Characterization of 4-Chloromethcathinone

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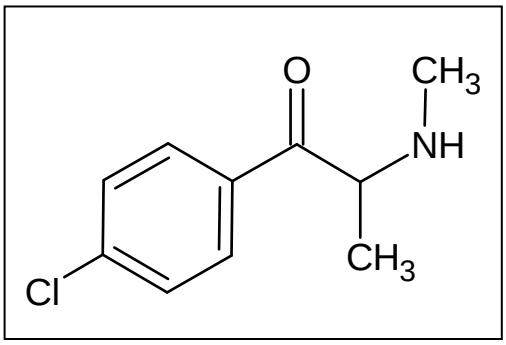
Part 1. Cayman Chemical Company Data



Name: 4-Chloromethcathinone

Synonyms: 4-CMC, clephedrone

CAS#: N/A

Molecular Formula: C10H12ClNO

Molecular Weight: 197.66 g/mol

SMILES: O=C(c1ccc(Cl)cc1)C(C)NC

InChl Key: UEJBEYOXRNGPEI-UHFFFAOYAF

InChl: InChI=1/C10H12ClNO/c1-7(12-2)10(13)8-3-5-9(11)6-4-8/h3-7,12H,1-2H3

Background:

4-Chloromethcathinone (also referred to as clephedrone or 4-CMC) is one of many designer synthetic cathinones that has been sold on the illicit drug market.[1] 4-CMC is a derivative of US regulated Schedule I controlled substance methcathinone. The only difference between the two is that 4-CMC has a chlorine in the para position on the phenyl ring. While pharmacological data for this compound does not exist, it has been published that the bromine analogue (4-bromomethcathinone or 4-BMC) acts as a serotonin and norepinephedrine reuptake inhibitor.[2,3]

1-Forensic Sci Int. 2014, 244, e56-e59.
2-Drug Develop Res. 2003, 60, 252-260
3-Naunyl Schmiedebergs Arch Pharmacol. 2002, 365(4), 457-461.

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 30 ^{o}C /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 4-Chloromethcathinone

