Characterization of the Synthetic Cannabinoid ADB-PINACA

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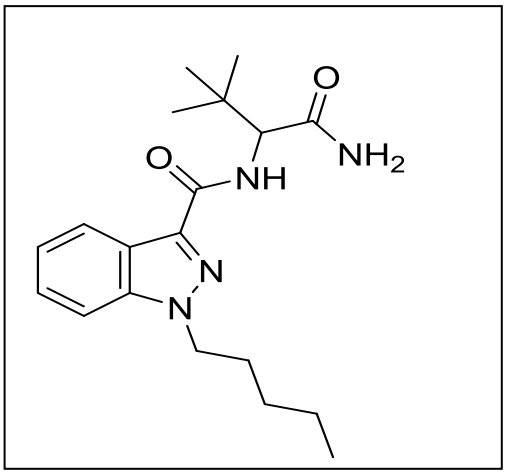
PART 1: CAYMAN CHEMICAL COMPANY DATA

COMPOUND INFORMATION

Name: N-(1-amino-3,3-dimethyl-1-oxobutan-2-yl)-1-pentyl-1H-indazole-3-carboxamide



Synonyms: N/A

CAS#: N/A

Molecular Formula: $C_{19}H_{28}N_4O_2$

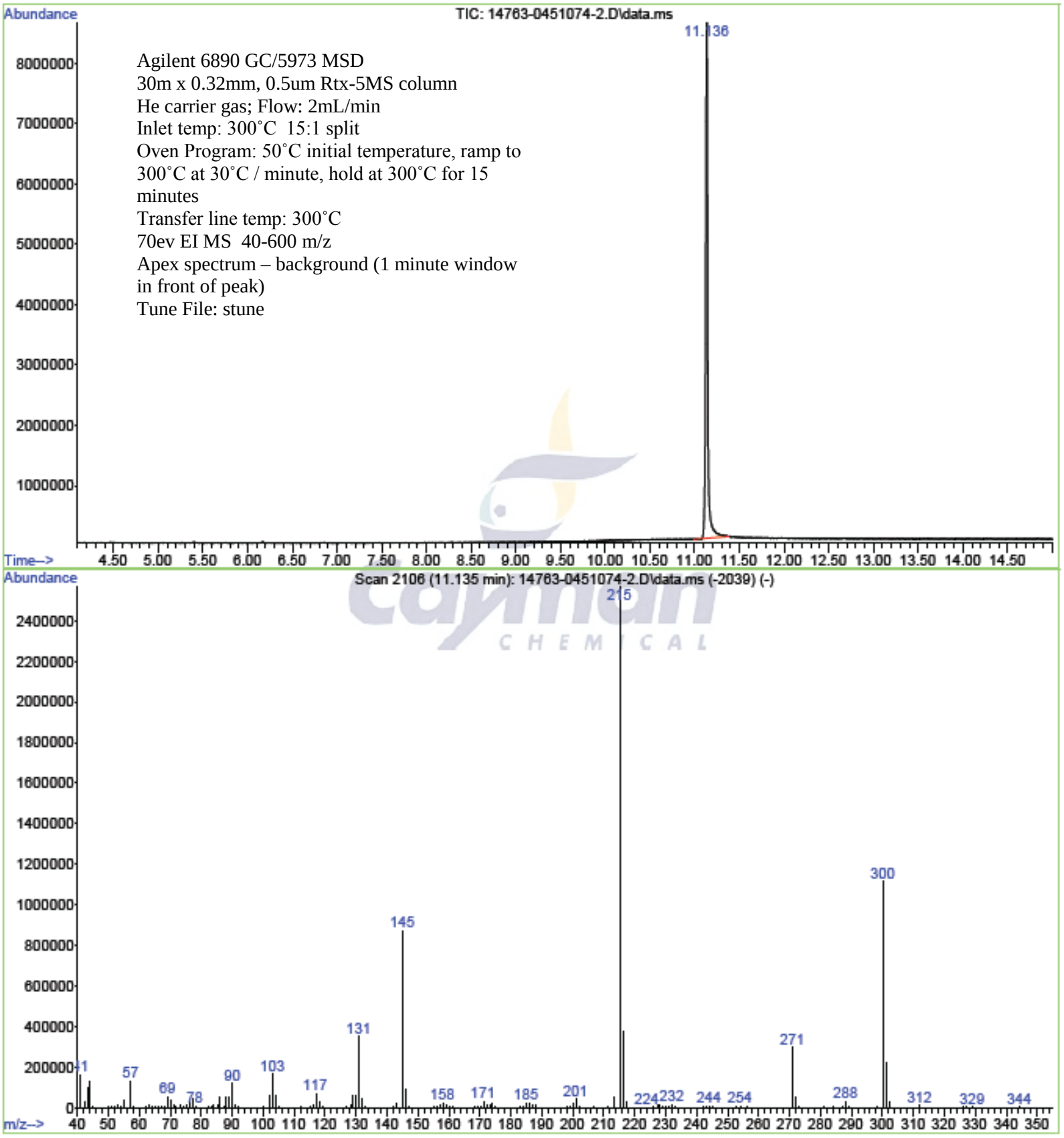
Molecular Weight: 344.50 g/mol

SMILES: O=C(NC(C(N)=O)C(C)(C)C)C1=NN(CCCCC)C2=C1C=CC=C2

InChl Key: FWTARAXQGJRQKN-UHFFFAOYSA-N

InChl: InChI=1S/C19H28N4O2/c1-5-6-9-12-23-14-11-8-7-10-13(14)15(22-23)18(25)21-16(17(20)24)19(2,3)4/h7-8,10-11,16H,5-6,9,12H2,1-4H3,(H2,20,24)(H,21,25)

Figure 1. GC/MS



Agilent 6890 GC/5973 MSD
30m x 0.32mm, 0.5um Rtx-5MS column
He carrier gas; Flow: 2mL/min
Inlet temp: 300˚C 15:1 split
Oven Program: 50˚C initial temperature, ramp to 300˚C at 30˚C / minute, hold at 300˚C for 15 minutes
Transfer line temp: 300˚C
70ev EI MS 40-600 m/z
Apex spectrum – background (1 minute window in front of peak)
Tune File: stune

