Characterization of FUB-AMB

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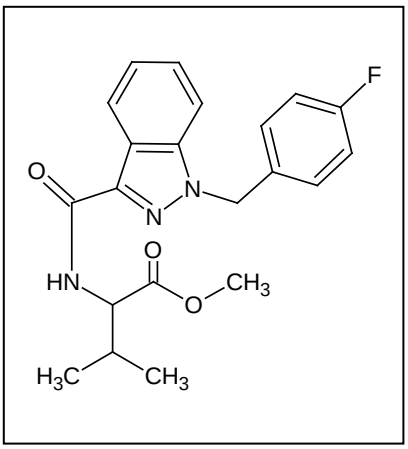
Part 1. Cayman Chemical Company Data



Name: FUB-AMB

Synonyms: AMB-FUBINACA; methyl(1-(4-fluorobenzyl)-1H-indazole-3-carbonyl)-L-valinate

CAS#: N/A

Molecular Formula: $C_{21}H_{22}FN_3O_3$

Molecular Weight: 383.4 g/mol

SMILES: O=C(OC)C(NC(=O)c3nn(Cc1ccc(F)cc1)c2ccccc23)C(C)C

InChl Key: FRFFLYJQPCIIQB-SFHVURJKSA-N

InChl: InChI=1S/C21H22FN3O3/c1-13(2)18(21(27)28-3)23-20(26)19-16-6-4-5-7-17(16)25(24-19)12-14-8-10-15(22)11-9-14/h4-11,13,18H,12H2,1-3H3,(H,23,26)/t18-/m0/s1

Background:

FUB-AMB is an analogue of AB-FUBINACA, a potent synthetic cannabinoid first synthesized by Pfizer. AB-FUBINACA exhibits a strong affinity (K_i =0.9 nM) for the CB_1 receptor [1]. The primary amide moiety in the L-valinamide side chain in AB-FUBINACA is replaced with a methyl ester in FUB-AMB. FUB-AMB was identified by Louisiana crime labs in an herbal mixture labelled "Train Wreck2" in 2014 and was banned as a controlled dangerous substance as of July 3rd, 2014[2]. The physiological and toxicological properties of this compound are not known.

1.) Buchler, I.P, Hayes, M.J., Hedge, S.G., et al. Indazole derivatives. Wo 2009/106982 A1 (2009), 1-283, PCT/IB2009/000432.

2.) Kliebert, K.H. Rulemaking-emergency rule adding controlled dangerous substances. State of Louisiana Department of Health and Hospitals. Baton Rouge, Louisiana. July 2014.

Gas chromatography/Mass spectrometry:

Experiment Parameters:

Instrument: Agilent 6890 GC / 5973 MSD

Column: 30mx0.32mm, 0.5um Rtx-5MS

Carrier Gas: Helium Flow: 2mL/min

Inlet temp: 300 ^{o}C, 15:1 split

Oven Program: Initial temp: 50 ^{o}C, Ramp to 300 ^{o}C at 30C/min, Hold at 300 ^{o}C for 5.67 minutes