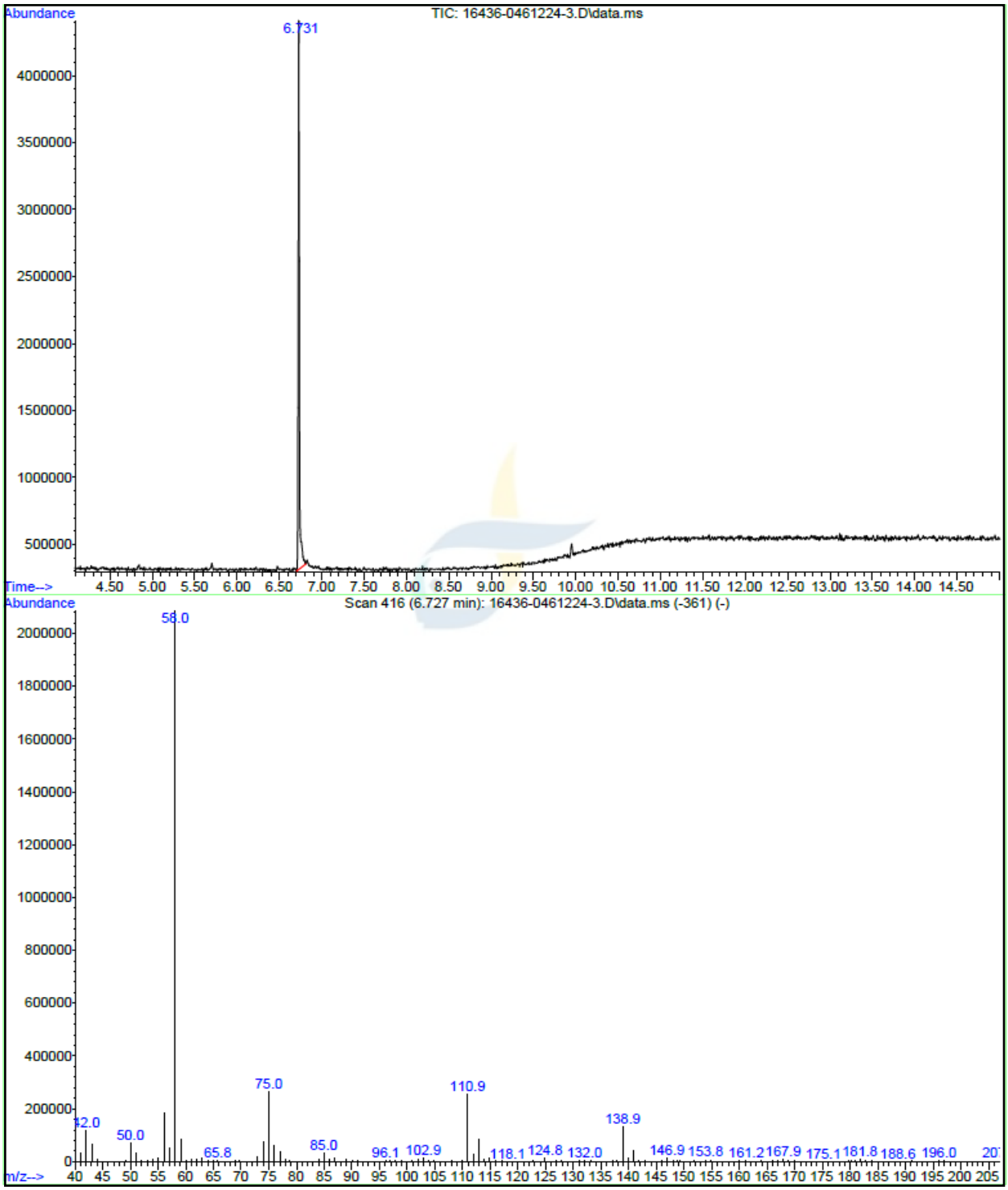


Figure 2. Fourier Transform Infrared Spectroscopy of 4-Chloromethcathinone

Experiment Parameters:
Instrument: Perkin Elmer Spectrum 65
Number of scans: 16 (background subtracted)
Resolution: 4 cm^{-1}
Scan Range: 600-4000 cm^{-1}
Sample prepared as KBr pellet

