Characterization of AM2201 Benzimidazole Analog (FUBIMINA)

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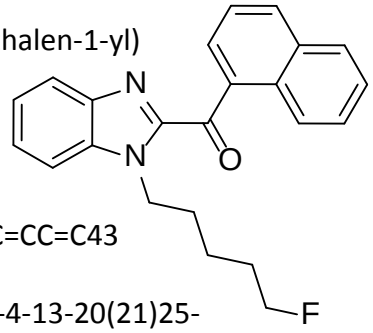
Table of contents:

Part 1. Cayman Chemical Company Data

Compound Information

Name: AM2201 benzimidazole analog

Synonyms: (1-(5-fluoropentyl)-1H-benzo[d]imidazol-2-yl)(naphthalen-1-yl) methanone; FUBIMINA; FTHJ



CASRegistryNo.: N/A

MF: $C_{23}H_{21}FN_2O$

FW: 360.4

SMILES: O=C(C1=NC2=C(C=CC=C2)N1CCCCCF)C3=CC=CC4=CC=CC=C43

InChI Key: KUESSZMROAFKQJ-UHFFFAOYSA-N

InChI: InChI=1S/C23H21FN2O/c24-15-6-1-7-16-26-21-14-5-4-13-20(21)25-23(26)22(27)19-12-8-10-17-9-2-3-11-18(17)19/h2-5,8-14H,1,6-7,15-16H2

Background

AM2201 Benzimidazole analog is a synthetic cannabinoid designer drug that introduces a benzimidazole in place of the indole central core observed in other structurally similar cannabinoids such as JWH-018 and AM2201. Although the physiological and toxicological properties of this AM2201 benzimidazole analog have not yet been tested, other benzimidazole analogs have been detected in herbal blends and have been shown to be selective CB_2 receptor agonists. The des-fluoro cannabinoid JWH-018 benzimidazole analog was previously identified simultaneously by the Canada Border Services Agency and USACIL in herbal smoking mixtures in late 2013, and subsequently confirmed through independent reference standard synthesis at Cayman Chemical Company.

Figure 1. Liquid Chromatography/Mass Spectrometry

Experiment Parameters:
Thermo Scientific LTQ Orbitrap XL mass spectrometer
Flow injection with an eluent of methanol
Atmospheric-pressure chemical ionization (APCI) in positive mode
Resolution setting of 30 000 (FWHM) at m/z 400 and internal lock mass of 391.2843 for the $[M+H]^+$ for dioctyl phthalate
Full scan: 50-700 m/z

