Characterization of 5-Fluoro SDB-005

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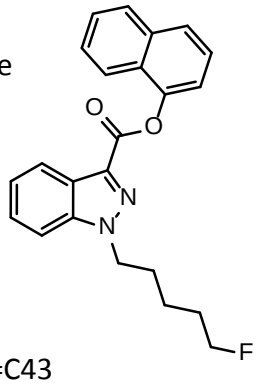
Part 1. Cayman Chemical Company Data

Compound Information

Name: 5-fluoro SDB-005



FormalName: naphthalen-1-yl 1-(5-fluoropentyl)-1H-indazole-3-carboxylate

Synonyms: N/A

CASRegistryNo.: N/A

MF: $C_{23}H_{21}FN_2O_2$

FW: 376.4

SMILES: O=C(OC1=C(C=CC=C2)C2=CC=C1)C3=NN(CCCCCF)C4=CC=CC=C43

InChI Key: FNMFGMMHNFDPNT-UHFFFAOYSA-N

InChI: InChI=1S/C23H21FN2O2/c24-15-6-1-7-16-26-20-13-5-4-12-19(20)22(25-26)23(27)28-21-14-8-10-17-9-2-3-11-18(17)21/h2-5,8-14H,1,6-7,15-16H2

Background:

5-fluoro-SDB-005 is a synthetic cannabinoid similar in structure to THJ-2201, the difference being the replacement of the aryl naphthyl group with a naphthyl ester at the 3 position of the indazole. Biological and toxicological data have not been reported for this compound. It has been observed in our lab that cannabinoids possessing an aromatic ester will slowly degrade when stored in alcohol solvents at room temperature (via transesterification). Acetonitrile or other aprotic solvents are recommended to be used with this structural class of compounds. *It should be noted that the nomenclature of SDB-005 is variable from scholarly publications to commercial and illicit drug websites. Banister et al. categorizes SDB-005 as an analogue of SDB-006, an n-alkylindole with an amide linking the 3 position to a benzyl group.[1] The difference between the two being a benzyl versus a phenyl substituent proximal to the amide linker. However, the structure provided is the common structure listed on illicit drug vendor websites.

1) Banister, S.D., Wilkinson, S.M., Longworth, M., et al. The synthesis and pharmacological evaluation of adamantane-derived indoles: Cannabimimetic drugs of abuse. ACS Chem Neurosci 4(7) 1081-1092 (2013).

Figure 1. Liquid Chromatography/Mass Spectrometry

Experiment Parameters:
Thermo Scientific LTQ Orbitrap XL mass spectrometer
Flow injection with an eluent of methanol
Electrospray ionization (ESI) 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: 230-530 m/z