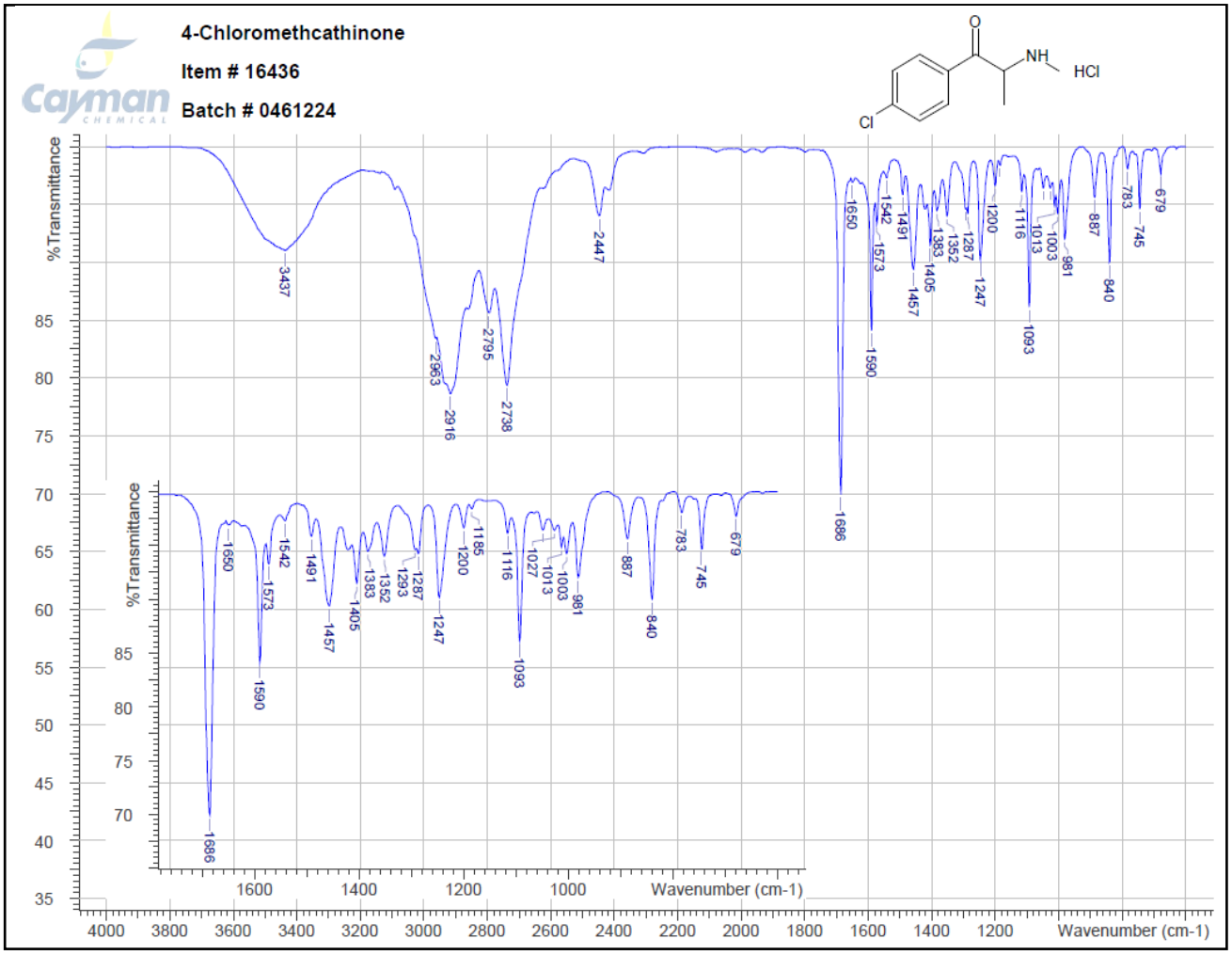


Figure 3. 1H Nuclear Magnetic Resonance Spectroscopy of 4-Chloromethcathinone

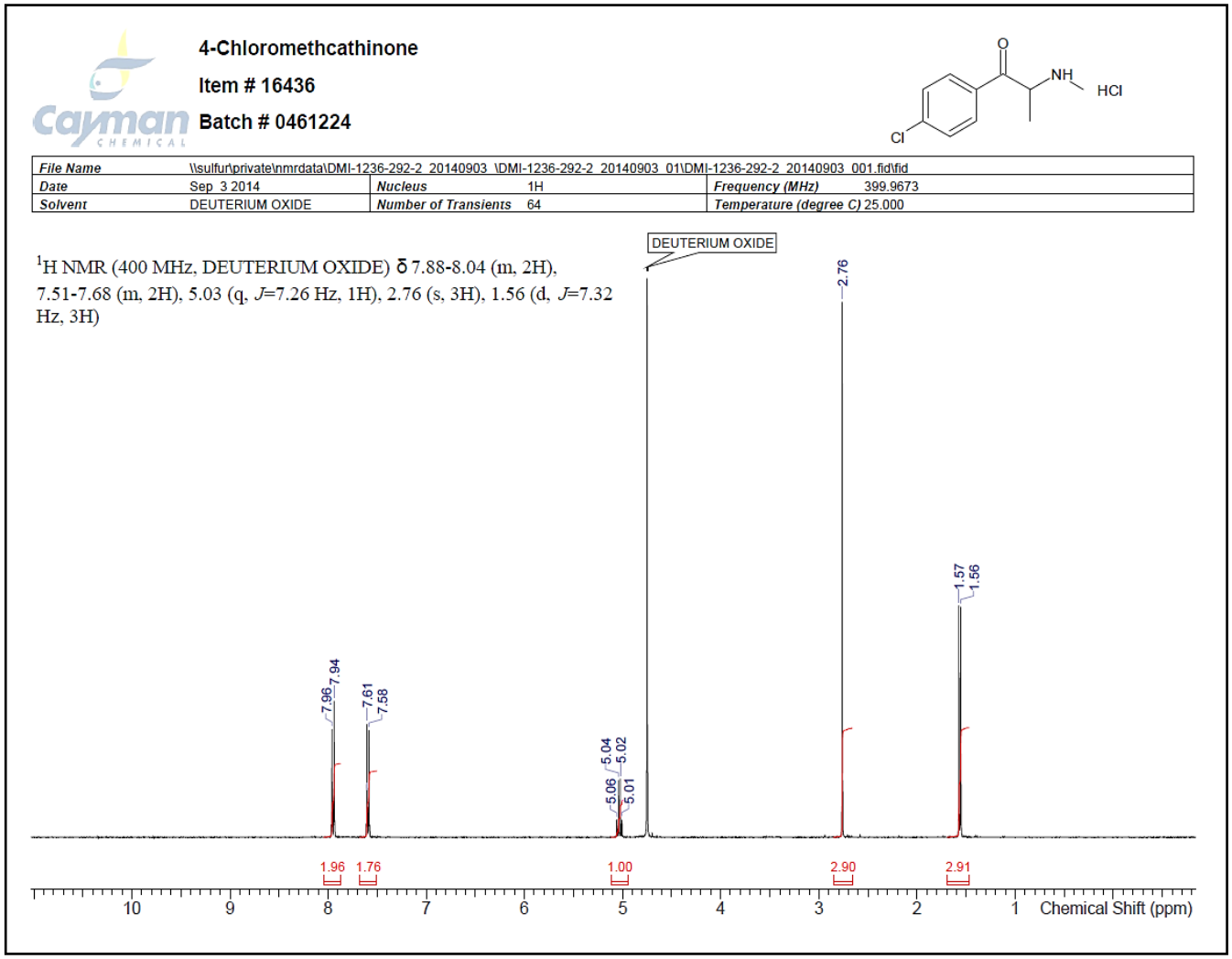


Figure 4. 1H Nuclear Magnetic Resonance Spectroscopy of 4-Chloromethcathinone, Enhanced for Detail