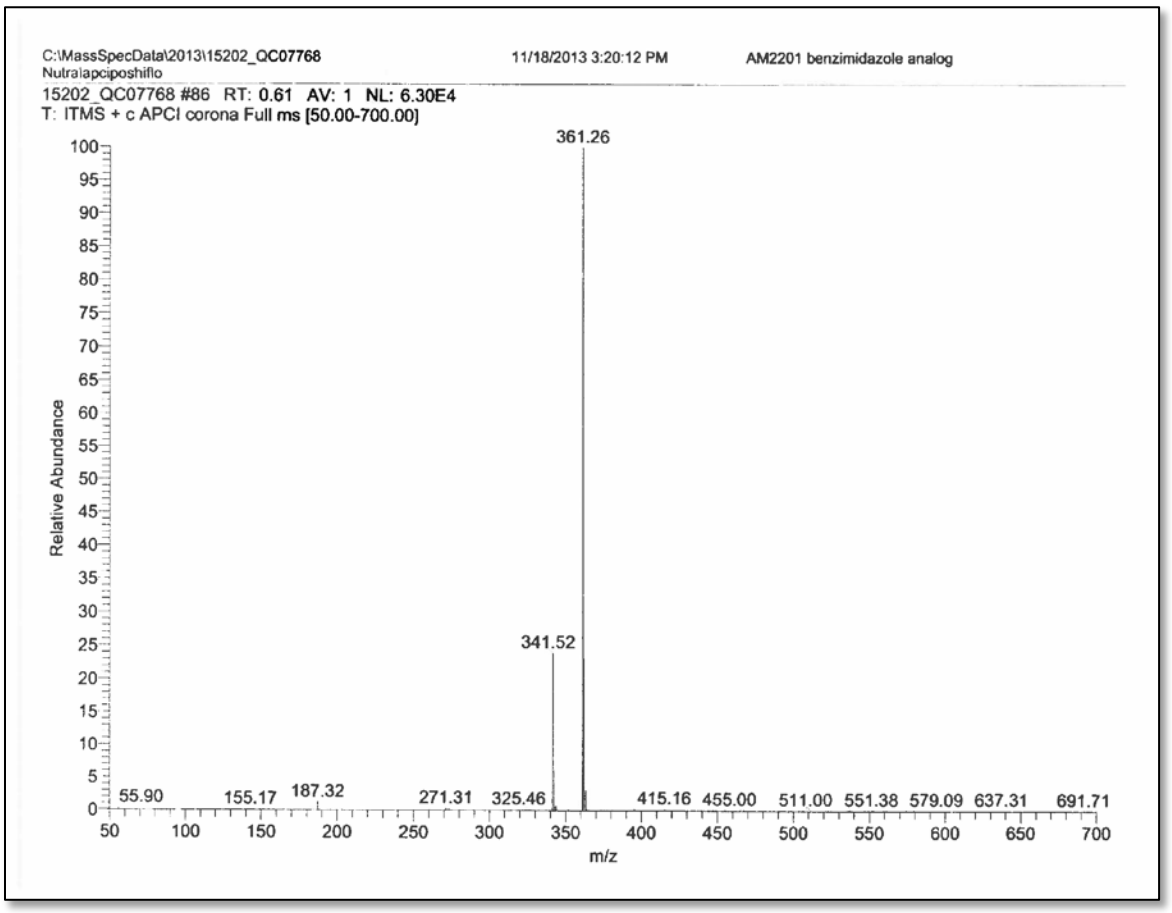


Figure 2. Gas Chromatography/Mass Spectrometry

Experiment Parameters:
Agilent 6890 GC/5973 MSD
15:1 split, 1 mL/min He carrier gas
300°C inlet
30 m x 0.32 mm, 0.5 µm Rtx-5MS column
240°C, ramp 30°C/min to 300°C (hold for 1 min, ramp, hold for 25 min)