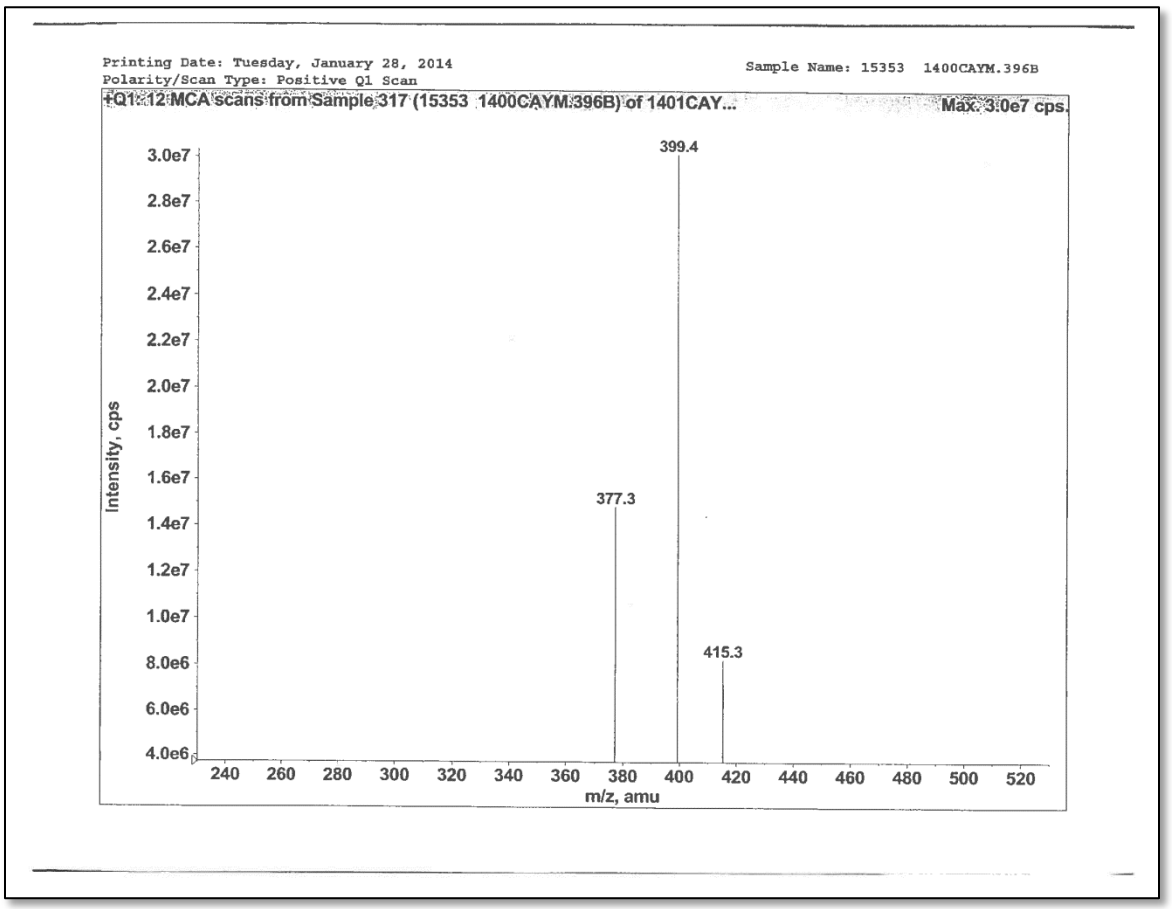


Figure 2. Gas Chromatography/Mass Spectrometry

Experiment Parameters:
Agilent 6890 GC/5973 MSD
15:1 split, 20 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)

