Characterization of the synthetic cannabinoid AB-CHMINACA

David M. LaGory, Donna M. Iula, Cayman Chemical Company, Ann Arbor, MI 48108

Carolyn Trader-Moore, Kentucky State Police Eastern Laboratory Branch, Ashland, KY

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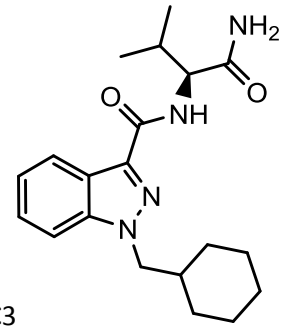
Part 1. Cayman Chemical Company Data

Compound Data

Name: AB-CHMINACA

Synonyms: N-[(1S)-1-(aminocarbonyl)-2-methylpropyl]-1-(cyclohexylmethyl)- 1H-indazole-3-carboxamide



CAS#: 1185887-21-1

Molecular Formula: $C_{20}H_{28}N_4O_2$

Molecular Weight: 356.5 g/mol

SMILES: O=C(N[C@H](C(N)=O)C(C)C)C1=NN(CC2CCCCC2)C3=C1C=CC=C3

InChI Key: KJNZIEGLNLCWTQ-KRWDZBQOSA-N

InChI: InChI=1S/C20H28N4O2/c1-13(2)17(19(21)25)22-20(26)18-15-10-6-7-11-16(15)24(23-18)12-14-8-4-3-5-9-14/h6-7,10-11,13-14,17H,3-5,8-9,12H2,1-2H3,(H2,21,25)(H,22,26)/t17-/m0/s1

Background:

AB-CHMINACA is a cannabinoid receptor modulator that was first synthesized by Pfizer for its potential therapeutic use.[1] The Ki toward the CB_1 receptor was reported in a 2009 patent to be 0.5 nM.[1] AB-CHMINACA is one of many new designer drugs being detected in illegal spice/herbal products. AB-CHMINACA is structurally related to another Pfizer cannabinoid, AB-FUBINACA, in that the *p*-fluorophenyl group has been replaced with a cyclohexyl group.[2] AB-FUBINACA is a similarly potent CB_1 receptor modulator that is now a US DEA regulated Schedule I controlled substance (Drug Code 7012) after having been identified in illegal products.[3]

References:
1. WO/2009/106980.
2. WO/2009/106982.
3. Forensic Toxicol, 31(1), 93-100, 2013.

Figure 1: GC/MS data

Experiment Parameters:
Agilent 6890 GC/5973 MSD
15:1 split, 20 mL/min He carrier
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)