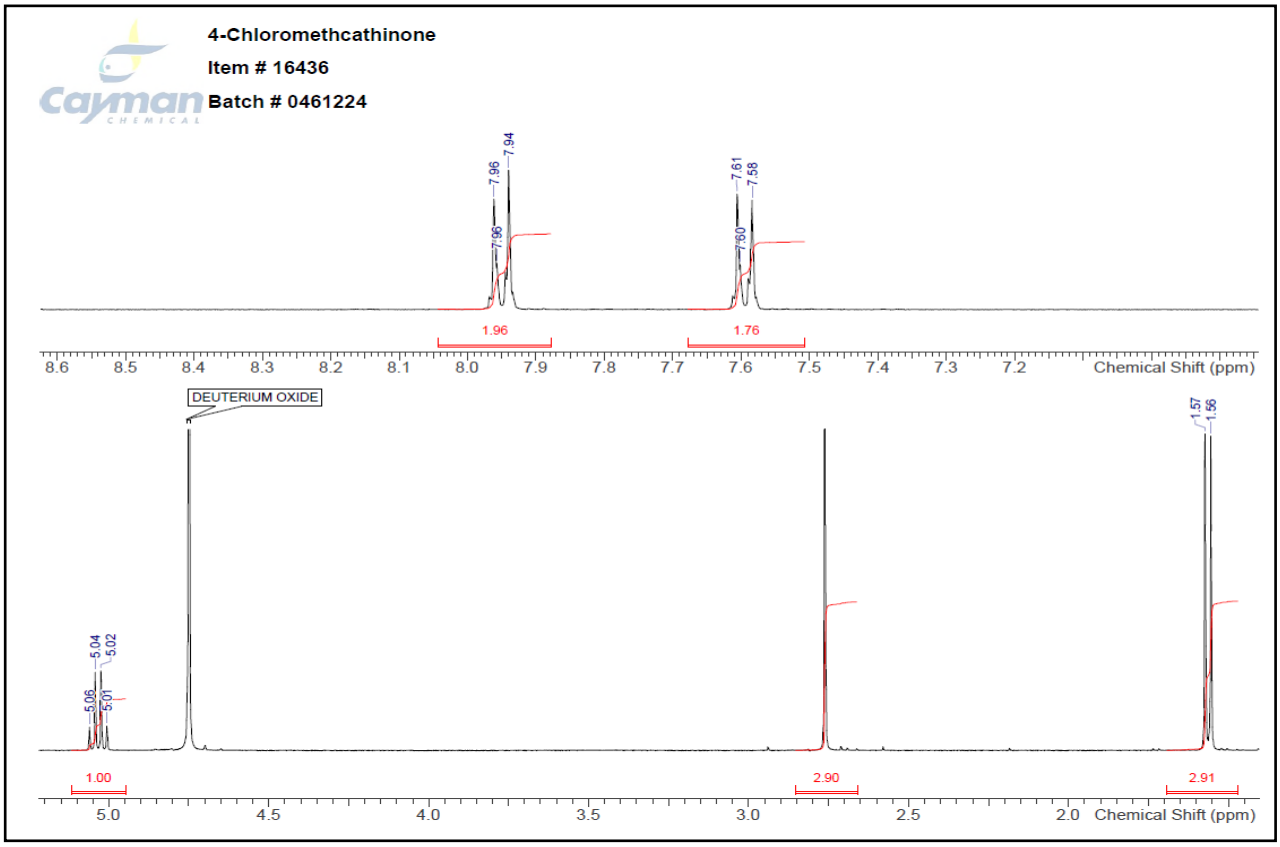
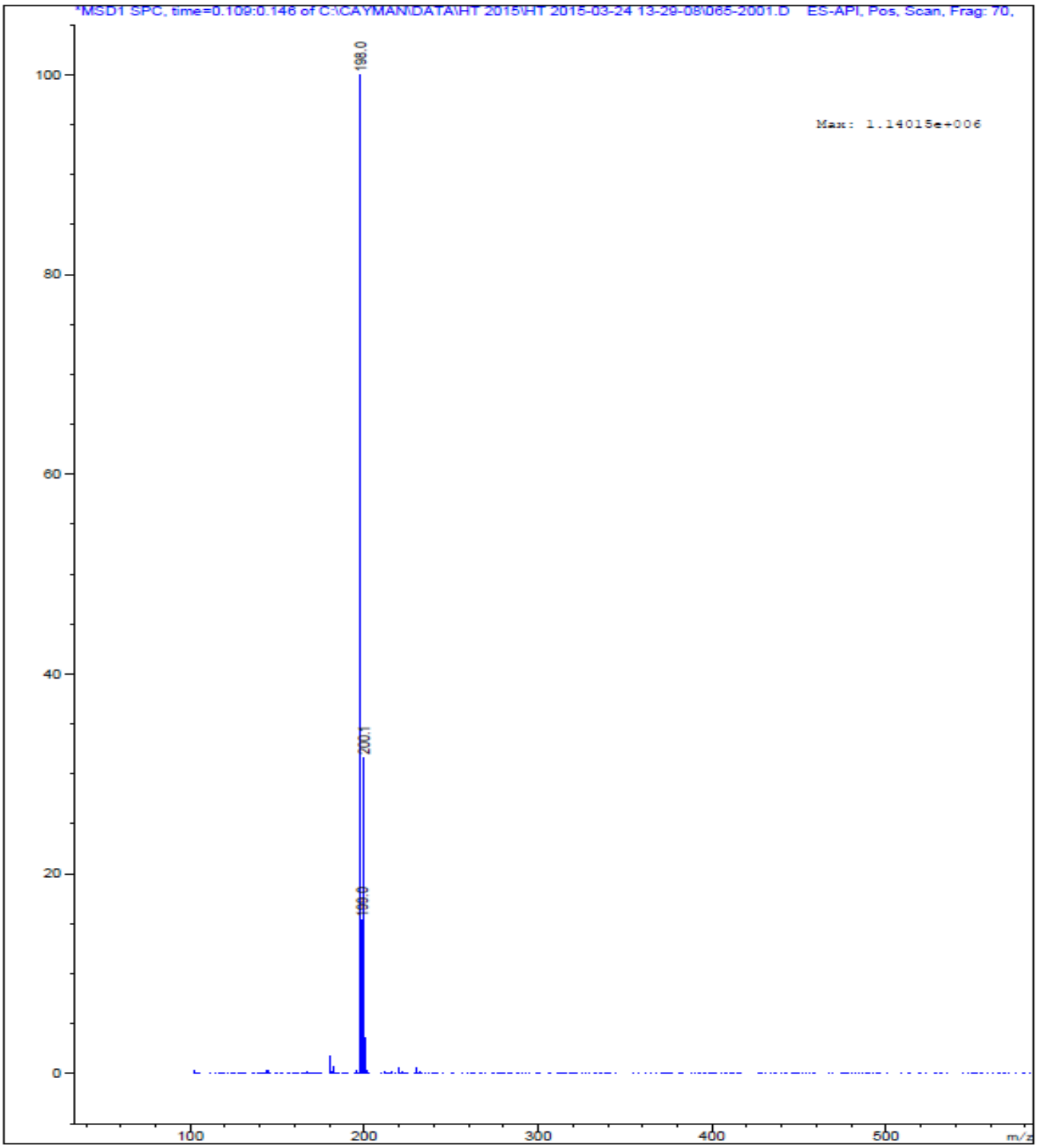
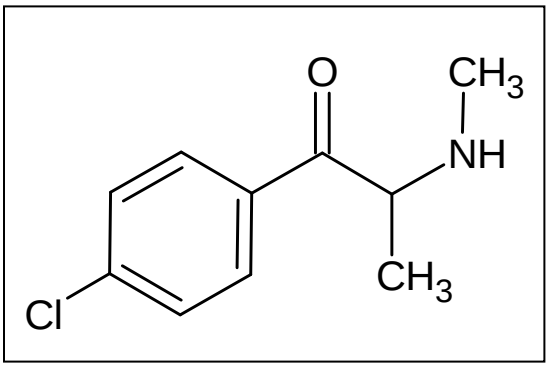