Figure 2. FTIR

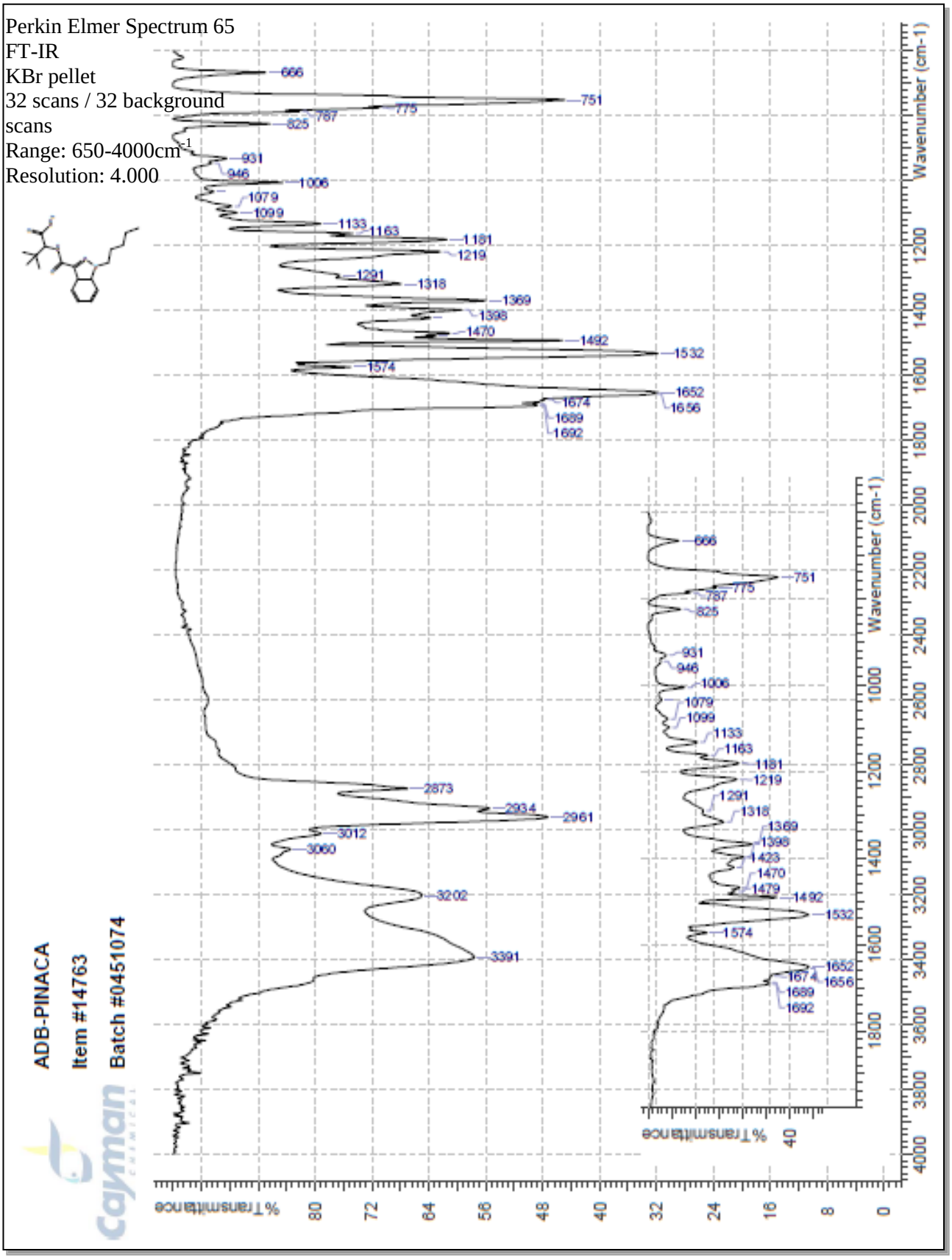