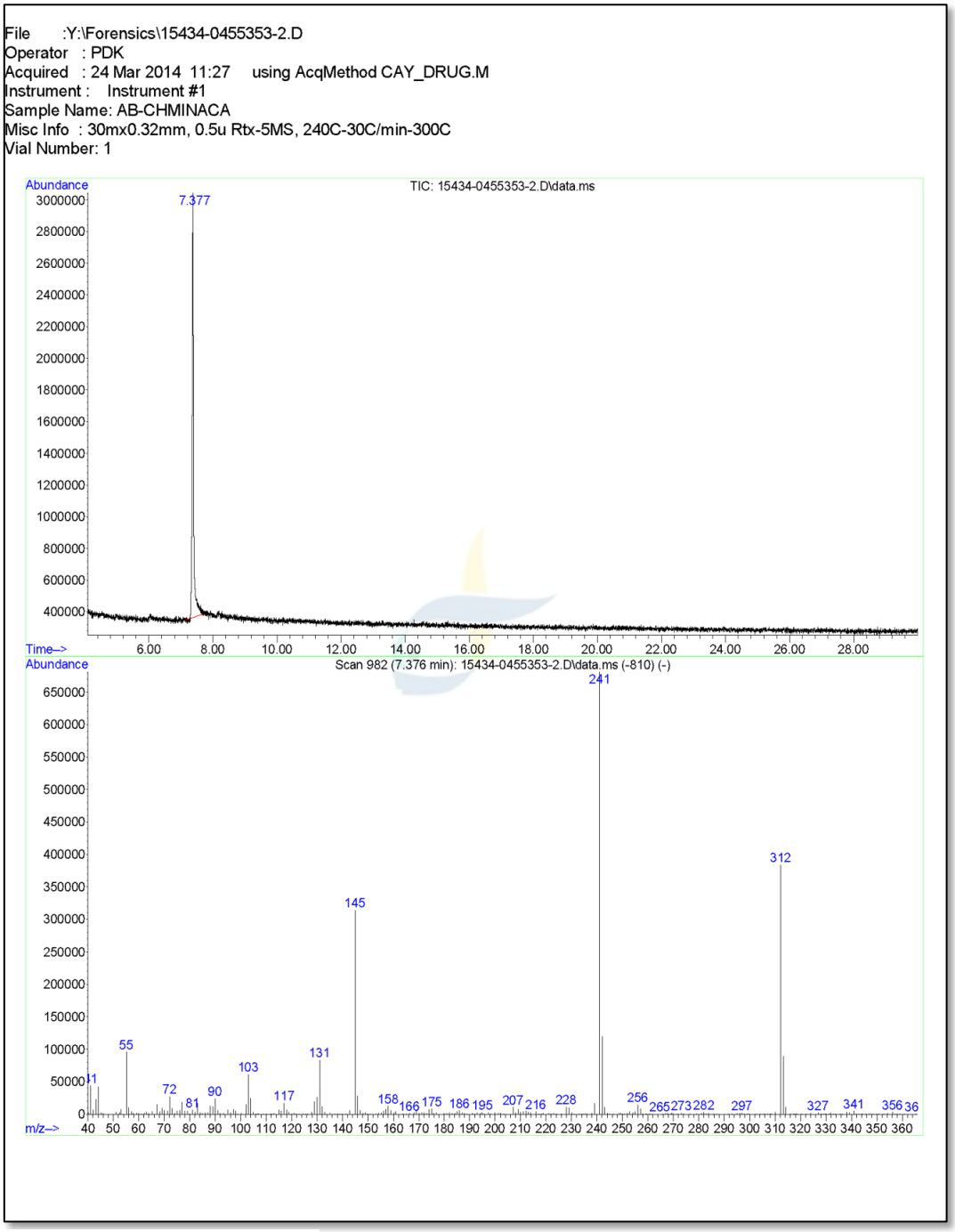


Figure 2: LC/MS data

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: 65-700 m/z

