** parameter file under **Experiment** from the tool bar
10. Remove "lollipop" from iS50 ATR sample area and place back in Thermo box and return it to the second drawer near the IR #7.

11. Make sure **Default iS50 GC-IR** parameter file is switched back and loaded in **Experiment** tool bar.

MONTHLY MAINTENANCE

Alignment:

1. At **Experiment** on the tool bar, load the **Transmission E.S.P.** parameter file.
2. Select **Collect** from the menu bar and select **Experiment Setup…**
3. After the window loads go to the **Bench** tab and make sure that the Gain is set to 1.0.
4. Then select the **Diagnostic** tab and select the "Align…" button. When the alignment is complete record the number in the appropriate GC/IR maintenance log.
5. Click "OK" button to exit out.
6. Next, check and make sure the desiccant on the instrument is blue (If pink, moisture is present).

Report & Main, ATR, GC iS50 Performance Tests (KBr)

1. Make sure that the main sample compartment is empty.
2. From the menu bar select **Collect** then select **Advanced Diagnostics….**
3. After "Nicolet iS50 Diagnostics" window opens, select **Performance Test.**
4. Check all the boxes for the **Main, ATR, GC iS50 Tests (KBr).**
5. Select the "Run Selected Test" button.
6. Fill out OMNIC with performance test values for each spectra (**Main, ATR, GC**) and print and place spectra in the appropriate GC/IR maintenance log book.

   Example:

   PERFORMANCE TEST (MAIN) 2200-2100 = 0.004 PASS RMH
   PERFORMANCE TEST (ATR) 2800-2700 = 0.024 PASS RMH
   PERFORMANCE TEST (GC) 2200-2100 = 0.012 PASS RMH

7. After tests are complete, select each spectra (**Main, ATR, GC**) and individually save by setting the filename to title under the "Monthly Performance Tests" folder under the "Spectra/Groups (*.SPA, *.SPG)" file type.
8. Select the back arrow button and select Report, Print, and then the back arrow button again. Place the print out in the GC/IR maintenance log book.
9. Exit out of "Nicolet iS50 Diagnostics" window.

ValPro Qualification:

1. Check to ensure the **Transmission E.S.P.** parameter file is loaded under **Experiment** from the tool bar.
2. Select **Analyze** on the menu bar and then **ValPro Qualification…**.
3. Once the "ValPro Qualification" window appears use the drop down box under "Qualification test:" and select the "Nicolet iS50 system with DTGS in built-in position KBr-EP".
4. Select the "Qualify" button once the test has been loaded.
5. When the ValPro Qualification has completed, highlight the test that just completed in the "Energy ratio" tab and click the "Report…" button.
6. A window will pop up with the report. Select the "Print" button and fill out ValPro Qualification Report and initial and place in the GC/IR maintenance log book.
7. Select the "Close" button.

For iS50 ATR Accessory

1. In the "Qualification test:" drop down box select the "Nicolet iS50 system with integrated diamond ATR and built-in DTGS-EP" option.
2. Select the "Qualify" button once the test has been loaded and click "OK" when the confirmation window pops up for the background.
3. Retrieve the SMART iTR polystyrene standard "lollipop" from the second drawer near the IR #7.
4. When a window pops up stating "Place the polystyrene in the accessory and apply pressure. Choose OK when you are ready to collect the sample data", place the polystyrene standard "lollipop" on the sample compartment area with the "ATR STD 269-173000" words facing upwards and apply pressure.

   NOTE: Be sure to place the iS50 ATR accessory on the "lollipop" polystyrene standard window in different locations when performing monthly maintenance so as to not place the iS50 ATR accessory on the same location on the "lollipop" window.

5. Select the "OK" button once the "lollipop" polystyrene standard is in place.
6. When the ValPro Qualification has completed, highlight the test that just completed in the "Wavenumber accuracy" tab and click the "Report…" button.
7. A window will pop up with the report. Select the "Print" button and place in the GC/IR maintenance log book.
8. Select the "Close" and then "Exit" button to close out of the ValPro Qualification.
9. Select and load the **Default iS50 GC-IR** parameter file under **Experiment** from the tool bar
10. Remove "lollipop" from iS50 ATR sample area and place back in Thermo box and return it to the second drawer near the IR #7.

11. Fill out ValPro Qualification Report and initial and place in the GC/IR maintenance log book.

To Run the Monthly Standard Check:

1. Check to ensure the **Default iS50 GC-IR** parameter file is loaded under **Experiment** from the tool bar.
2. Make sure the reservoir for the MCT detector is filled with liquid nitrogen.
3. Make sure that the **transfer line** and **flow cell** heaters are at 280°C.
4. Analyze the Monthly QC test standard (Amphetamine, Phentermine, Methamphetamine) that is kept refrigerated.
5. Check its expiration date. If it is past its expiration date, make up a new QC test standard following the correct procedure to ensure the proper concentrations.
6. Make sure that the **60@20AMIN** or **MAN60@20AMIN** is loaded and used to run the Monthly QC standard.
7. Run this sample following the procedures for analyzing data from the GC/FTIR and place in the GC/IR maintenance log book.

This is not meant to be all-inclusive. There may be other ways to accomplish the same task.