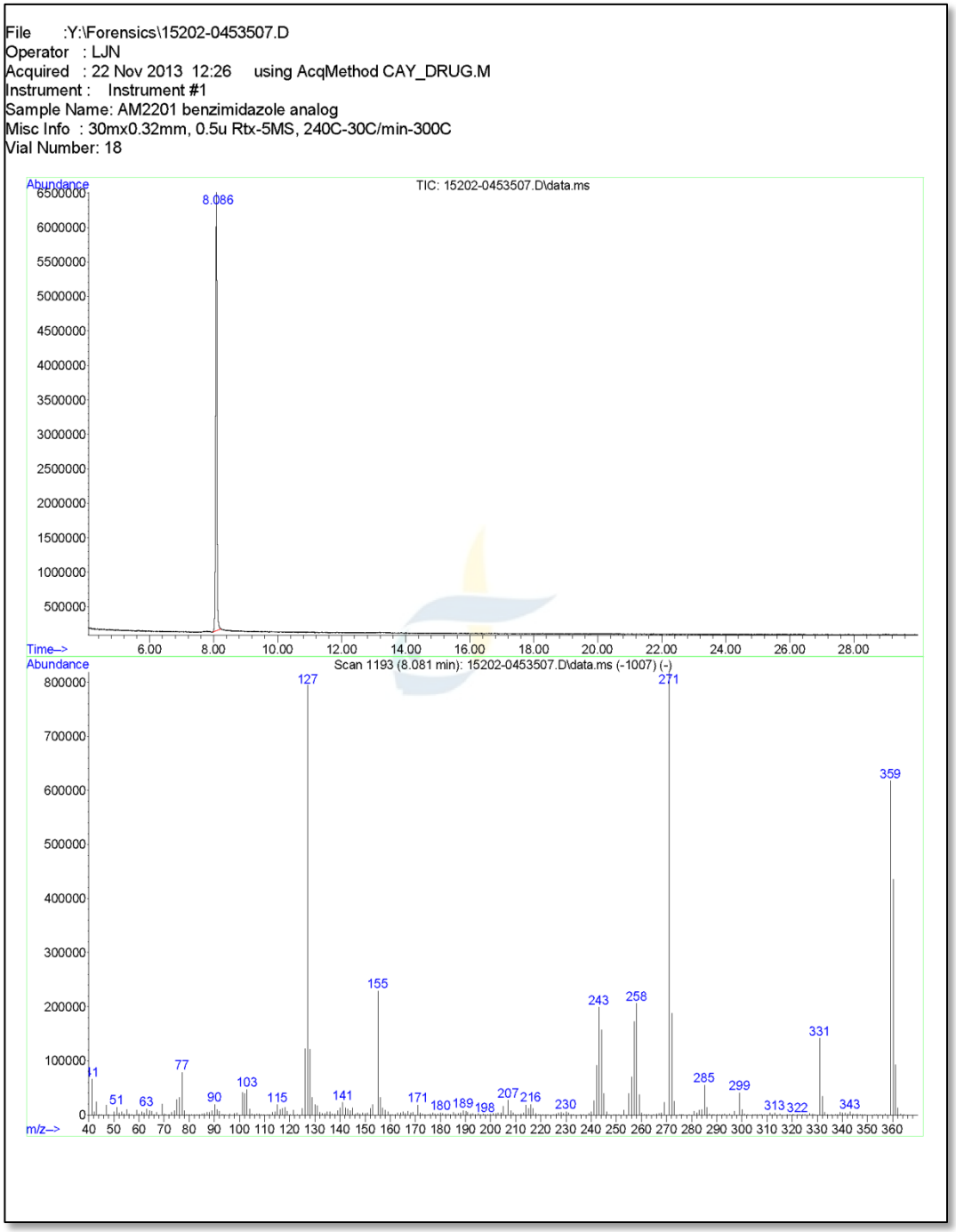


Figure 3. Fourier transform infrared spectroscopy

Experiment Parameters:
PerkinElmer Spectrum 65
Sample prepared as KBr pellet
Range: 4000-600 cm^{-1}, 16 scans, 4 cm^{-1} resolution