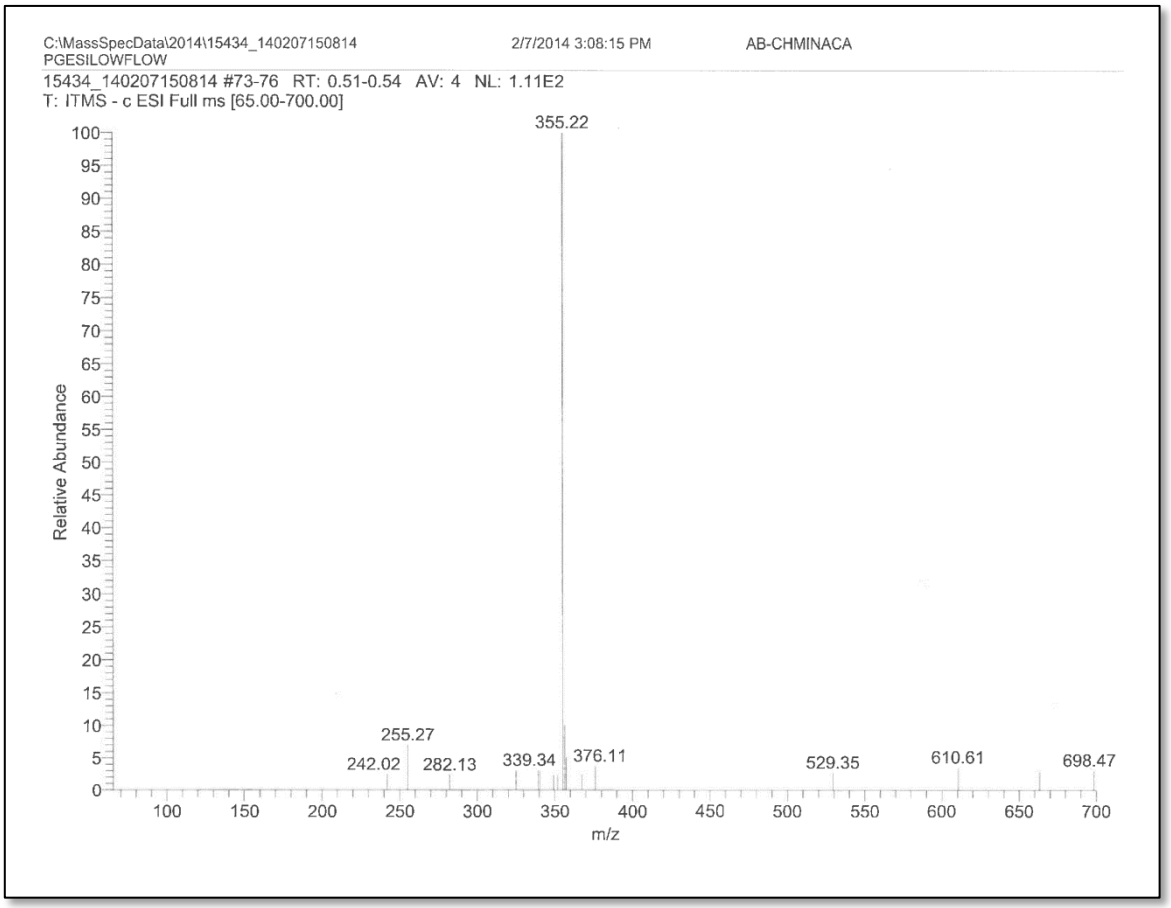


Figure 3: Fourier Transform Infrared Spectroscopy

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