Transfer Line Temp: 300 ^{o}C

MS Source: 230^{o}C

MS Quad: 150^{o}C

Mass Scan Range: 40-600 amu

Threshold: 150

Tune File: stune.u

Figure 1: Gas Chromatography/Mass Spectrometry of FUB-AMB

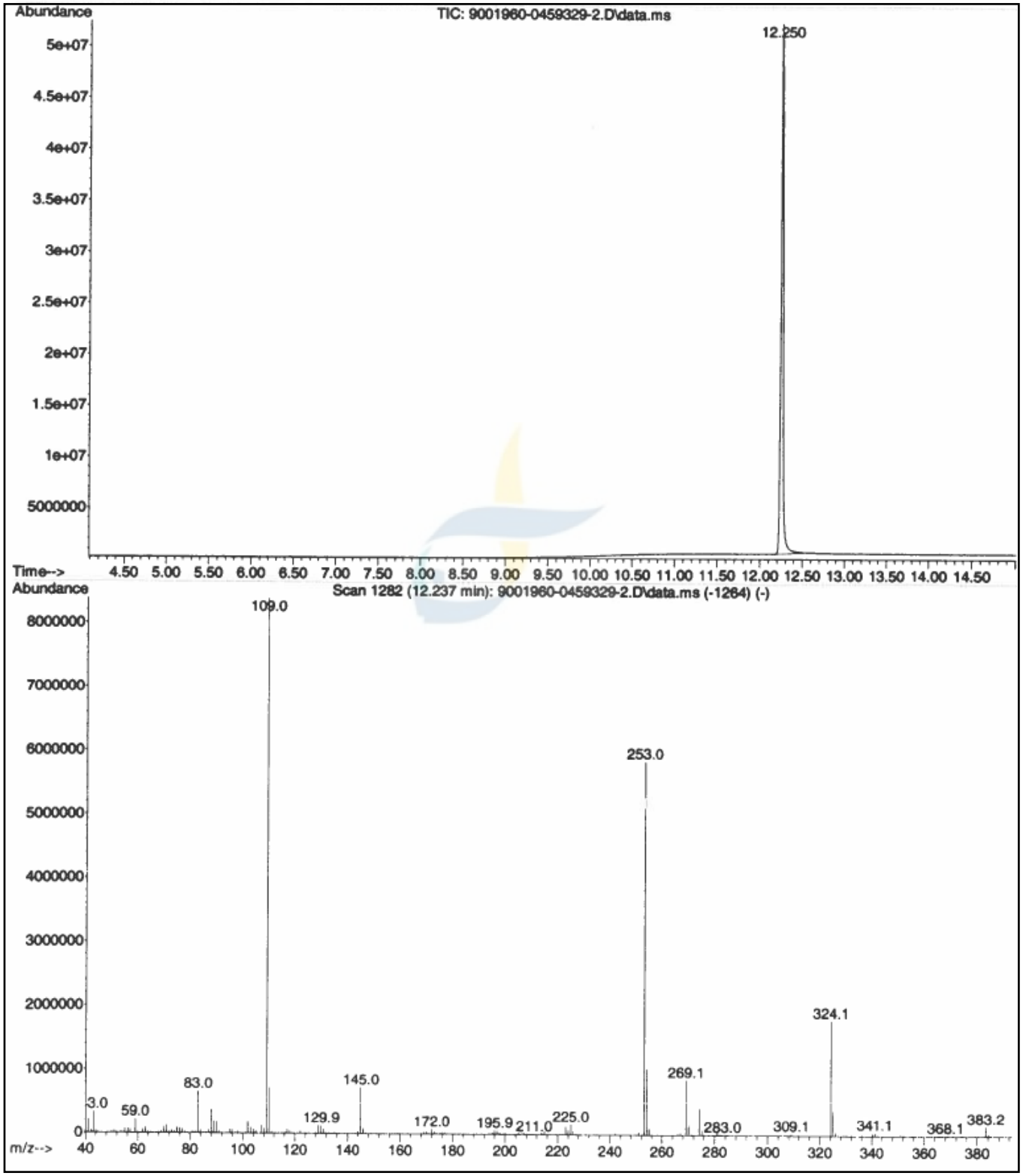


Figure 2. Fourier Transform Infrared Spectroscopy of FUB-AMB

Experiment Parameters:
PerkinElmer Spectrum 65
Number of scans: 16 (background subtracted)
Resolution: 4 cm^{-1}
Scan Range: 600-4000 cm^{-1}
Sample prepared as NaCl plate