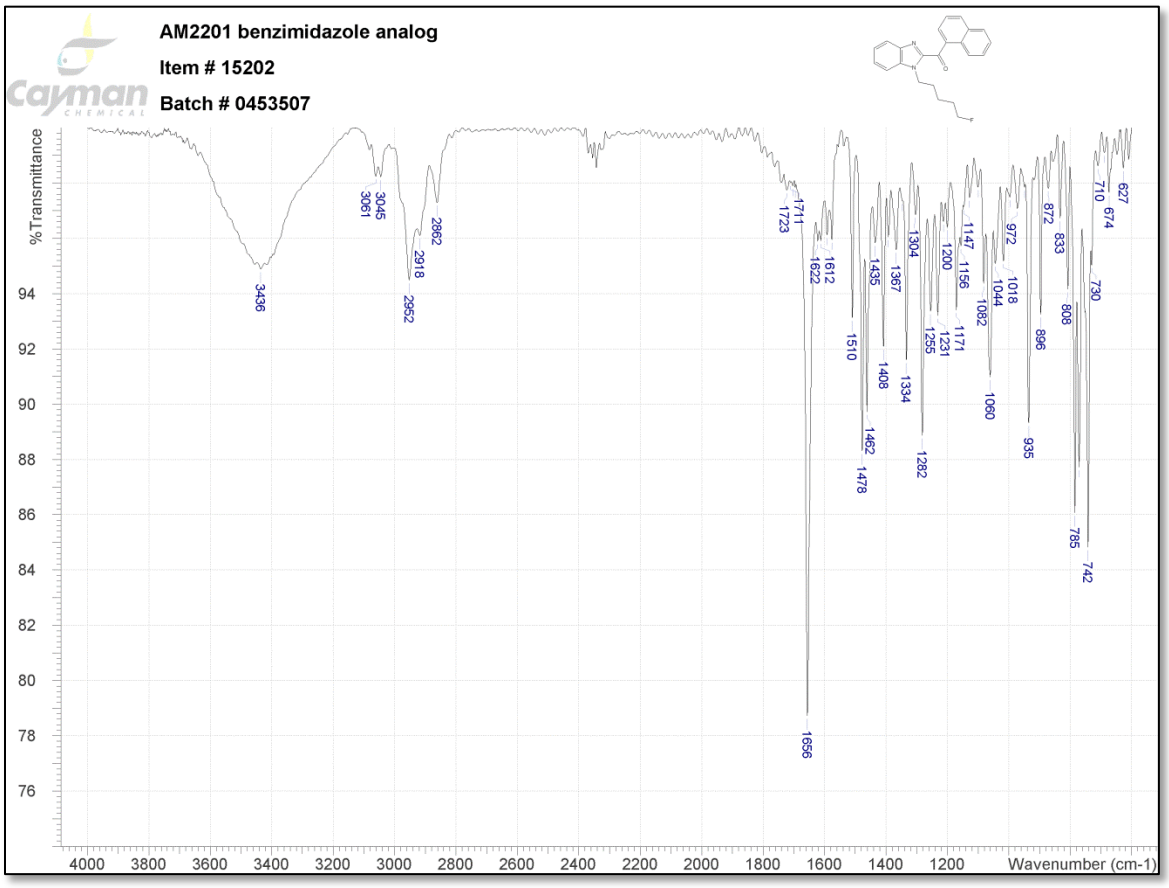


Figure 4. ^{1}H Nuclear Magnetic Resonance Spectroscopy

Experiment Parameters:
Varian ^{UNITY}INOVA 400 MHz Spectrometer with Oxford magnet
Spectrum set to solvent peak at 7.26ppm ($CDCl_3$)