Figure 5. ESI-MS of 4-Chloromethcathinone



Part 2. Kentucky State Police Eastern Laboratory Branch Data



Name: 4-Chloromethcathinone

Synonyms: 1-(4-chlorophenyl)-2-(methylamino)-1-propanone; Clephedrone; 4-CMC

CAS#: N/A

Molecular Formula: $C_{10}H_{12}ClNO$

Molecular Weight: 197.66 g/mol

SMILES: O=C(c1ccc(Cl)cc1)C(C)NC

InChl Key: WJAQVQFSQUVTAY-UHFFFAOYSA-N

InChl: InChI=1/C10H12ClNO/c1-7(12-2)10(13)8-3-5-9(11)6-4-8/h3-7,12H,1-2H3

Gas chromatography/Mass spectrometry:

Sample Preparation: Approximately 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: 50:1

MS Parameters: **Temperatures:**

Injector: 250°C

MSD transfer line: 280^{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: EI Mass Spectrum of 4-Chloromethcathinone

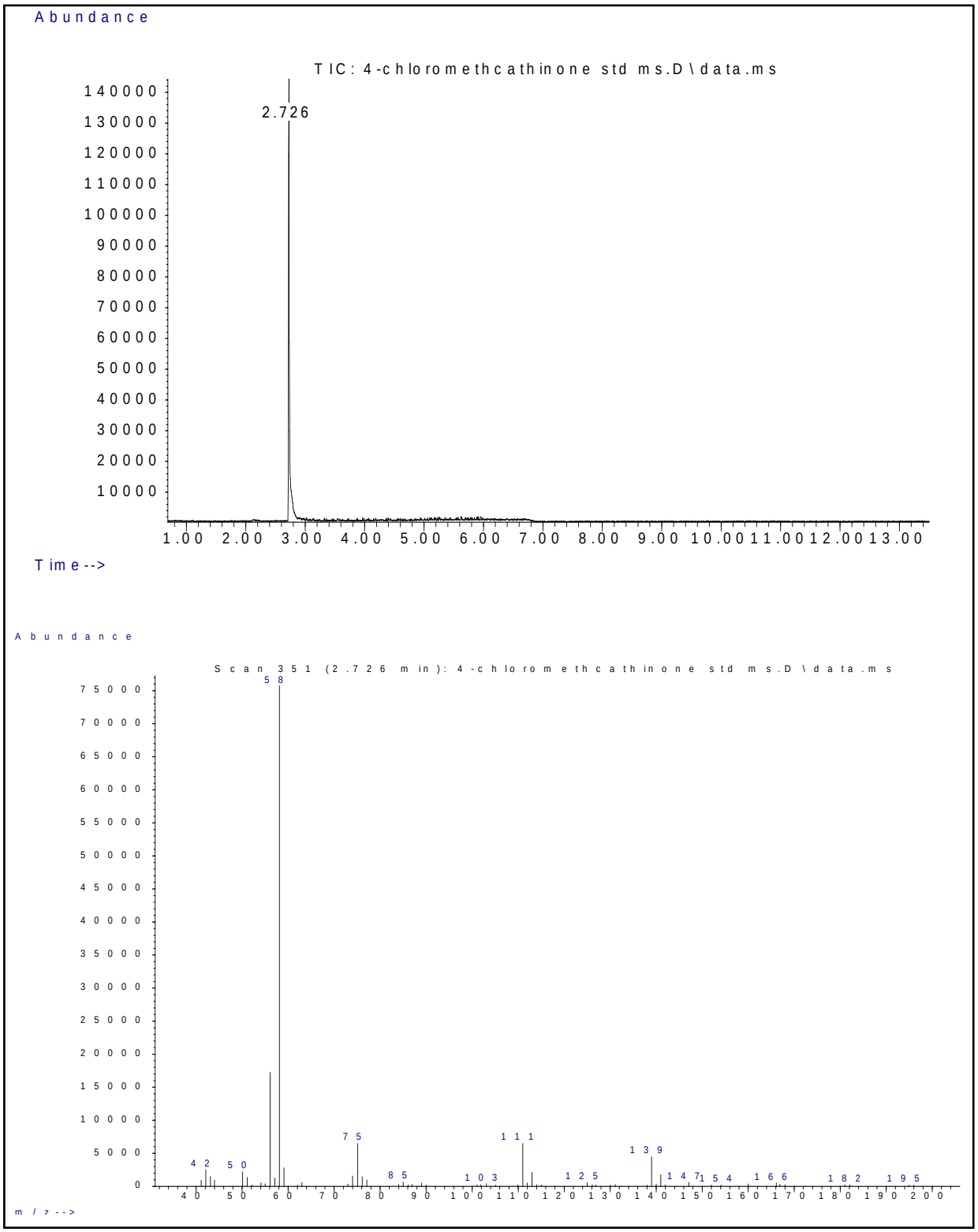


Figure 7: Expanded Mass Spectrum of 4-Chloromethcathinone

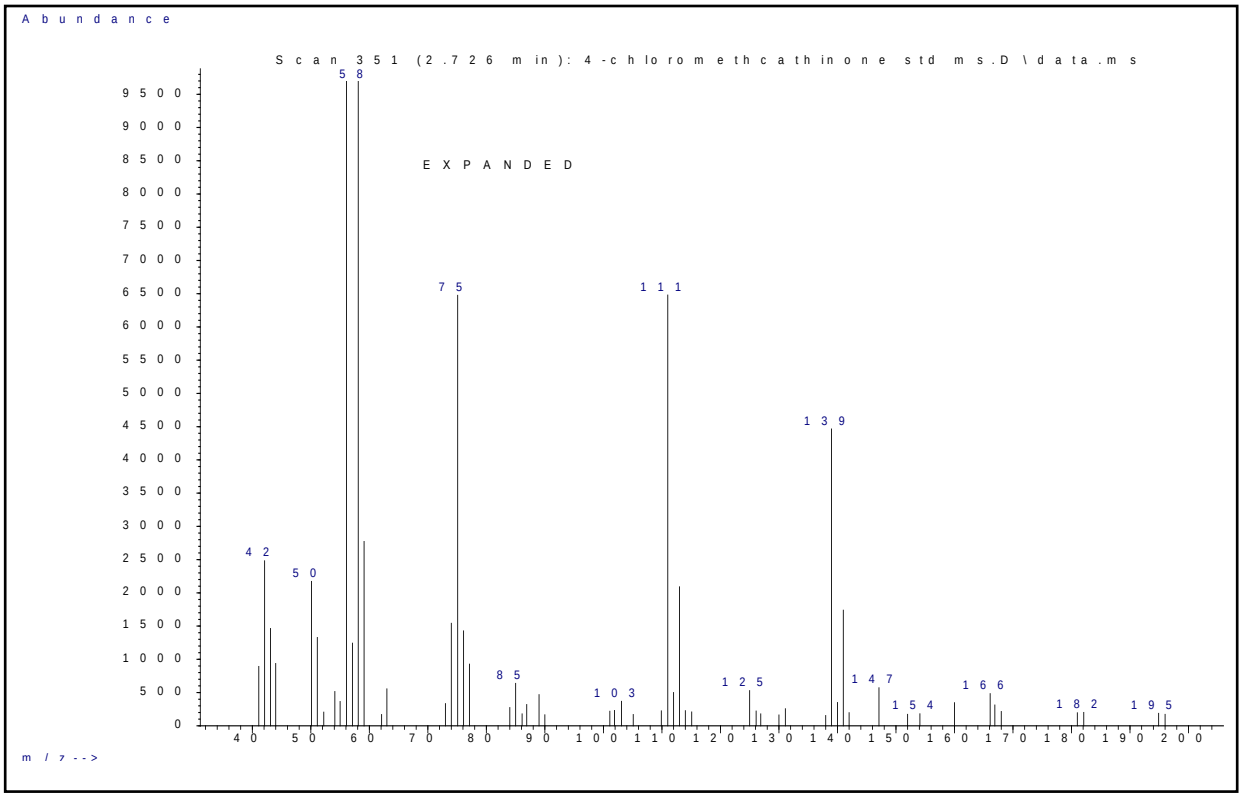


Figure 8. FTIR/ATR Spectrum of 4-Chloromethcathinone

Experiment Parameters:
Instrument: FT-IR with diamond ATR attachment
Number of Scans: 64
Number of Background Scans: 64
Resolution: 4 cm^{-1}