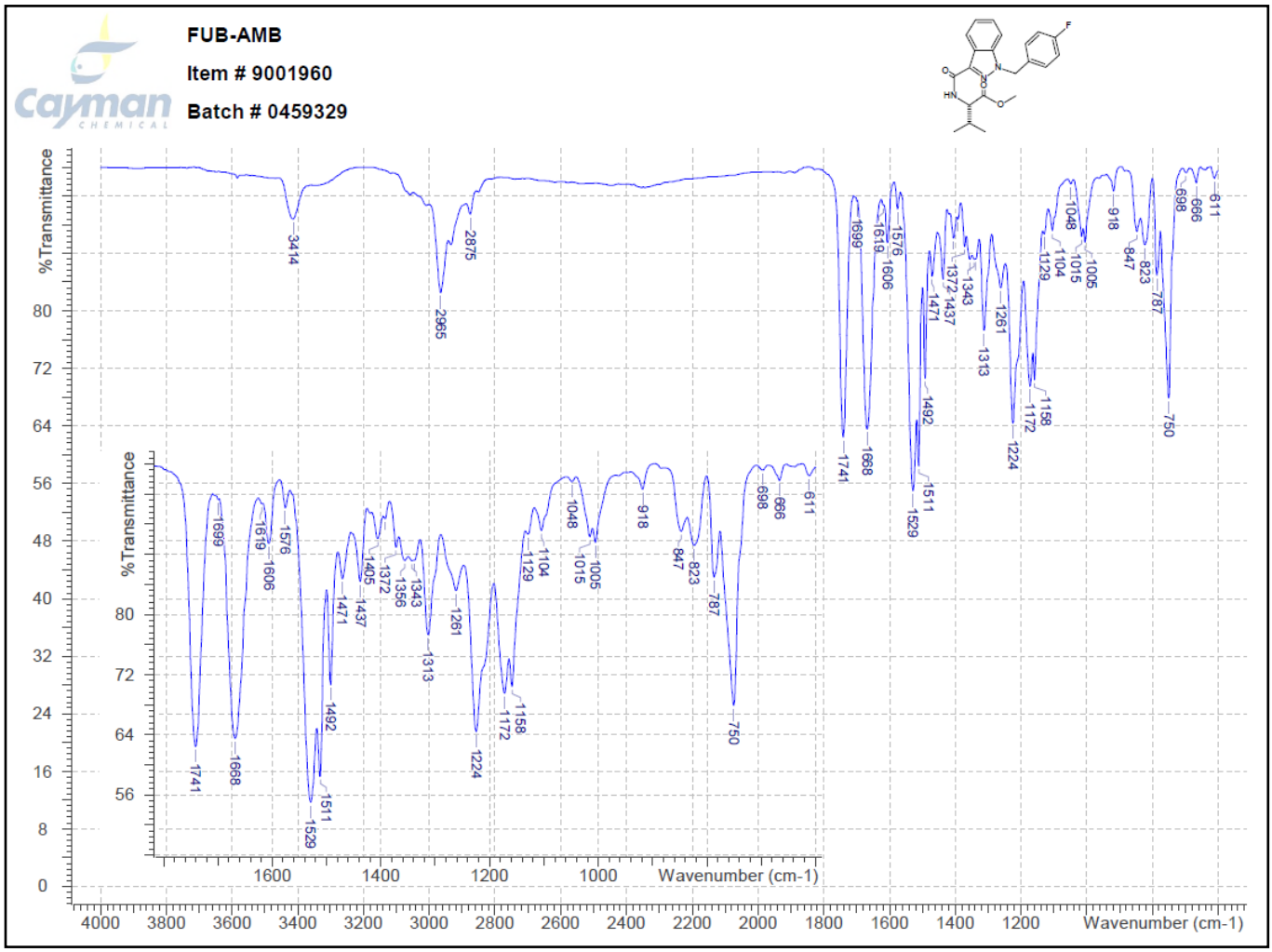


Figure 3. 1H Nuclear Magnetic Resonance Spectroscopy of FUB-AMB

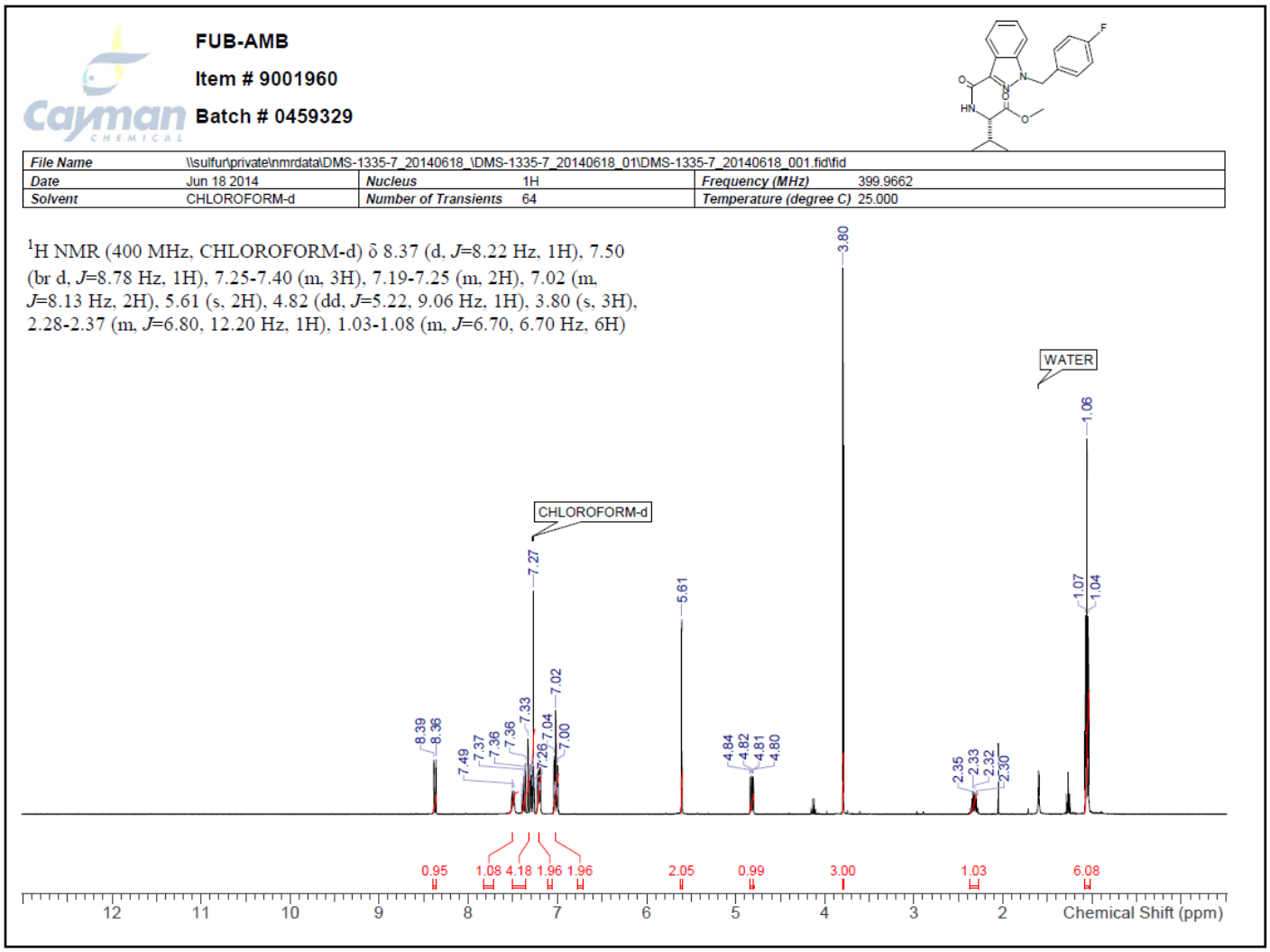


Figure 4. 1H Nuclear Magnetic Resonance Spectroscopy of FUB-AMB, Enhanced for Detail