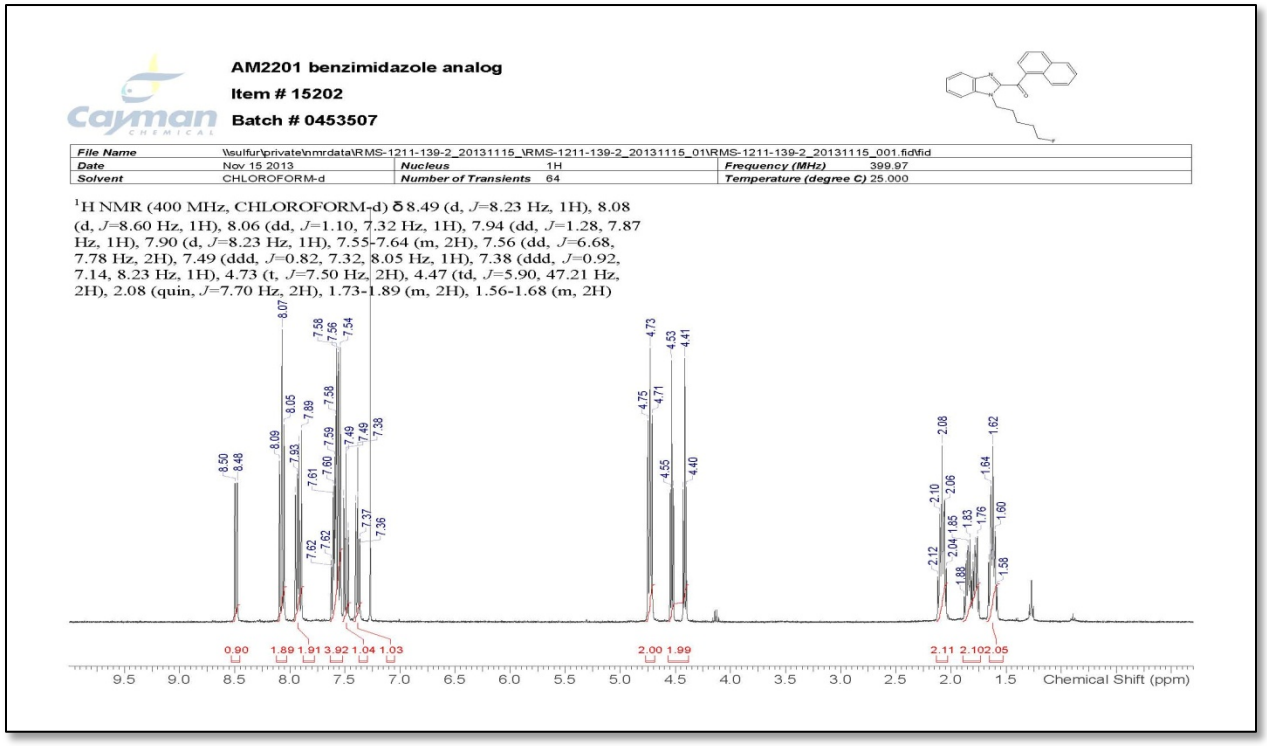
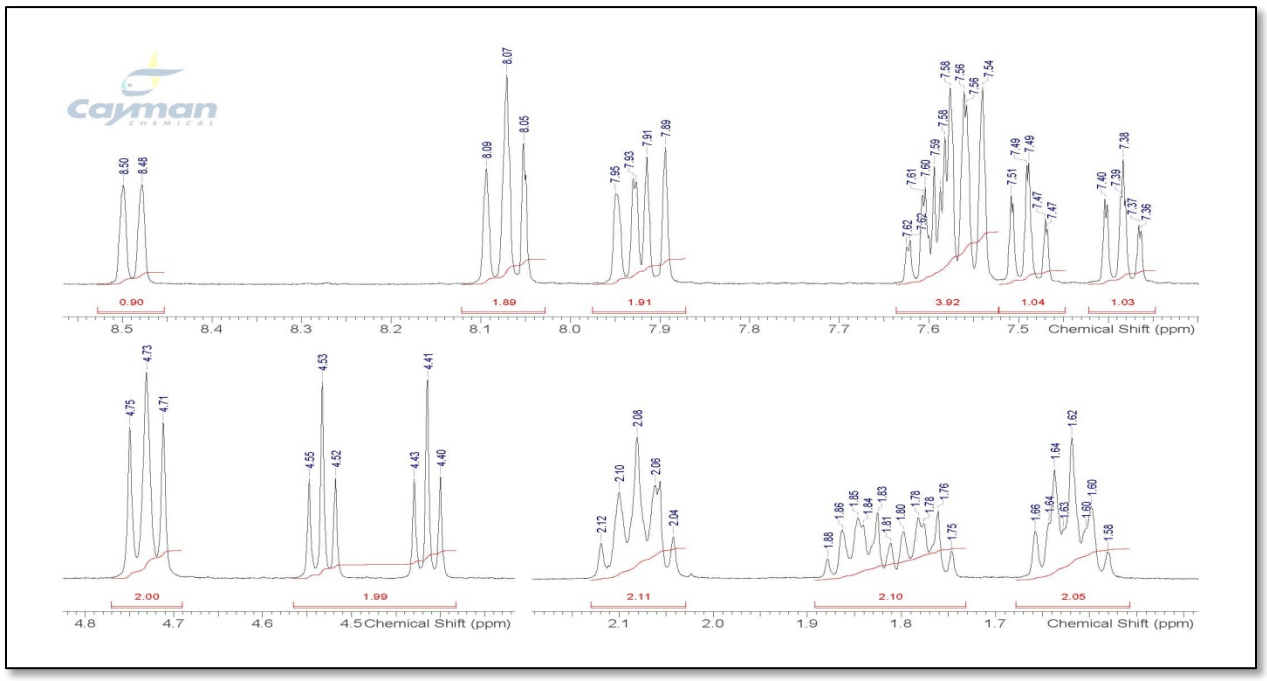