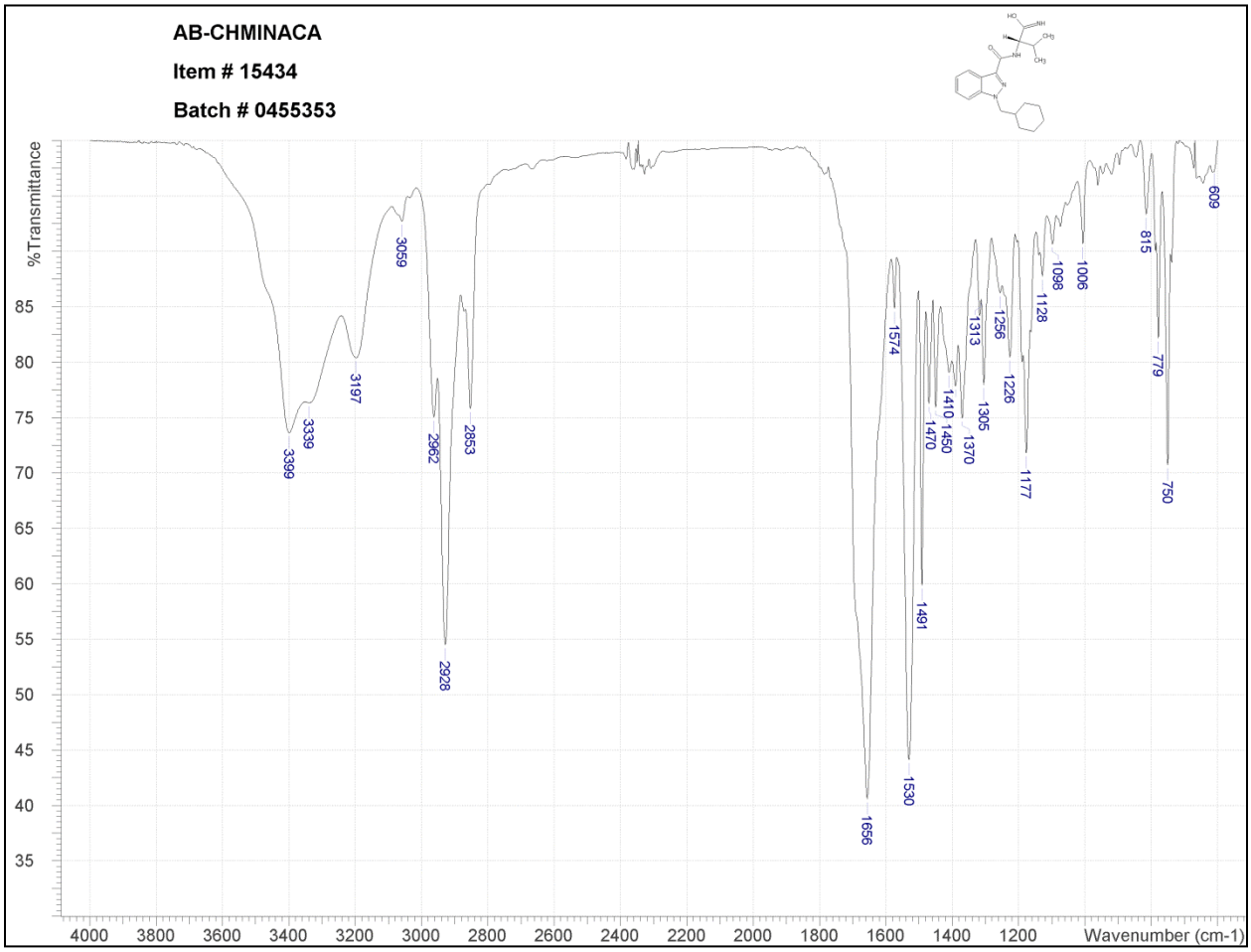


Figure 4: ^{1}H Nuclear Magnetic Resonance Spectroscopy

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