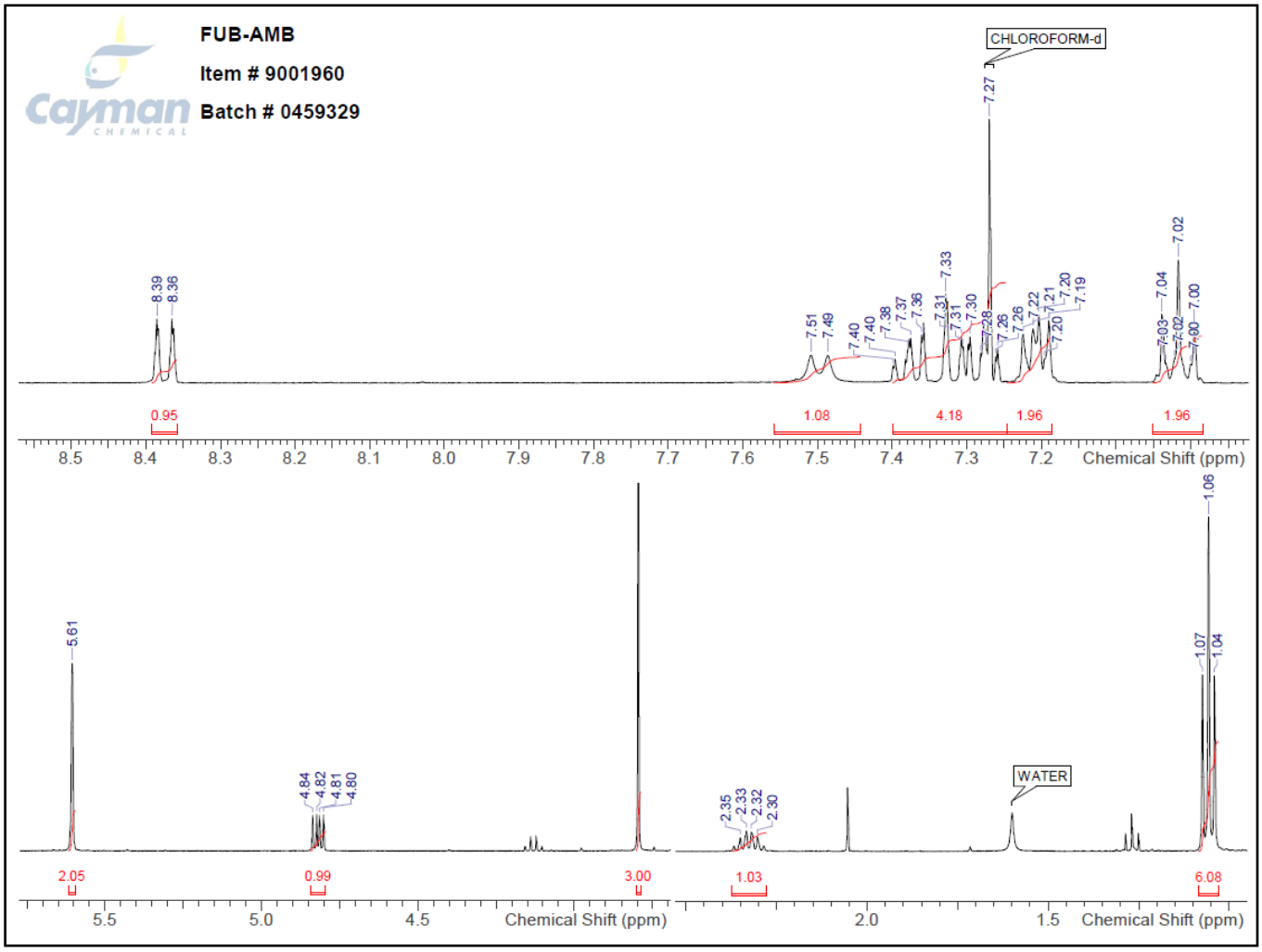
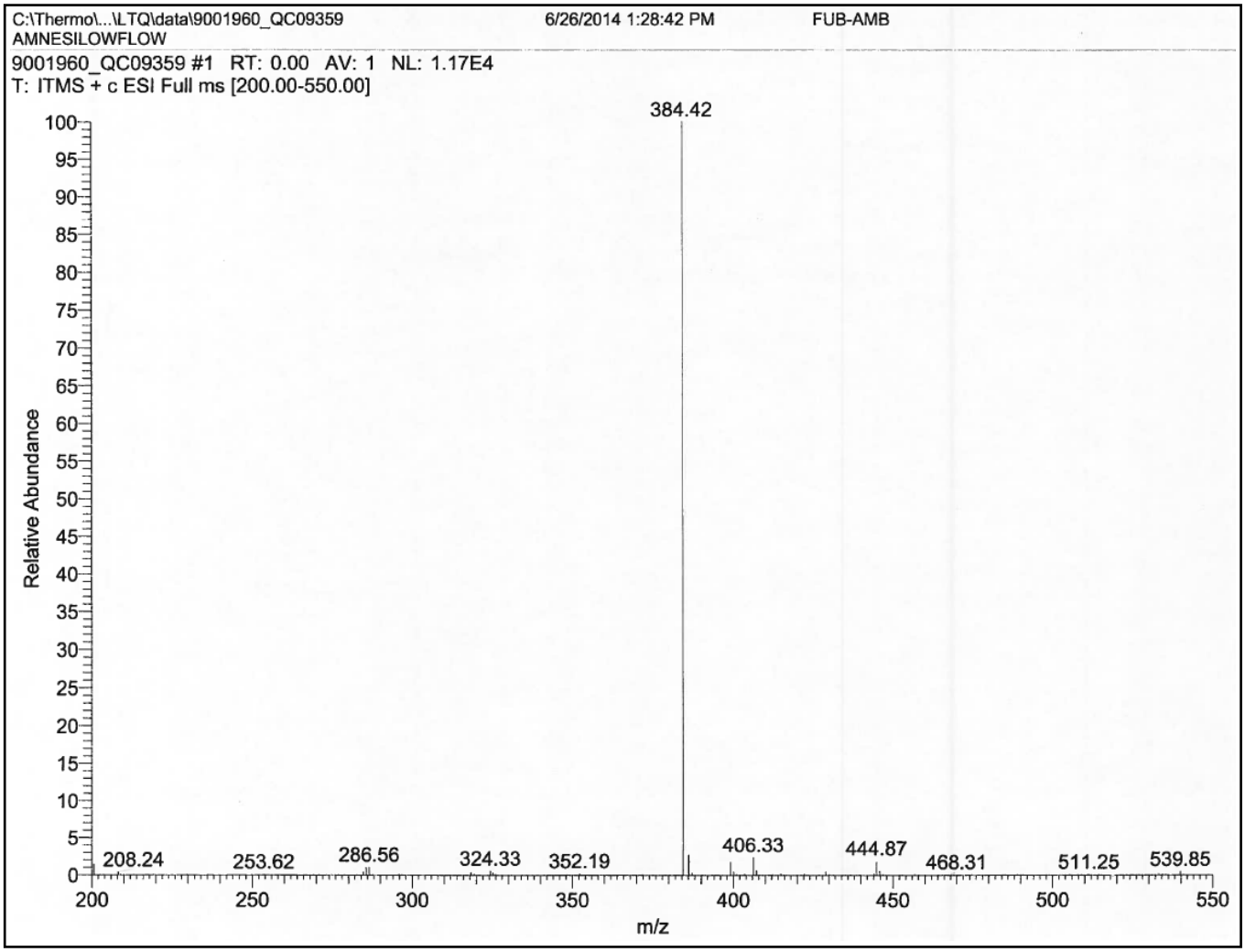
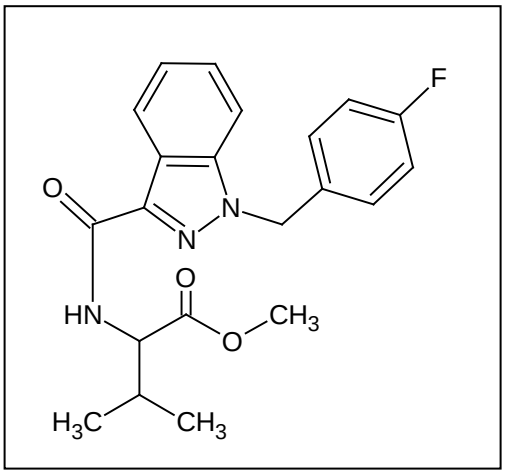