Figure 5. ^{1}H Nuclear Magnetic Resonance Spectroscopy, Enhanced for Detail



Part 2. Kentucky State Police Eastern Laboratory Branch Data

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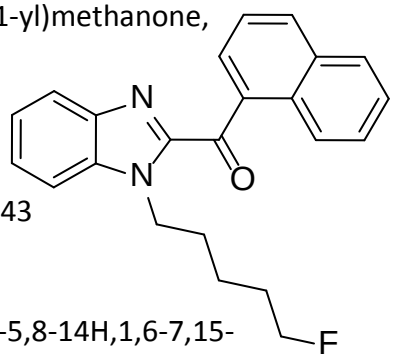

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Gas chromatography / Mass spectrometry:

Sample Preparation: < 1mg/mL in Methanol

Instrument Agilent gas chromatograph operated in split mode with MS detector**:**

GC Parameter:

Column: Zebron ZB-DRUG-1 (10m x 0.18mm x 0.18µm)

Carrier Gas: Helium

Oven Program: Temperature Program: 100°C initial temperature for 0.5 min, ramp to 280°C at 40°/min, hold final temperature for 8.5 min
Pressure Program: 5psi initial pressure for 0.5 min, ramp to 15 psi at 75psi/min and hold for 6 min, ramp to 40psi at 150psi/min and hold for 0.5 min

Injection parameter: Injector Volume: 1µL **Split ratio:** 25:1

MS Parameters:

Injector 250^{o}C

MSD transfer line: 280^{o}C

MS Source: 230^{o}C

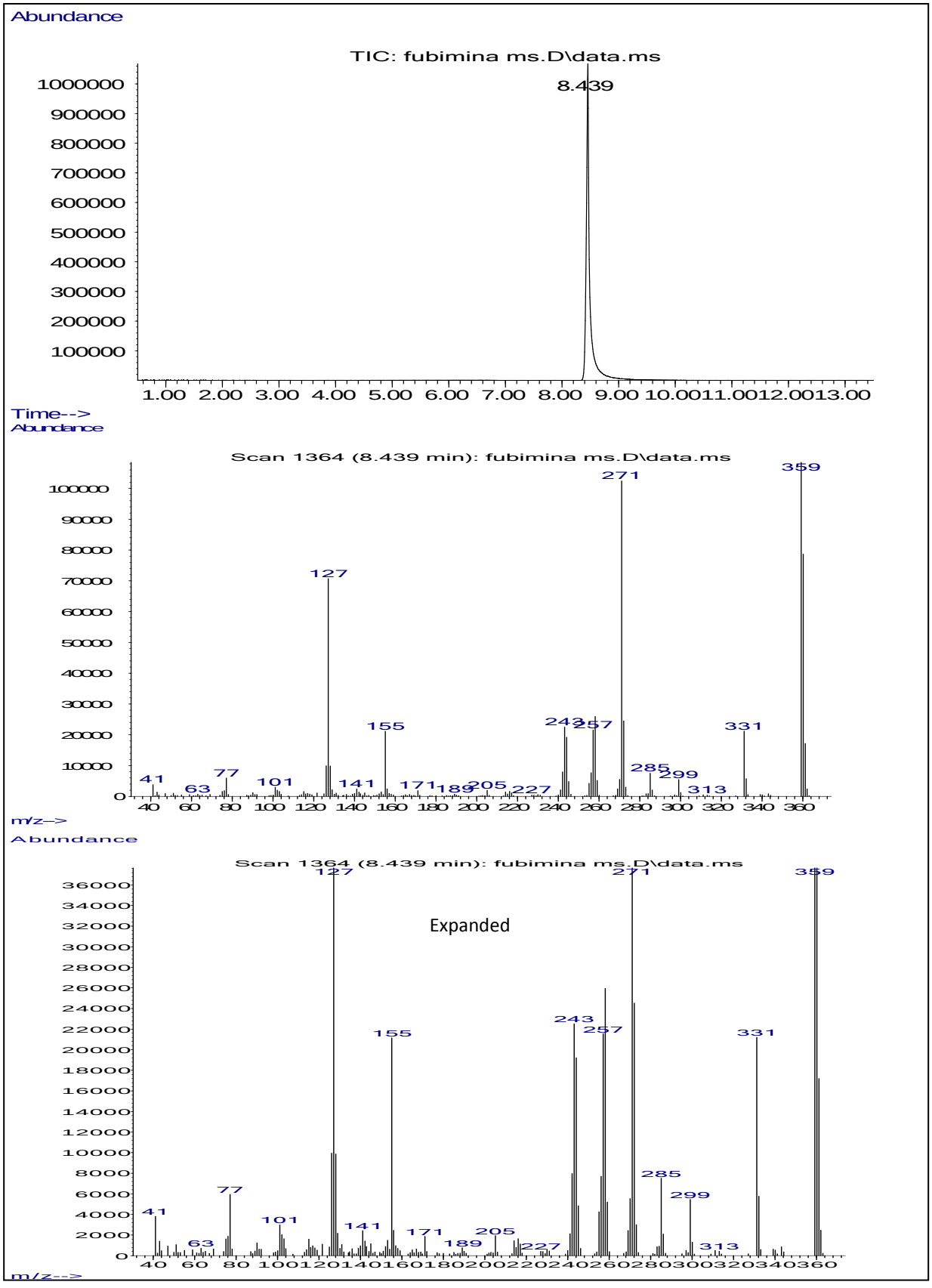
MS Quad: 150^{o}C

Mass Scan Range: 40-550 amu

Threshold: 150

Tune File: atune.u

Figure 6. EI Data



Infrared spectroscopy (ATR)