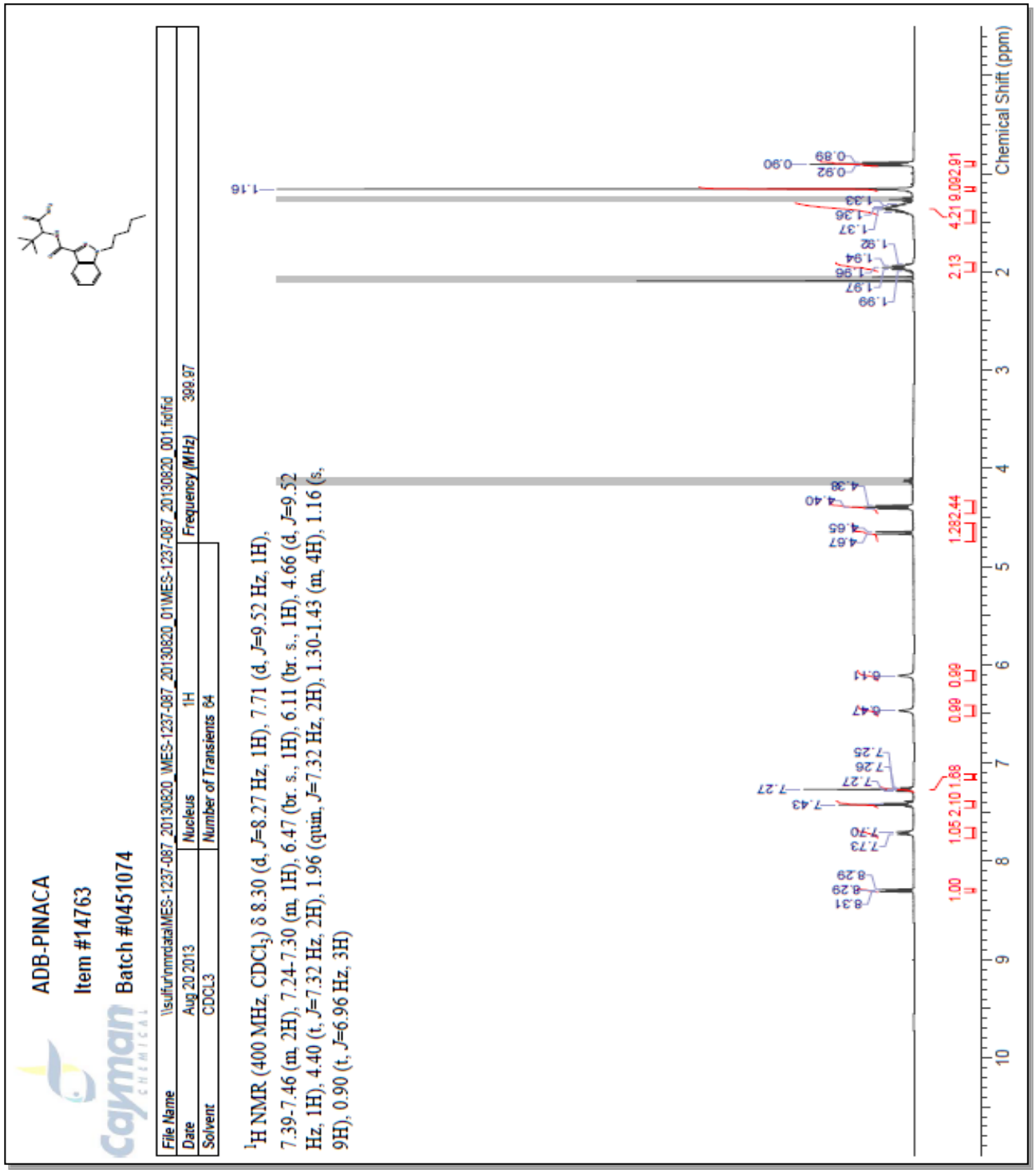