Figure 5. ESI-MS of FUB-AMB

Experiment Parameters:
Instrument: Thermo LCQ Ion Trap MS
Sample Infusion: 500 µl/min
Mode: +ESI
Mass range: 200-550 amu
Capillary Temperature: 275 C



Part 2. Miami Valley Regional Crime Laboratory Data



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SMILES:
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InChl Key: FRFFLYJQPCIIQB-SFHVURJKSA-N

InChl: InChI=1S/C21H22FN3O3/c1-13(2)18(21(27)28-3)23-20(26)19-16-6-4-5-7-17(16)25(24-19)12-14-8-10-15(22)11-9-14/h4-11,13,18H,12H2,1-3H3,(H,23,26)/t18-/m0/s1

GAS CHROMATOGRAPHY / MASS SPECTROMETRY:

Sample Preparation: Approximately 1mg/mL in Methanol

Instrument: Agilent 7890A GC/5975C MSD

GC Parameter: **Column:** HP-1MS 30m x 0.250mm x 0.25µm

Carrier Gas: Helium

Oven Program: 240°C for 2 min

20°C/min to 300°C-Hold for 15 min

Injection parameter: **Injector Volume:** 1µL

Split ratio: 50:1

MS Parameters: **Temperatures:**

Injector: 250°C

MSD transfer line: 250^{o}C

MS Source: 230^{o}C

MS Quad: 150^{o}C

Mass Scan Range: 40-550amu

Threshold: 150

Tune File: atune.u

Figure 6: Gas Chromatography/Mass Spectrometry of FUB-AMB

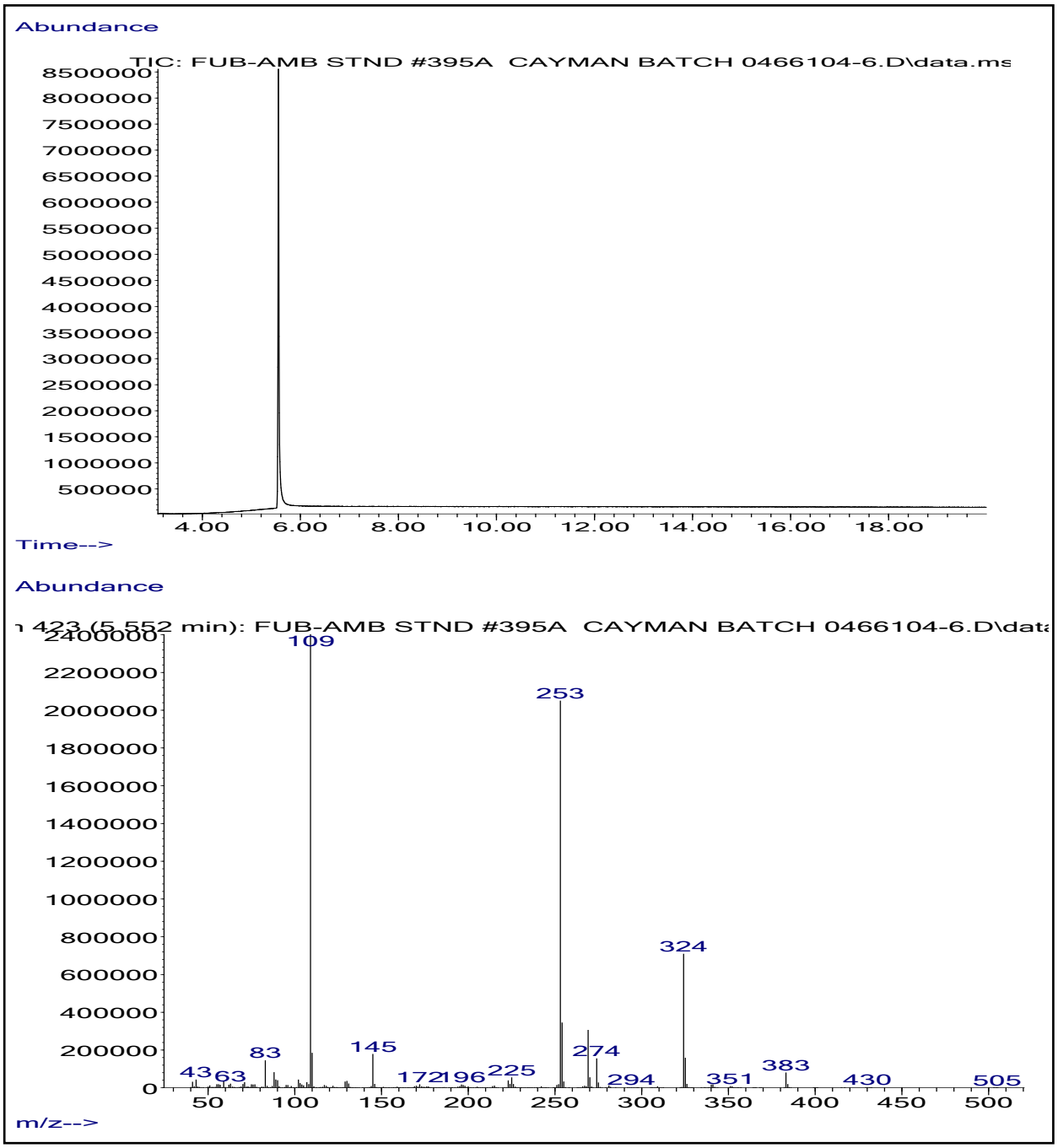
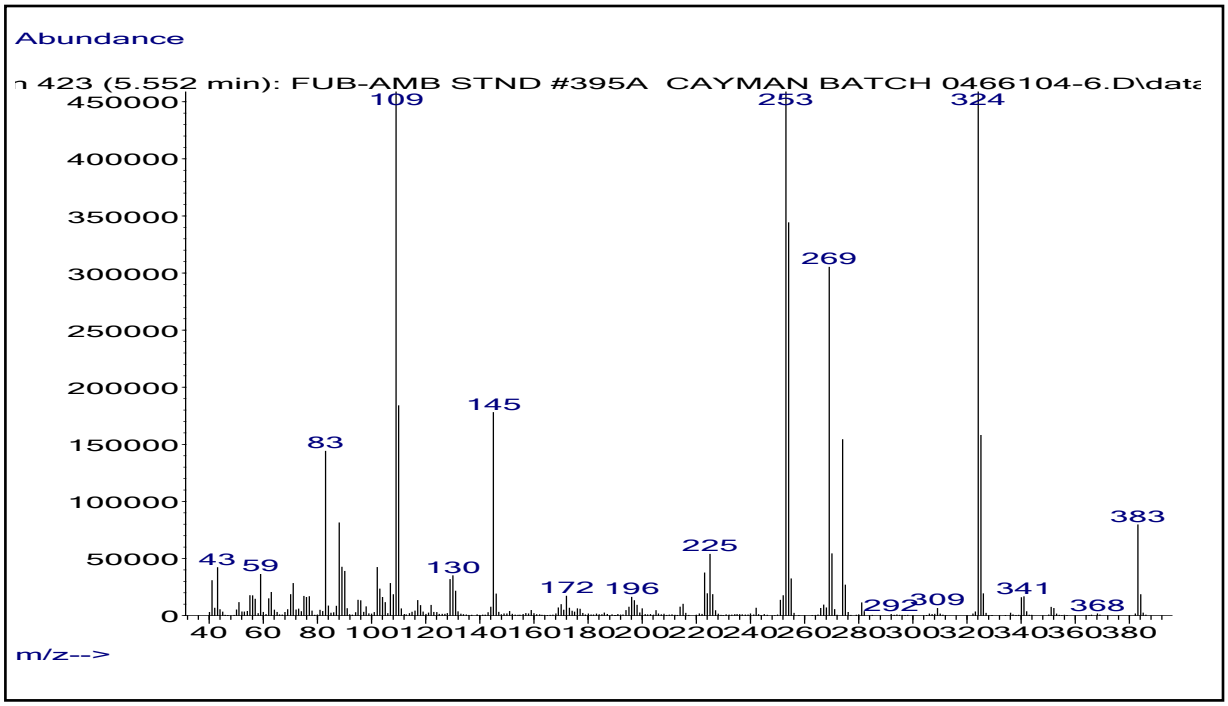


Figure 7: Expanded GC/MS of FUB-AMB



GAS CHROMATOGRAPHY/INFRARED SPECTROSCOPY (SOLID PHASE):

Sample Preparation: Approximately 2mg/mL in Methanol

Instrument: Spectra Analysis DiscovIR-GC

Parameters:

GC Parameters:

Column: HP-5MS 30m x 0.250mm x 0.25µm
Carrier Gas: He
Split Mode: SPLIT
Split Ratio: 3:1
Oven Program: 240°C for 2 min. Then 20°C/min to 300°C for 13 minutes