Instrument: FTIR with diamond ATR attachment

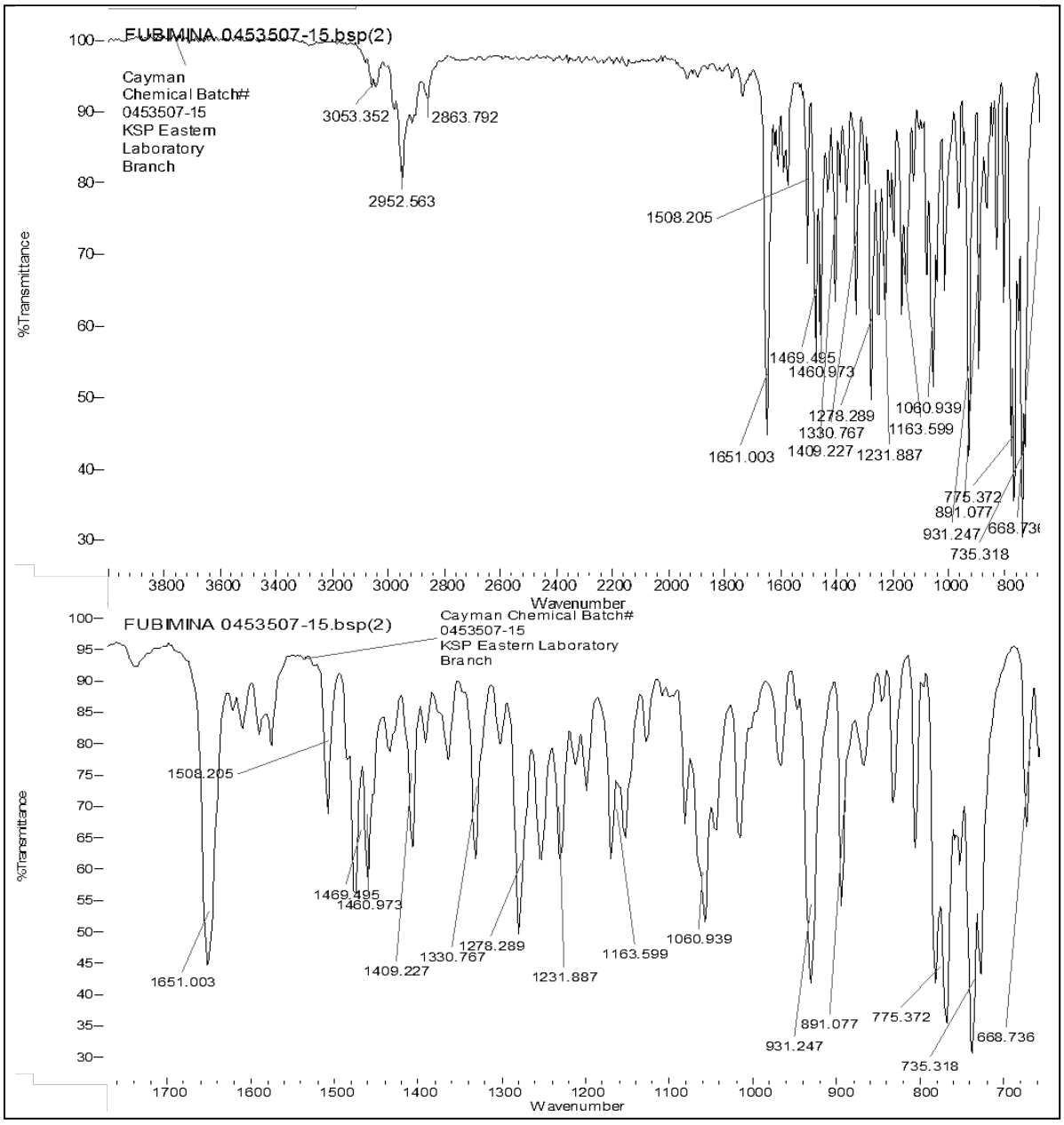
Scan Parameters:

Numbers of Scans: 64

Number of Background Scans: 64

Resolution: 4

Figure 3: FTIR Diamond ATR Data



Part 3.

References:

1. N. Uchiyama, Y. Shimokawa, S. Matsuda, M. Kawamura, R. Kikura-Hanajiri, Y. Goda. Two new synthetic cannabinoids, AM-2201 benzimidazole analog (FUBIMINA) and (4-methylpiperazin-1-yl)(1-pentyl-1H-indol-3-yl)methanone (MEPIRAPIM), and three phenethylamine derivatives, 25H-NBOMe 3,4,5-trimethoxybenzyl analog, 25B-NBOMe, and 25C-N-NBOMe, identified in illefal products. Forensic Toxicol. 32 (2014) 105-115.

2. V. Shevyrin, V. Melkozerov, A. Nevero, O. Eltsov, Y. Morzherin, Y. Shafran. 3-Naphthylindazoles and 2-naphthoylbenzoimidazoles as novel chemical groups of synthetic cannabinoids: Chemical structure elucidation, analytical characteristics and identification of the first representatives in smoke mixtures. Forensic Science International. 242 (2014) 72-80.

External Links:

Forendex link to FUBIMINA