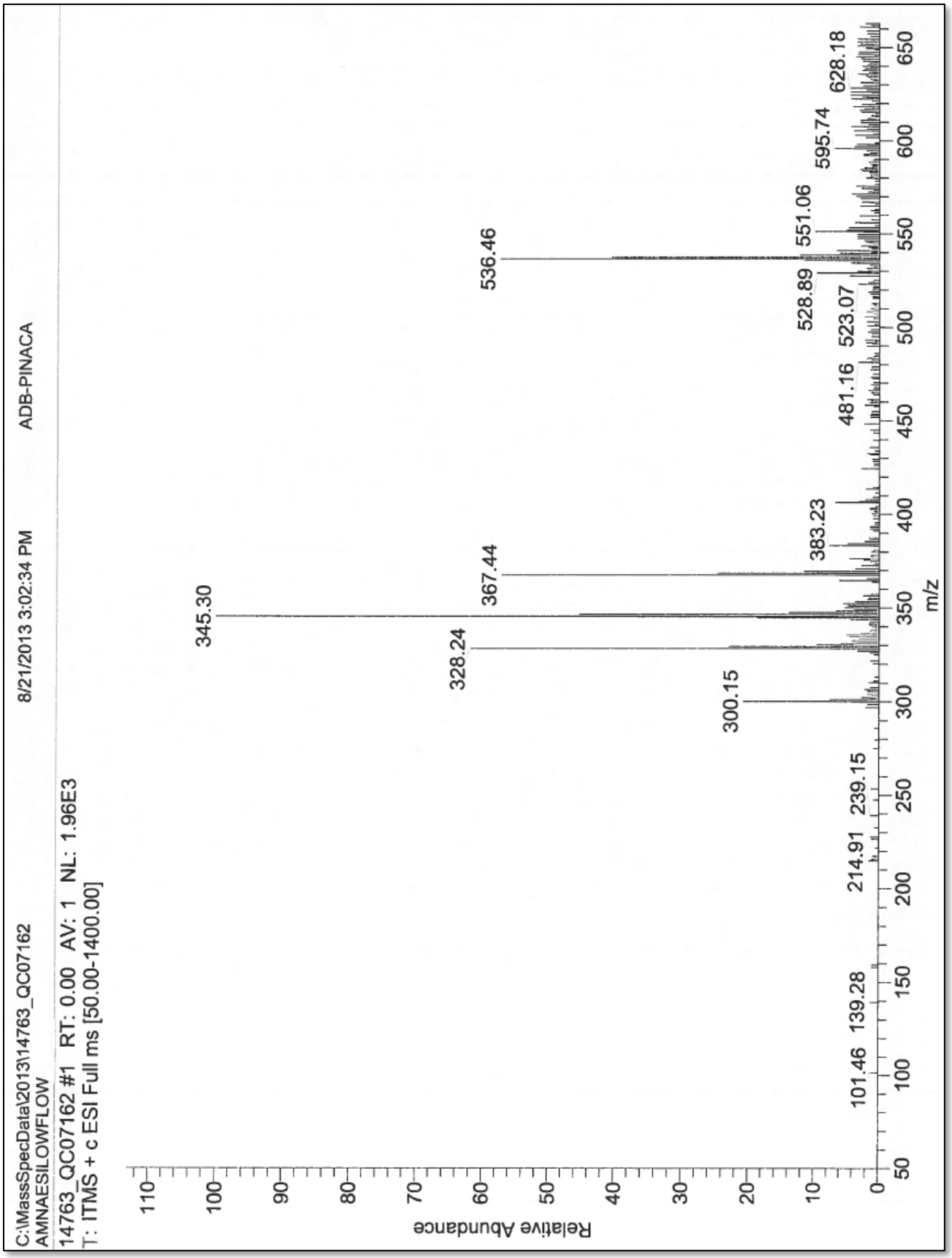
Figure 3. ^{1}H NMR

Varian Inova 400MHz NMR
64 scans



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J*=8.27 Hz, 1H), 7.71 (d, *J*=9.52 Hz, 1H), 7.39-7.46 (m, 2H), 7.24-7.30 (m, 1H), 6.47 (br. s., 1H), 6.11 (br. s., 1H), 4.66 (d, *J*=9.52 Hz, 1H), 4.40 (t, *J*=7.32 Hz, 2H), 1.96 (quin, *J*=7.32 Hz, 2H), 1.30-1.43 (m, 4H), 1.16 (s, 9H), 0.90 (t, *J*=6.96 Hz, 3H)

Figure 4. Positive ESI-MS



PART 2: GBI-DOFS DATA:

COMPOUND INFORMATION

GBI-DOFS purchased a pre-weighed solution of 5mg ADB-PINACA, [N-(1-amino-3,3-dimethyl-1-oxobutan-2-yl)-1-pentyl-1H-indazole-3-carboxamide], in 500µL of methanol from Cayman Chemical – item # 14763, lot # 0451074. The solution was evaporated to dryness and reconstituted in 2mL of acetone. The final concentration was approximately 2.5mg/mL in acetone.*

BACKGROUND:

ADB-PINACA is an emerging designer drug that has been found in synthetic cannabinoid samples. The molecule combines a 1-amino-3,3-dimethyl-1-oxobutan-2-yl (ADB) with a 1-pentyl-1H-indazole-3-carboxamide (PINACA). It differs from AB-PINACA by the replacement of the iso-propyl group with a tert-butyl group. Very little is known about the pharmacological activity of ADB-PINACA in humans or other animals.

GAS CHROMATOGRAPHY / MASS SPECTROMETRY:

Instrument: Agilent 7890A GC / 5975C MSD

GC Parameter:	**Column:** HP Ultra 1 12m x .200mm x .33µm, 100% Dimethylpolysiloxane stationary phase **Carrier Gas:** Helium **Oven Program:** 250°C initial temp, hold for 1 min, ramp 5°C / min to 275°C, hold for 24 min
Injection parameter:	**Injection volume:** 1 uL **Split ratio:** 100:1
MS Parameters:	**Temperature: Injector** 275°C **MSD transfer line:** 280°C **MS Source:** 230°C **MS Quad:** 150°C **Mass Scan Range:** 40-500 amu **Threshold:** 150 **Tune File:** stune.u

* The original document was changed post publication on November 05, 2013 to correct the concentration from 1.25 mg/mL to 2.5 mg/mL.