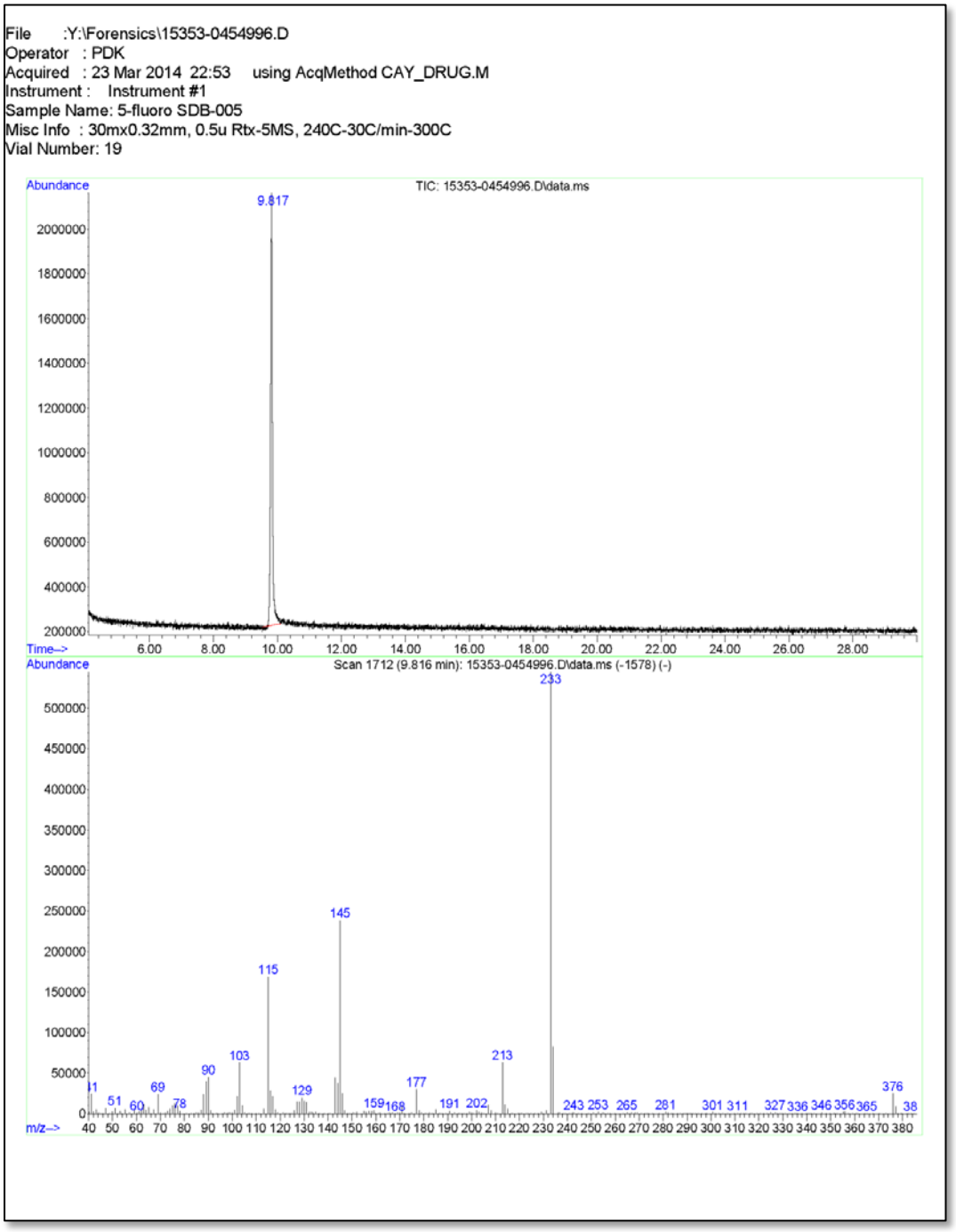


Figure 3. Fourier transform infrared spectroscopy

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

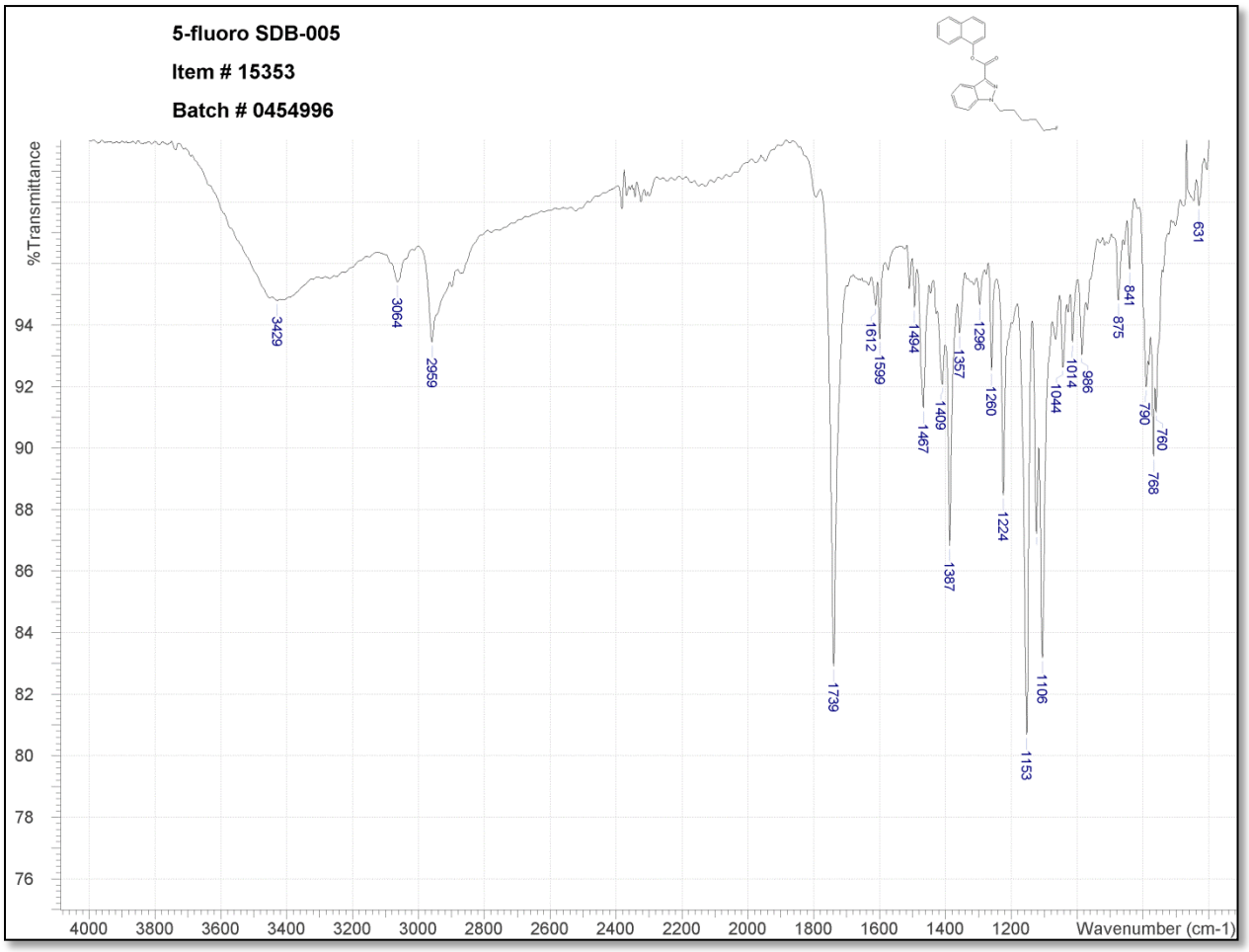


Figure 4. ^{1}H Nuclear Magnetic Resonance Spectroscopy

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