Injection Parameters:

Injection Volume: 1µL
Injection Port Temperature: 250°C

IR Parameters:

Transfer Line: 325°C
Oven: 325°C
Restrictor: 325°C

Disk: -40°C

Figure 8: DiscovIR-GC Gas Chromatogram of FUB-AMB

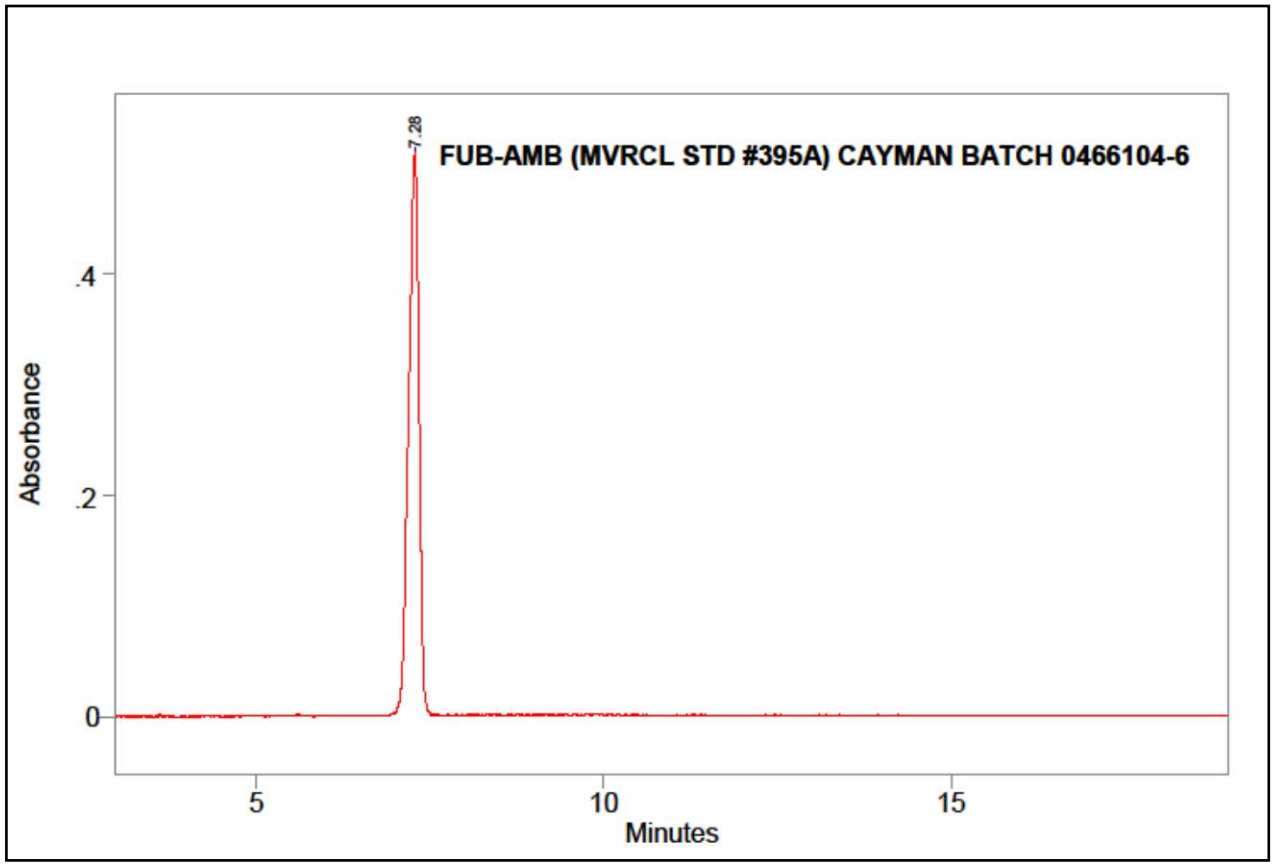