Figure 5: GBI GC/MS

```
2013-CHEMSTDS  0009
MISC INFO:  ADB-PINACA 090413,
INSTRUMENT: HQ_DI_GCMS#21_03725
SOFTWARE: CHEMSTATION, E.02.01.1177
HIGH.M
 5 Sep 2013  10:19
ALS VIAL:      52
Inj. Vol:  1 µL
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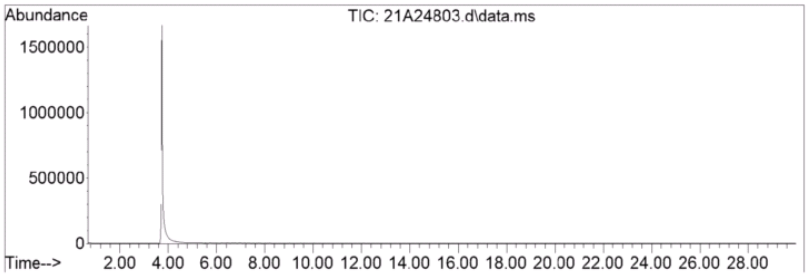
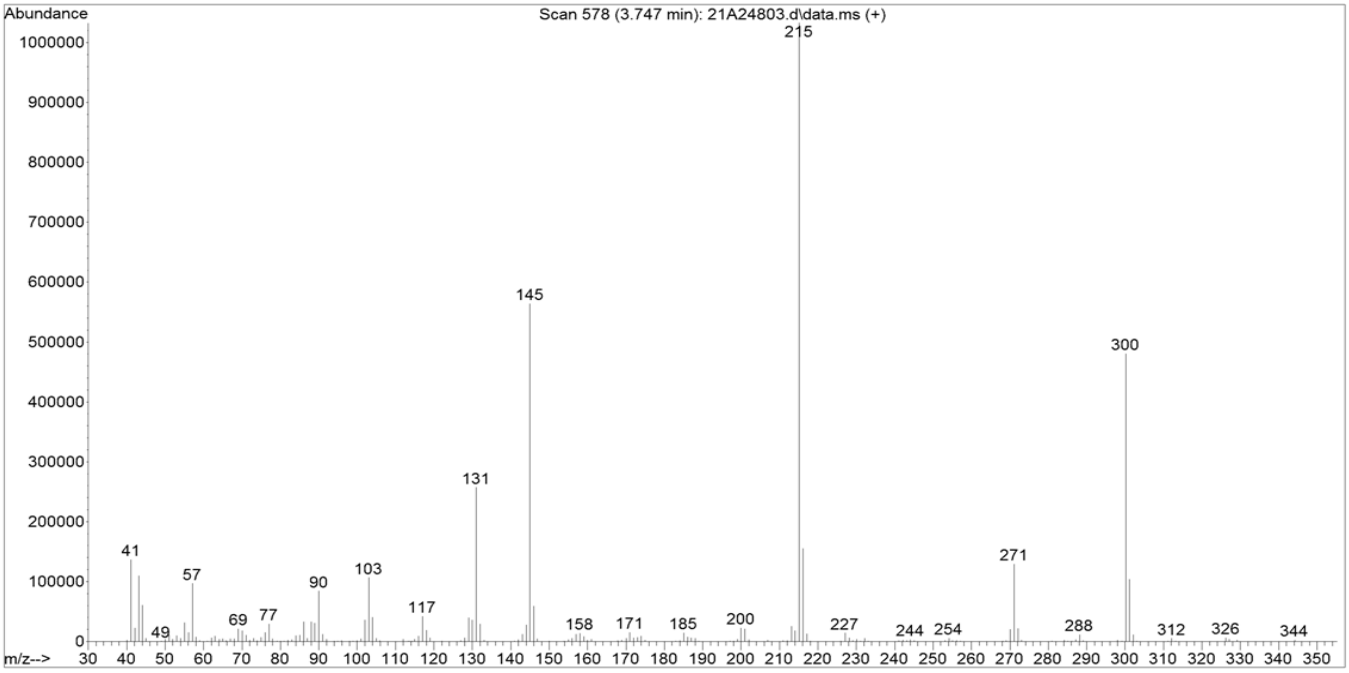
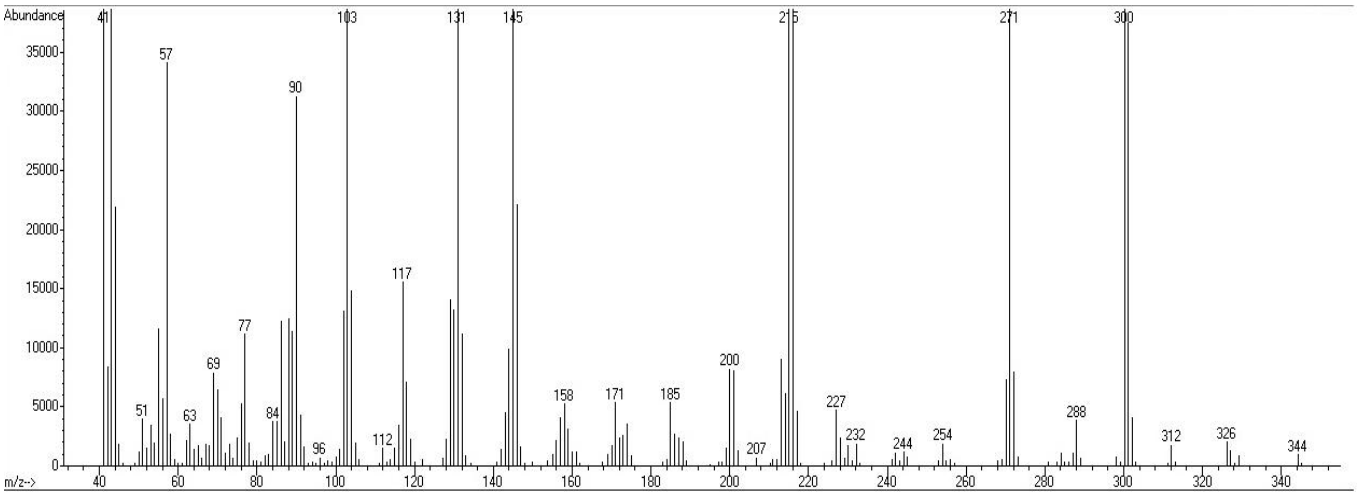




Expanded Mass Spectrum



GAS CHROMATOGRAPHY/INFRARED SPECTROMETRY

Instrument: Agilent 7890 GC / Spectra Analysis DiscovIR

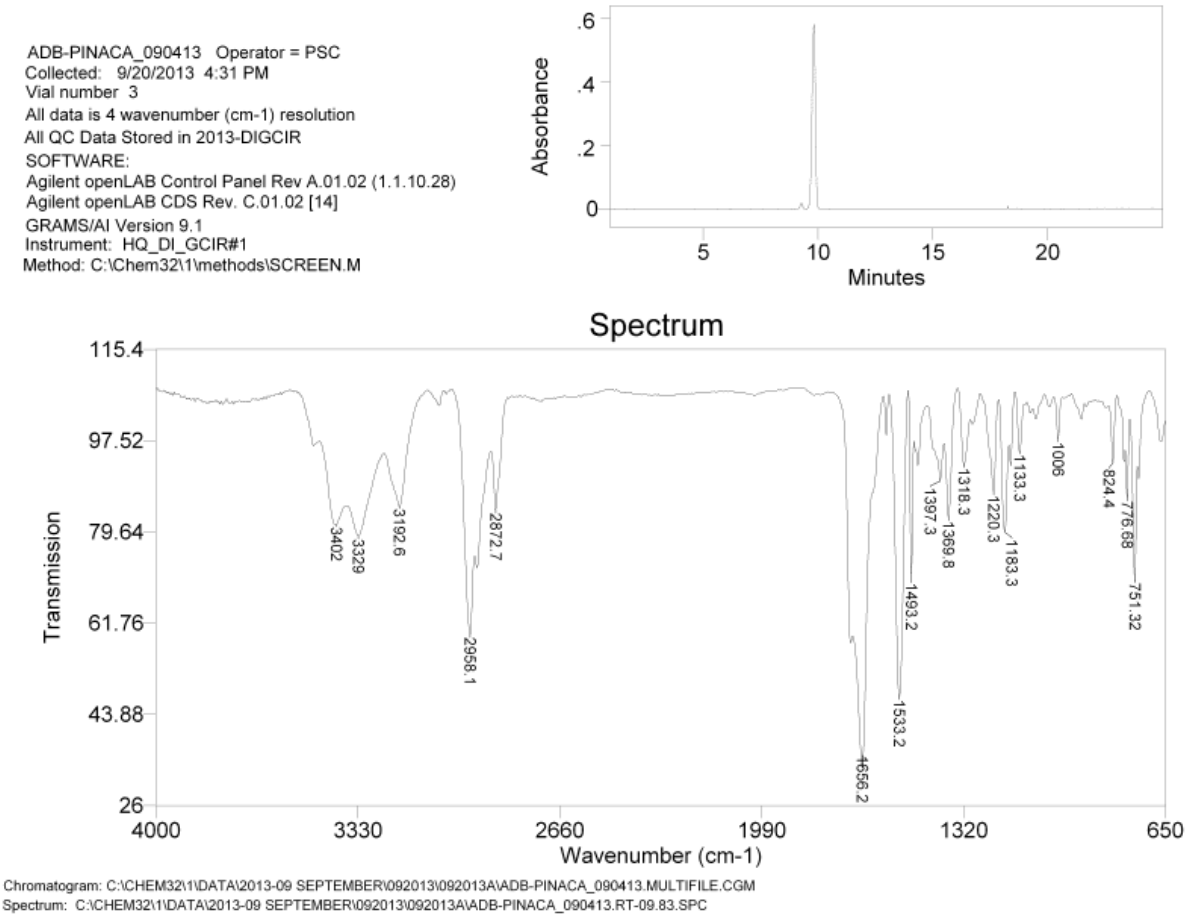
GC Parameter:

Column: HP Ultra 1 12m x .200mm x .33µm, 100% Dimethylpolysiloxane stationary phase