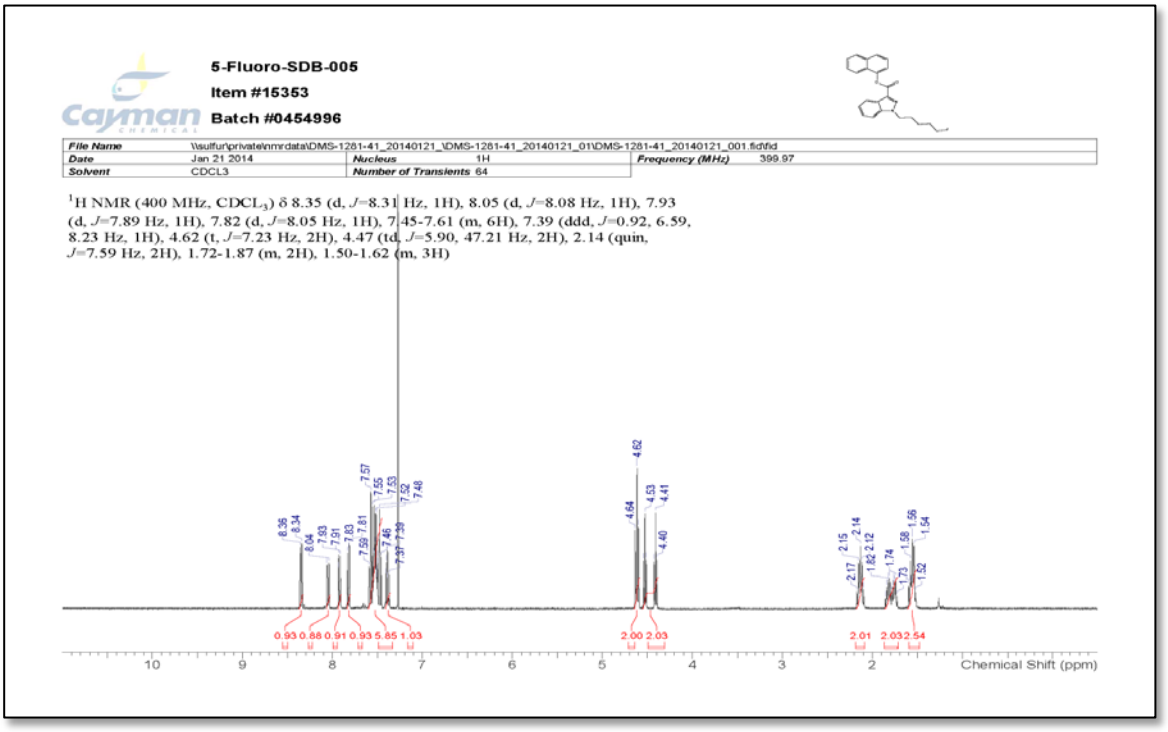
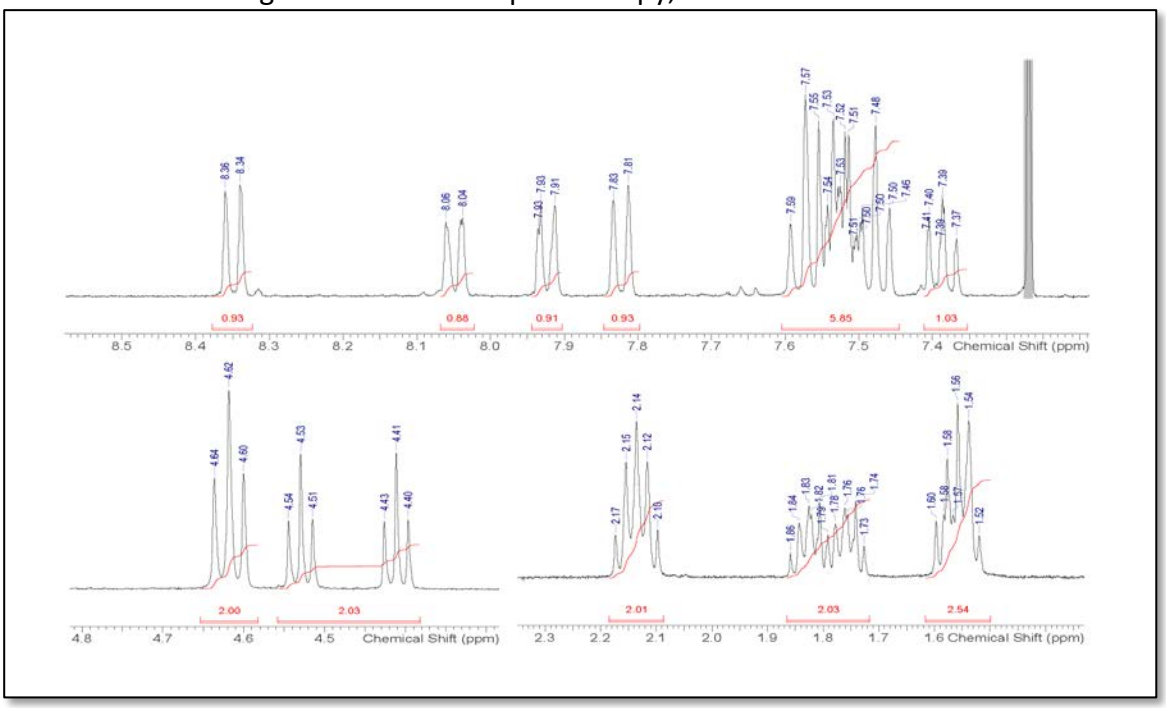


Figure 5. ^{1}H Nuclear Magnetic Resonance Spectroscopy, Enhanced for Detail



Part 2. Ohio Bureau of Criminal Investigation Data

Compound Information

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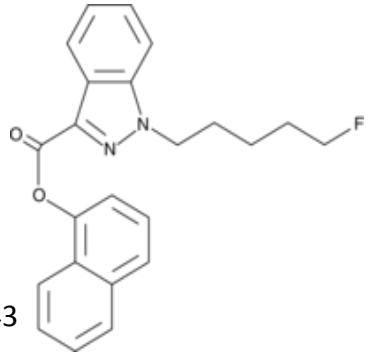

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Gas chromatography/ Mass spectrometry

Sample Preparation: Approximately 1 mg/ml in chloroform. Substantial breakdown of the sample occurred when using methanol. Methanol and other nucleophilic solvents should be avoided.