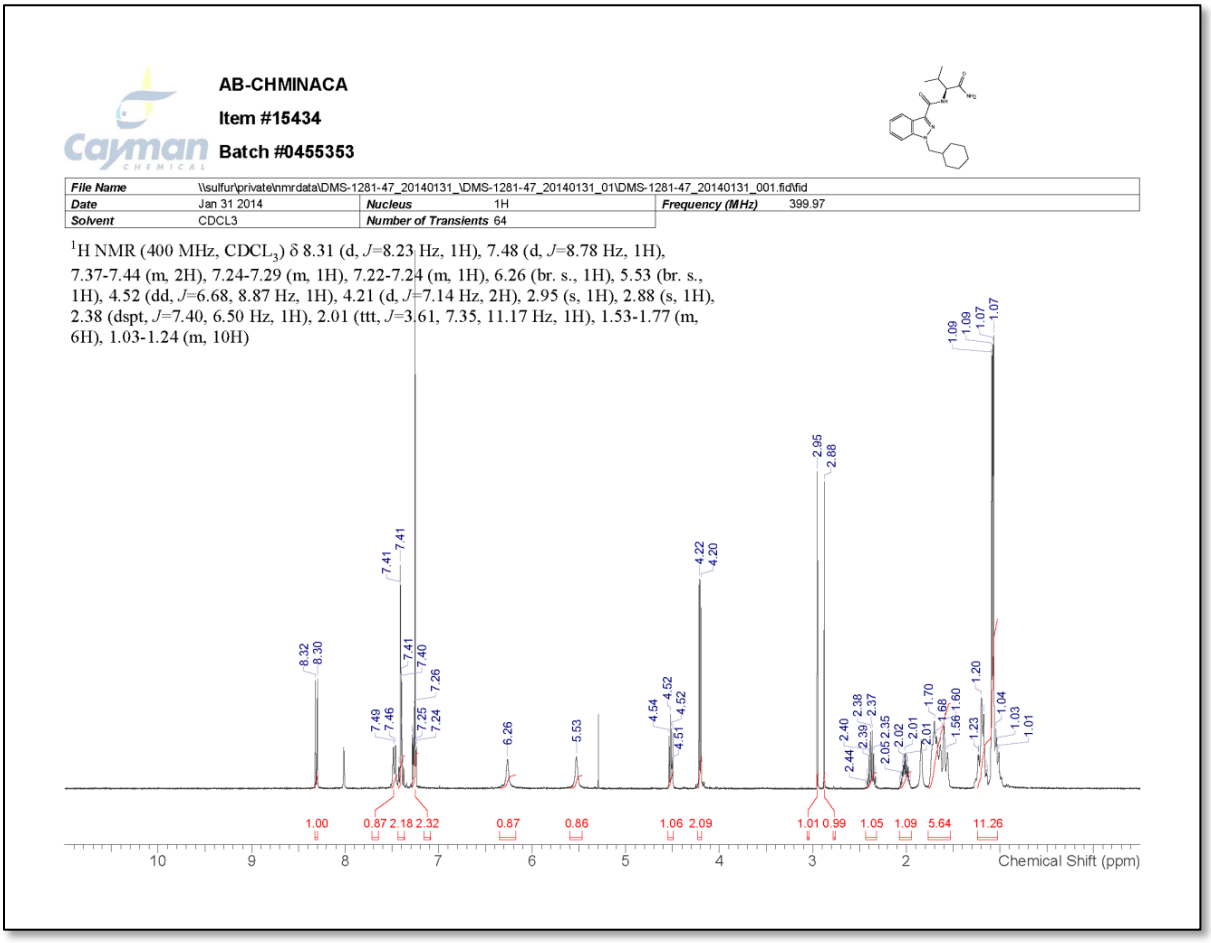
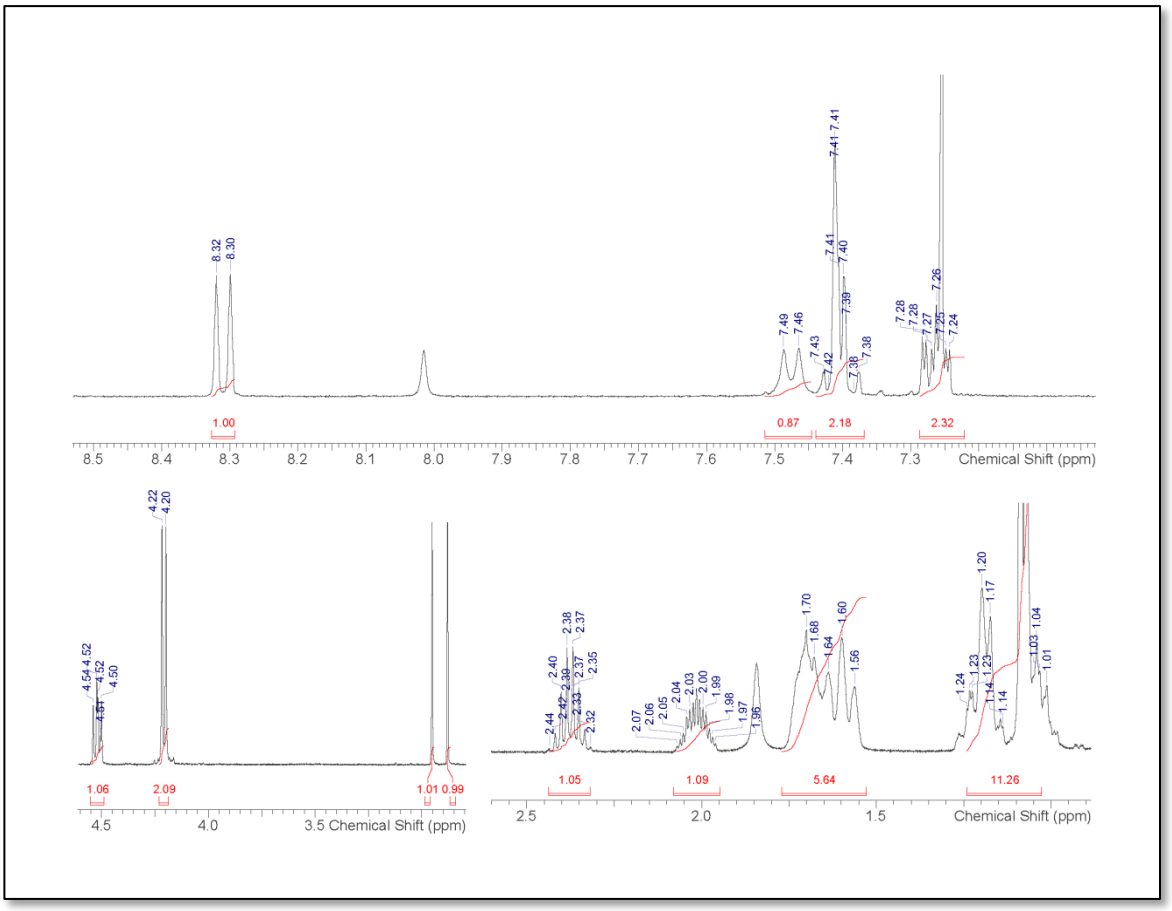
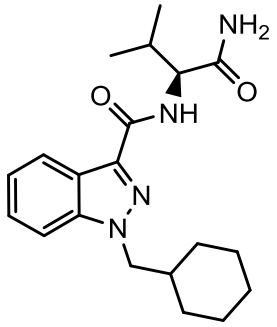