Figure 9: DiscovIR-GC IR Spectrum of FUB-AMB

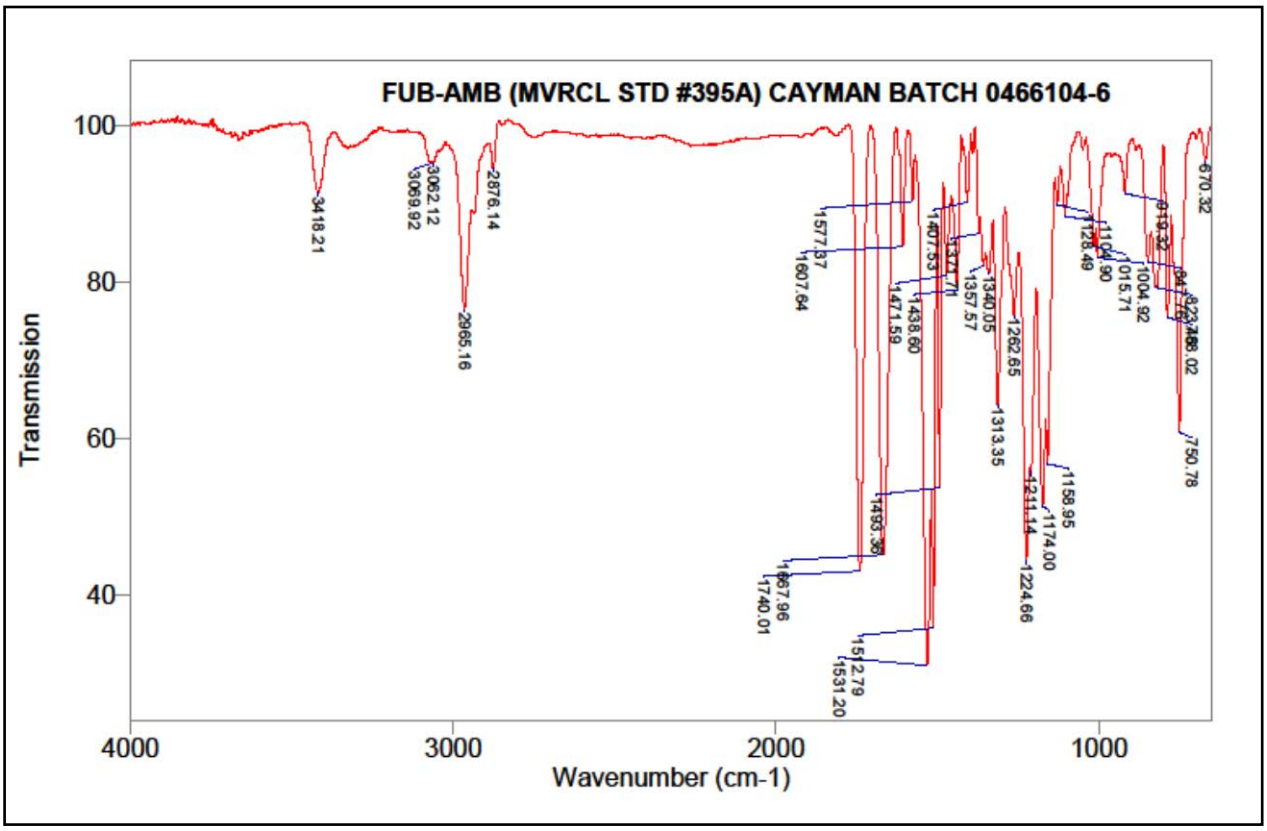
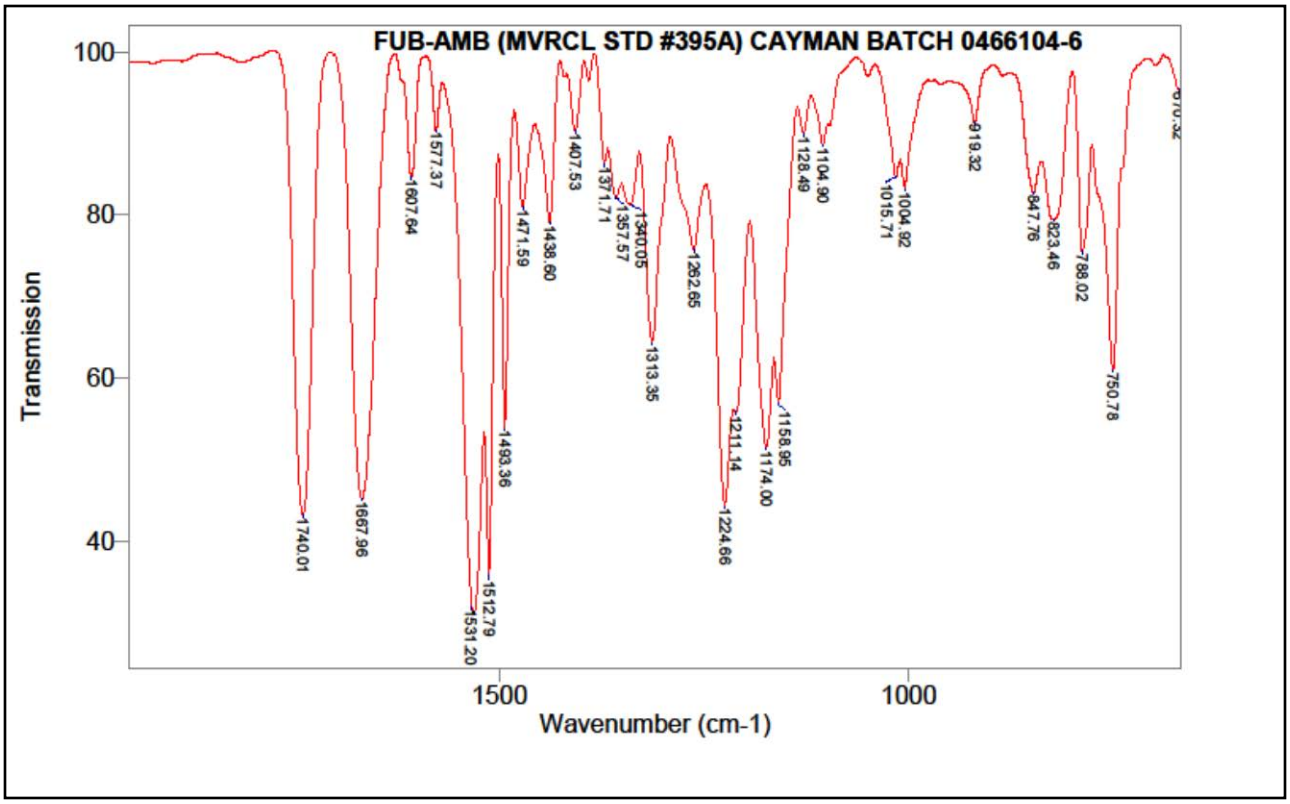


Figure 10: Expanded DiscovIR-GC IR Spectrum of FUB-AMB



Part 3. Reference:

Forendex