11. Fill out ValPro Qualification Report and initial and place in the GC/IR maintenance log book.

To Run the Monthly Standard Check:

1. Check to ensure the **Default iS50 GC-IR** parameter file is loaded under **Experiment** from the tool bar.
2. Make sure the reservoir for the MCT detector is filled with liquid nitrogen.
3. Make sure that the **transfer line** and **flow cell** heaters are at 280°C.
4. Analyze the Monthly QC test standard (Amphetamine, Phentermine, Methamphetamine) that is kept refrigerated.
5. Check its expiration date. If it is past its expiration date, make up a new QC test standard following the correct procedure to ensure the proper concentrations.
6. Make sure that the **60@20AMIN** is loaded and used to run the Monthly QC standard.
7. Run this sample following the procedures for analyzing data from the GC/FTIR and place in the GC/IR maintenance log book.

This is not meant to be all-inclusive. There may be other ways to accomplish the same task.

Addendum

S/SL Injection Port with HP-1MS 30 meter column, 0.32 column ID, and 0.25 um film thickness:

*Stored Methods for **AUTOSAMPLE SPLIT INJECTION***

120TO270 Initial 120C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 10.00 minutes.

120TO270(30MIN) Initial 120C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 30.00 minutes.

200TO270 Initial 200C degrees hold for 1 minutes ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 15.00 minutes.

ISO270 270C degrees isothermal. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 20.00 minutes.

60@20AMIN Initial 60C degrees hold for 1 minute ramped to 270C degrees at 20C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 15.00 minutes.

200TO270@20AMIN Initial 200C degrees hold for 1 minute ramped to 270C degrees at 20C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 10.00 minutes.

Always verify that the temperature for the GC interface is at least 10 degrees higher than the maximum temperature of the GC oven.

MAN120TO270(30MIN) Initial 120C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 30.00 minutes.

MAN200TO270 Initial 200C degrees hold for 1 minutes ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 15.00 minutes.

MANISO270 270C degrees isothermal. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 20.00 minutes.

MAN60@20AMIN Initial 60C degrees hold for 1 minute ramped to 270C degrees at 20C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 15.00 minutes.

MAN200TO270@20AMIN Initial 200C degrees hold for 1 minute ramped to 270C degrees at 20C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 10.00 minutes.

*Stored Methods for **AUTOSAMPLE SPLITLESS INJECTION***

SL120TO270 Initial 120C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Splitless (1 minute), Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 10.00 minutes.

SL120TO270(30MIN) Initial 120C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Splitless (1 minute), Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 30.00 minutes.

SL200TO270 Initial 200C degrees hold for 1 minutes ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Splitless (1 minute), Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 15.00 minutes.

SLISO270 270C degrees isothermal. Constant carrier flow rate of 3.0 mL/min, Splitless (1 minute), Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 20.00 minutes.

Back Column: PTV Injection Port with TR-1MS 7 meter column, 0.32 column ID, and 1 um film thickness (S/N# 1264708):

(NOTE: The back S/SL inlet settings are set to Split with an inlet temperature of 250C degrees with a purge flow of 5.0 mL/min and a constant flow of 0.500 mL/min.)

Always verify that the temperature for the GC interface is at least 10 degrees higher than the maximum temperature of the GC oven.

SL60@20AMIN Initial 60C degrees hold for 1 minute ramped to 270C degrees at 20C/min. Constant carrier flow rate of 3.0 mL/min, Splitless (1 minute), Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 15.00 minutes.

SL200TO270@20AMIN Initial 200C degrees hold for 1 minute ramped to 270C degrees at 20C/min. Constant carrier flow rate of 3.0 mL/min, Splitless (1 minute), Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 10.00 minutes.

*Stored Methods for **MANUAL SPLITLESS INJECTION***

SLMAN120TO270 Initial 120C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Splitless (1 minute), Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 10.00 minutes.

SLMAN120TO270(30MIN) Initial 120C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Splitless (1 minute), Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 30.00 minutes.

SLMAN200TO270 Initial 200C degrees hold for 1 minutes ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Splitless (1 minute), Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 15.00 minutes.

SLMANISO270 270C degrees isothermal. Constant carrier flow rate of 3.0 mL/min, Splitless (1 minute), Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 20.00 minutes.

SLMAN60@20AMIN Initial 60C degrees hold for 1 minute ramped to 270C degrees at 20C/min. Constant carrier flow rate of 3.0 mL/min, Splitless (1 minute), Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 15.00 minutes.

SLMAN200TO270@20AMIN Initial 200C degrees hold for 1 minute ramped to 270C degrees at 20C/min. Constant carrier flow rate of 3.0 mL/min, Splitless (1 minute), Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 10.00 minutes.

Addendum

Front Column: S/SL Injection Port with HP-1MS 30 meter column, 0.32 column ID, and 0.25 um film thickness (S/N# USE149117H):

*Stored Methods for **AUTOSAMPLE SPLIT INJECTION***

120TO270 Initial 120C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 10.00 minutes.

120TO270(30MIN) Initial 120C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 30.00 minutes.

200TO270 Initial 200C degrees hold for 1 minutes ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 15.00 minutes.

ISO270 270C degrees isothermal. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 20.00 minutes.

60@20AMIN Initial 60C degrees hold for 1 minute ramped to 270C degrees at 20C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 15.00 minutes.

200TO270@20AMIN Initial 200C degrees hold for 1 minute ramped to 270C degrees at 20C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 10.00 minutes.

*Stored Methods for **MANUAL SPLIT INJECTION***

MAN120TO270 Initial 120C degrees hold for 1 minute ramped to 270C degrees at 70C/min. Constant carrier flow rate of 3.0 mL/min, Split ratio of 2.0, Split flow 6.0 mL/min, Purge flow 5 mL/min, Inlet temperature of 250C degrees. Total run time 10.00 minutes.