Figure 5. ^{1}H Nuclear Magnetic Resonance Spectroscopy, Enhanced for Detail



Part 2. Kentucky State Police Eastern Laboratory Branch Data

Compound Data



Name N-[(1S)-1-(aminocarbonyl)-2-methylpropyl]-1-(cyclohexylmethyl)- 1H-indazole-3-carboxamide

Synonyms: AB-CHMINACA

CAS#: 1185887-21-1

Molecular Formula: $C_{20}H_{28}N_4O_2$

Molecular Weight: 356.5 g/mol

Gas chromatography / Mass spectrometry:

Sample Preparation: approximately 1 mg/ml in methanol

Instrument: Agilent 6890N GC / 5973 MSD

GC Parameter: **Column:** ZB-DRUG-1 10m x 0.18mm x 0.18µm

Carrier Gas: Helium

Oven Program: 100 ˚C Hold 0.5 min. Ramp 40 ˚C/min to 280 ˚C Hold for 7.5 minutes.

Pressure Program: Initial pressure 5 psi, Ramp 150 psi/min to 15 psi Hold for 6 min. Ramp 150 psi/min to 40 psi.

Injection parameter: **Injector Volume:** 1 µL **Split ratio:** 1:50

MS Parameters: **Temperature:** **Injector** 250^{o}C

MSD transfer line: 290^{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. Gas Chromatography/ Mass Spectrometry