Instrument: Agilent 7890A GC / 5975C MSD**:**

GC Parameter: **Column:** HP-5MS 30m x .250mm x .25µm

Carrier Gas: Helium

Oven Program:

100°C initial temp, hold 2.0 min, ramp 30°C / min to 305°C, hold for 11.0min

Injection parameter:

Injector Volume: 1uL **Split ratio:** 30:1

MS Parameters: **Injector** 275^{o}C

MS Source: 230^{o}C

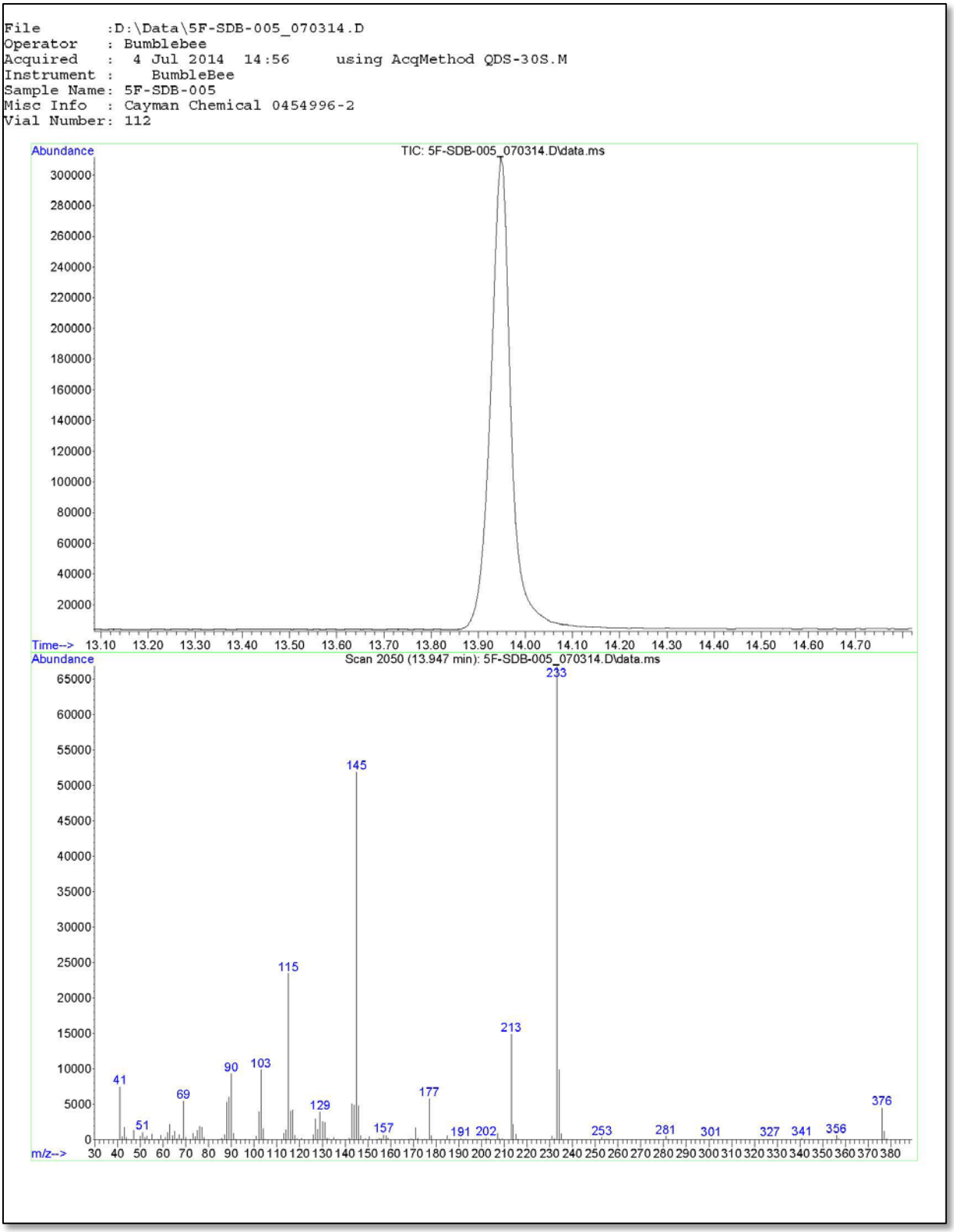
MS Quad: 150^{o}C

Mass Scan Range: 40-500 amu

Threshold: 100

Tune File: stune.u

Figure 6: 5F-SDB-005 GC/MS



Infrared spectroscopy (ATR)