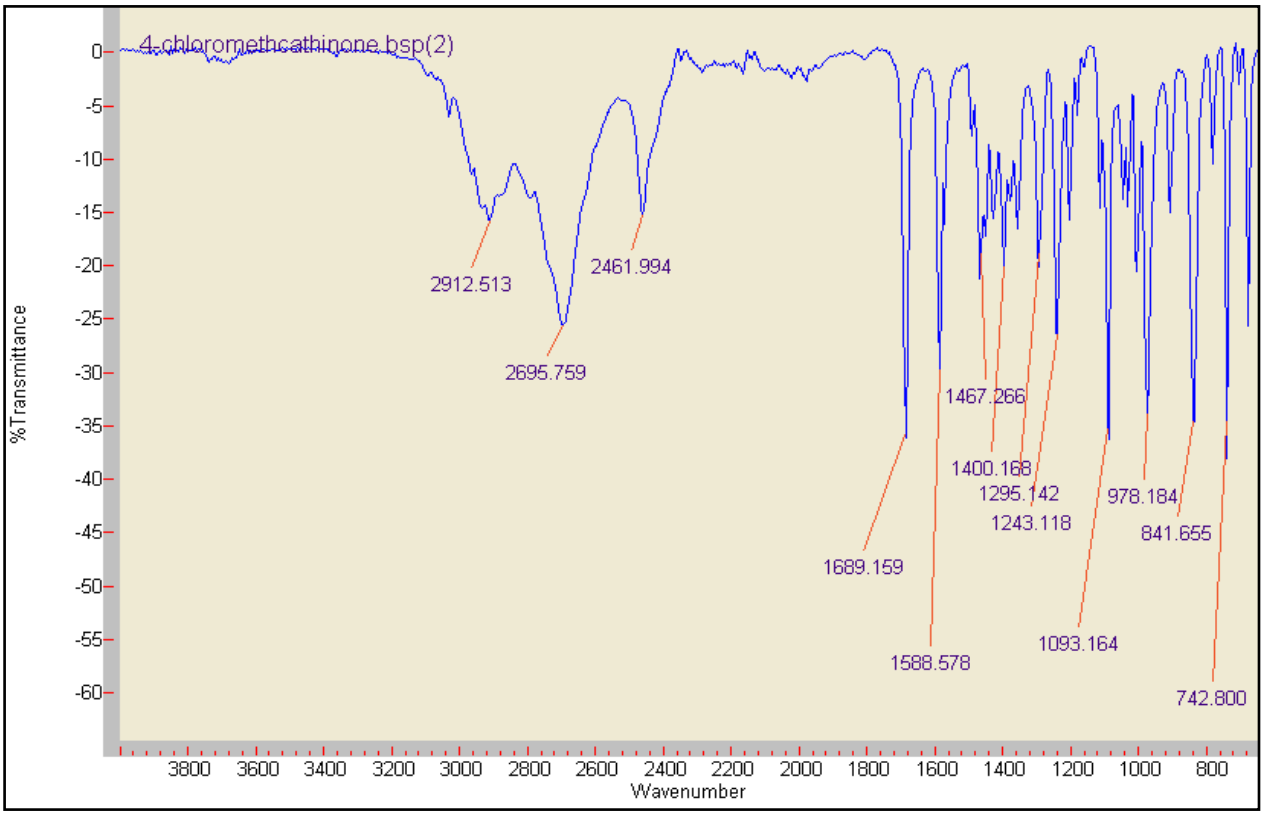
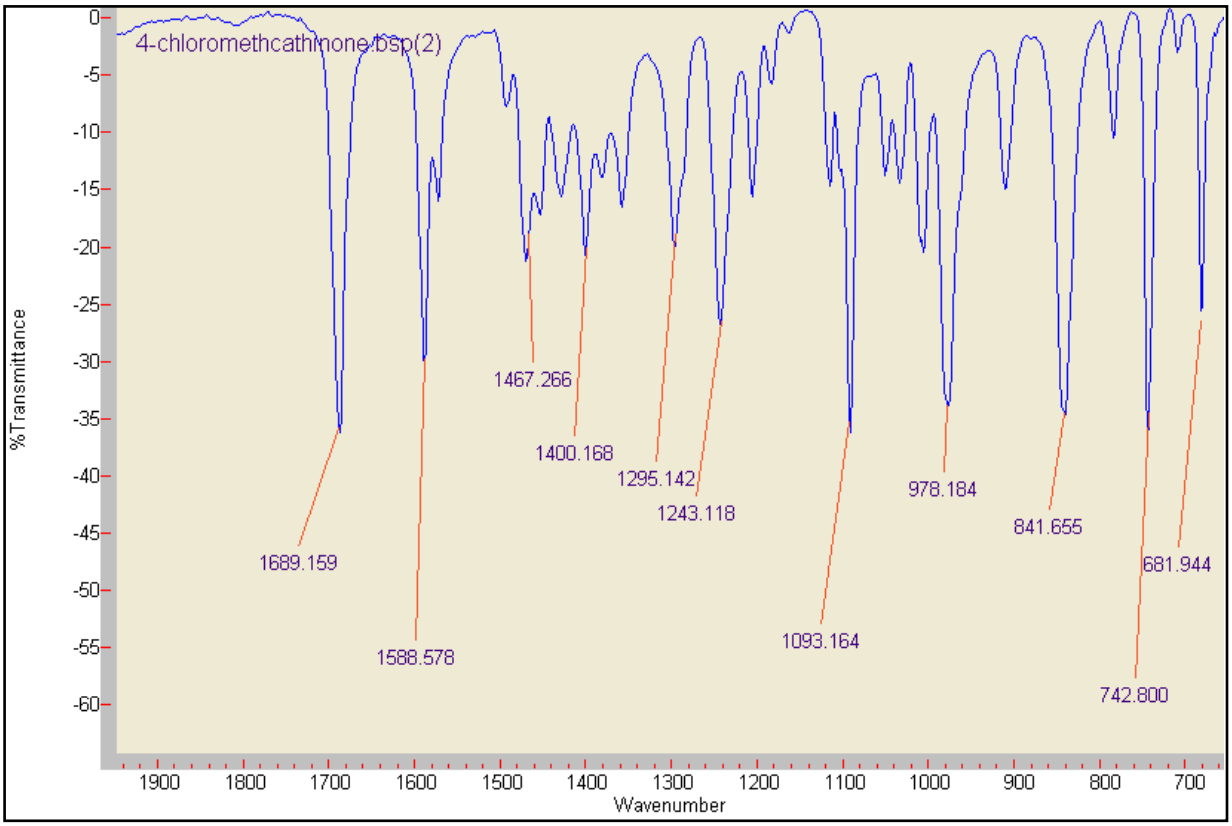


Figure 9. Expanded FTIR/ATR Spectrum of 4-Chloromethcathinone



Part 3. References:

M. Taschwer, J. A. Weiß, O. Kunert, M. G. Schmid. Analysis and characterization of the novel psychoactive drug 4-chloromethcathinone (clephedrone). Forensic Science International. 244 (2014) e56–e59.