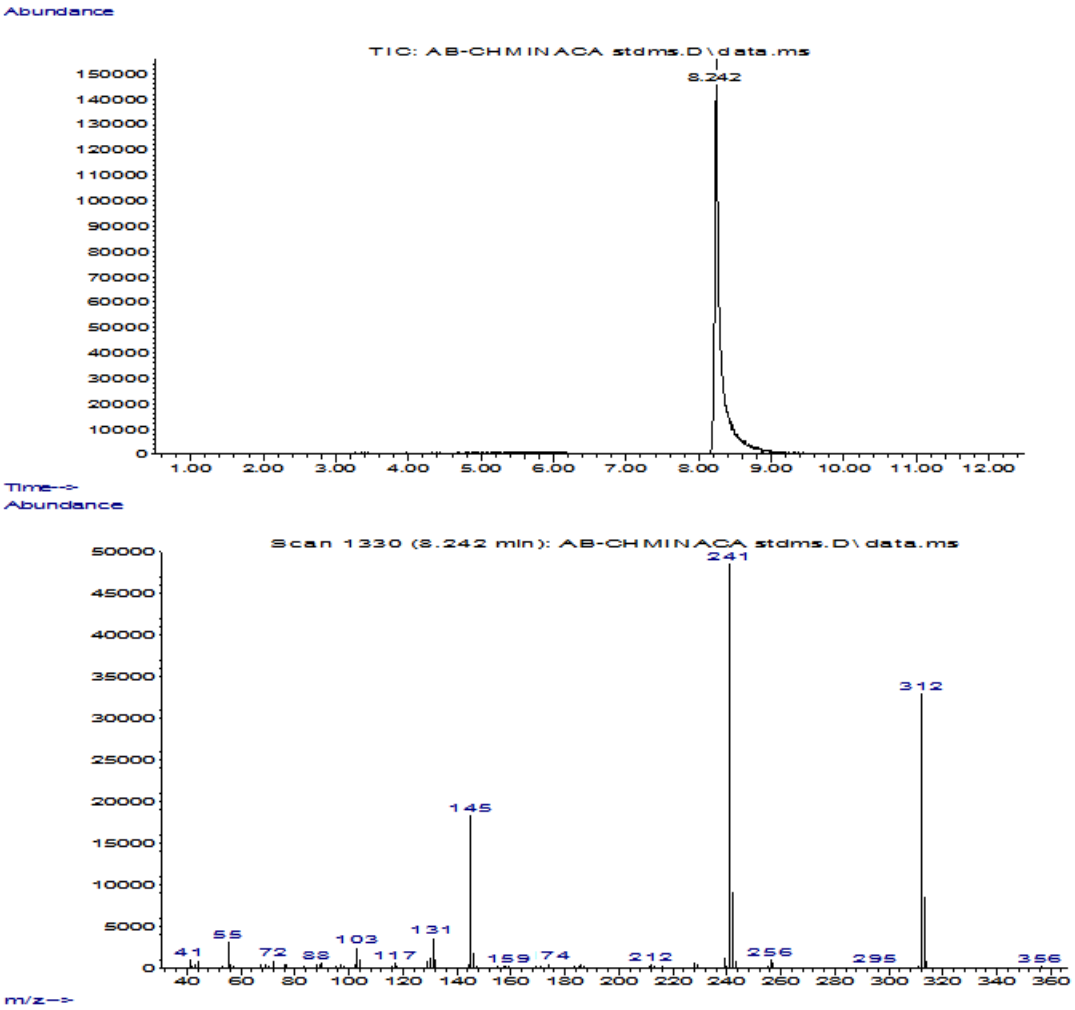
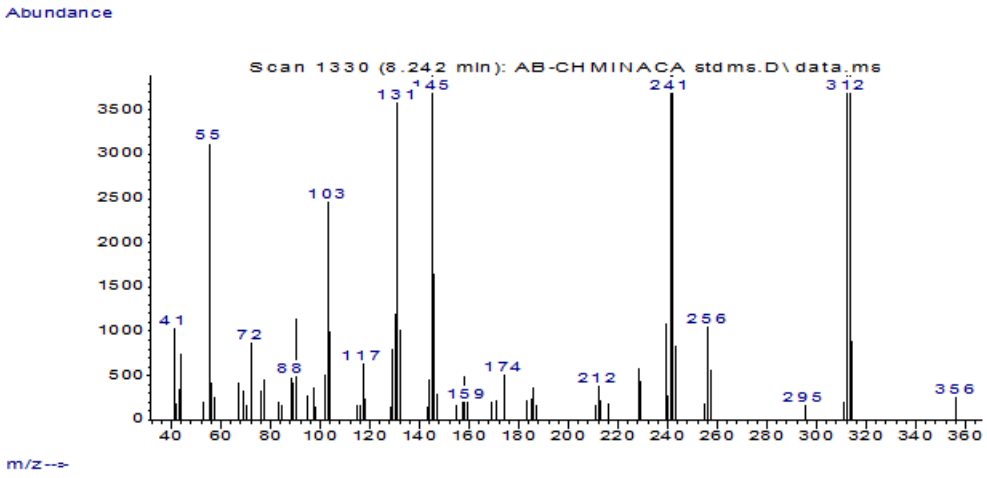


Figure 7. Expanded Mass Spectrum



Fourier Transform Infrared Spectroscopy (ATR)

Instrument: Digilab FTS 2000 series FTIR, Specac Golden Gate ATR accessory

Scan Parameters:

Numbers of Scans: 64

Number of Background Scans: 64

Resolution: 4 cm-1

Beamsplitter: KBr

Figure 8. FTIR/ ATR spectrum

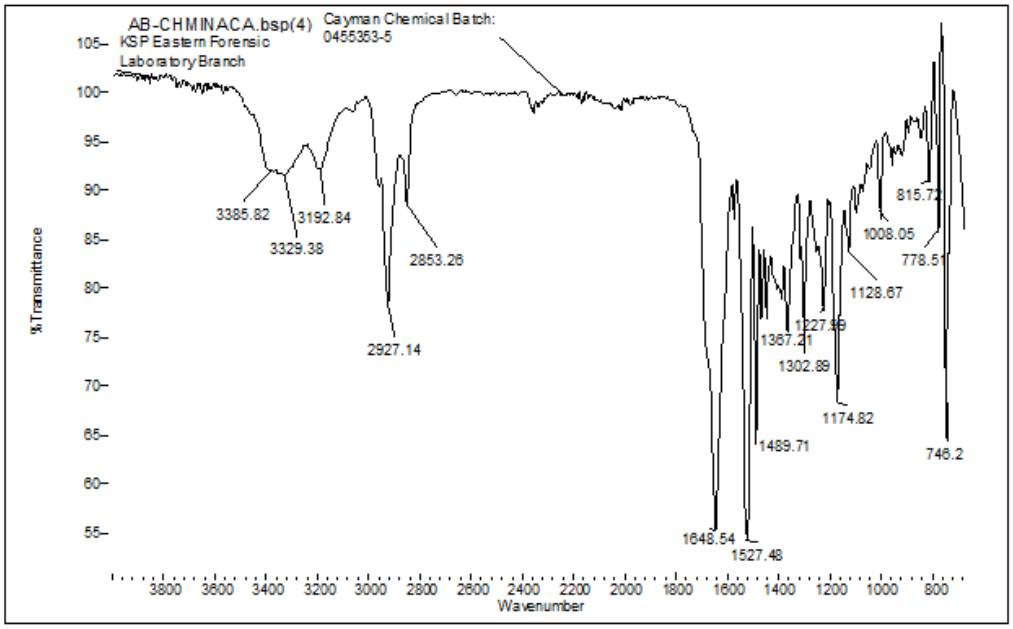
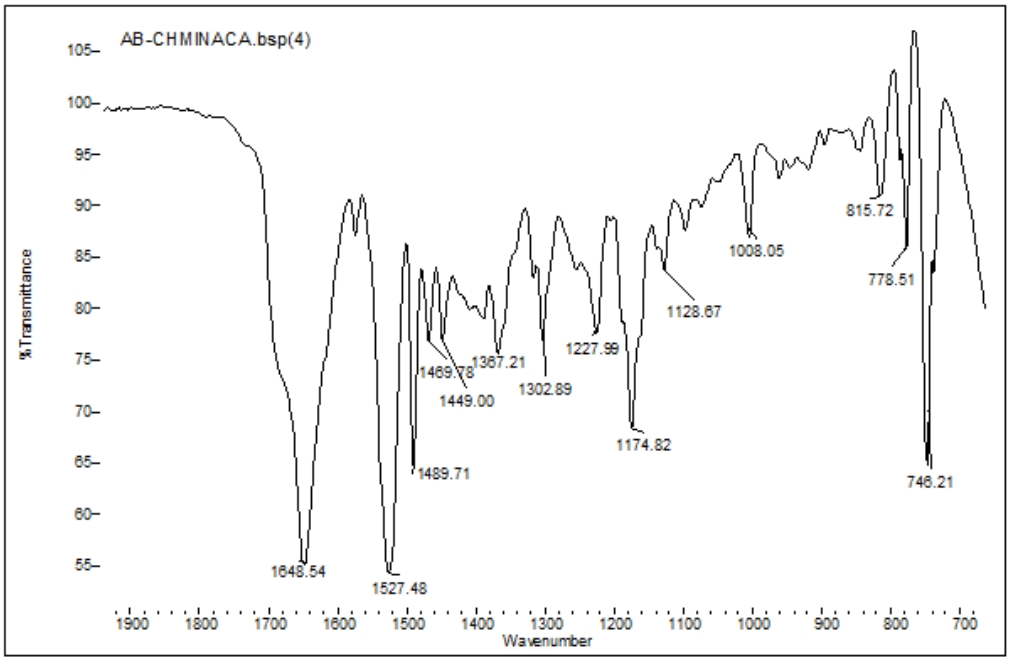


Figure 9. Expanded FTIR/ ATR spectrum



Part 3.

External Links:

Forendex link to AB-CHMINACA