Instrument: Perkin Elmer Spectrum 100 with diamond ATR attachment

Scan Parameters:

Scan Range: 4000 – 450 cm-1

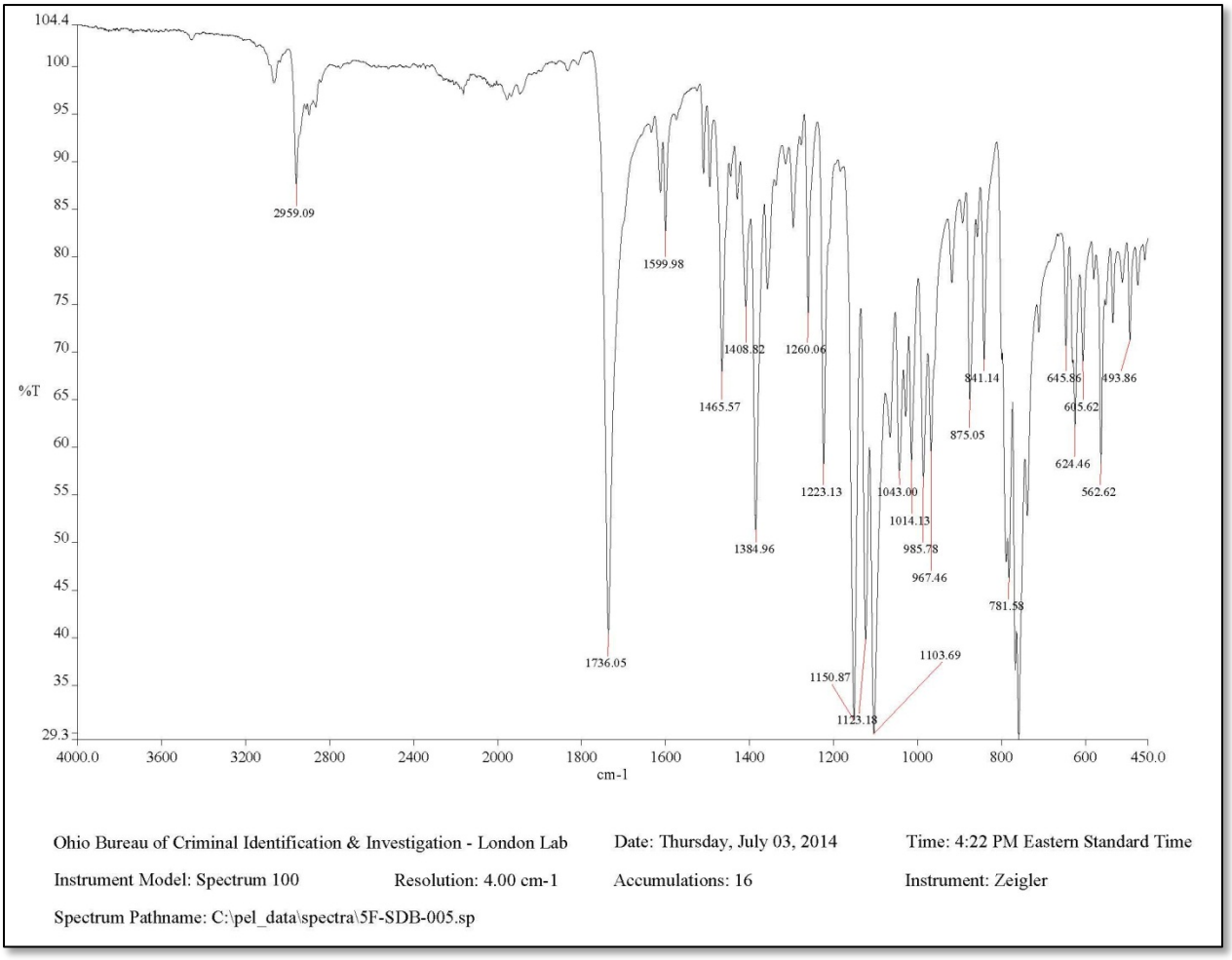
Numbers of Scans: 16

Number of Background Scans: 16

Resolution: 4

Beamsplitter: Autogain

Figure 7: 5F-SDB-005 FTIR



Part 3. External Links:

Forendex link to 5F-SDB-005