Carrier Gas: Helium
Oven Program: 70°C initial temp, hold for 2 min, ramp 30°C / min to 275°C, hold for 16.1min

IR Parameter:

Transfer line: 290°C
Restrictor: 290°C
Disk: -40°C +/- 10 °C

Figure 6: GBI GC/IR



PART 3: REFERENCES AND EXTERNAL LINKS

REFERENCES:

1. Uchiyama, N., Matsuda, S., Kawamura, M., Kikura-Hanajiri, R., Goda, Y. "Two new-type cannabimimetic quinolinyl carboxylates, QUPIC and QUCHIC, two new cannabimimetic carboxamide derivatives, ADB-FUBINACA and ADBICA, and five synthetic cannabinoids detected with a thiophene derivative α-PVT and an opioid receptor agonist AH-7921 identified in illegal products" *Forensic Toxicology*, March 2013.
2. Uchiyama, N., Matsuda, S., Wakana, D., Kikura-Hanajiri, R., Goda, Y. "New cannabimimetic indazole derivatives, *N*-(1-amino-3-methyl-1-oxobutan-2-yl)-1-pentyl-

1*H*-indazole-3-carboxamide (AB-PINACA) and *N*-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(4-fluorobenzyl)-1*H*-indazole-3-carboxamide (AB-FUBINACA) identified as designer drugs in illegal products" *Forensic Toxicology*, November 2012.

EXTERNAL LINKS:

Forendex ADB-PINACA page

Forendex ADBICA page

Forendex ADB-FUBINACA page

SWGDRUG AB-FUBINACA monograph

SWGDRUG 5F-AB-PINACA monograph