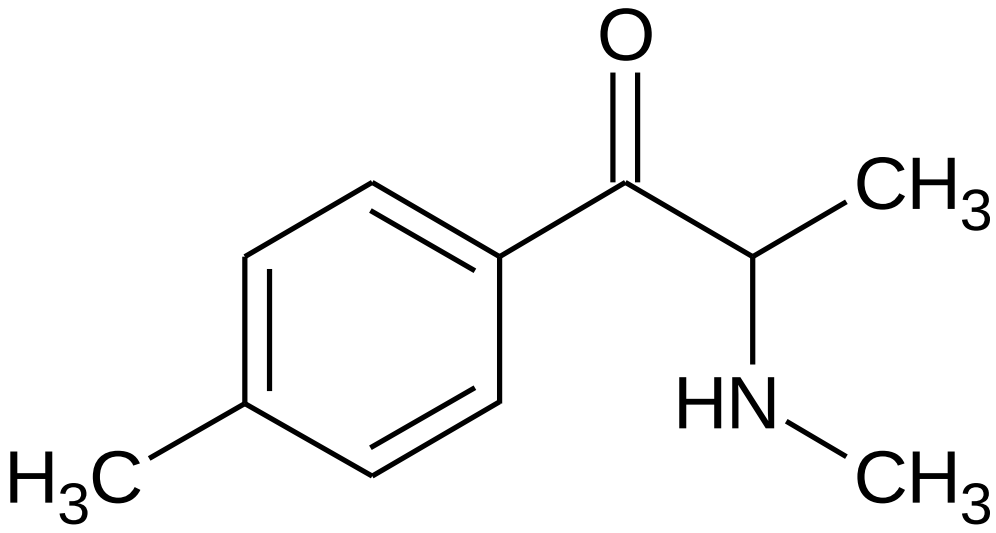


1. GENERAL INFORMATION

IUPAC Name: 2-(methylamino)-1-(4-methylphenyl)propan-1-one

CFR: Schedule I

CAS #: 1189805-46-6 (Base)
1189726-22-4 (HCl)

Synonyms: Mephedrone, 4-MMC, 4-methylephedrone

Source: DEA Reference Material Collection

Appearance: Pale yellow powder (HCl)

Kovat's Index: Pending

UV_{max} (nm): 262.8

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{11}H_{15}NO$	177	Not Determined
HCl	$C_{11}H_{15}NO \cdot HCl$	213	249.6

3. ADDITIONAL RESOURCES

K. Tsujikawa, T. Mikuma, K. Kuwayama, et al. Degradation pathways of 4-methylmethcathinone in alkaline solution and stability of methcathinone analogs in various pH solutions. Forensic Science International 2012; 220: 103-110.

P. Dargan, R. Sedefov, A. Gallegos, D. Wood. The pharmacology and toxicology of the synthetic cathinone mephedrone (4-methylmethcathinone). Drug Testing and Analysis 2011; 3:454-463.

Forendex

Wikipedia

4. QUALITATIVE DATA

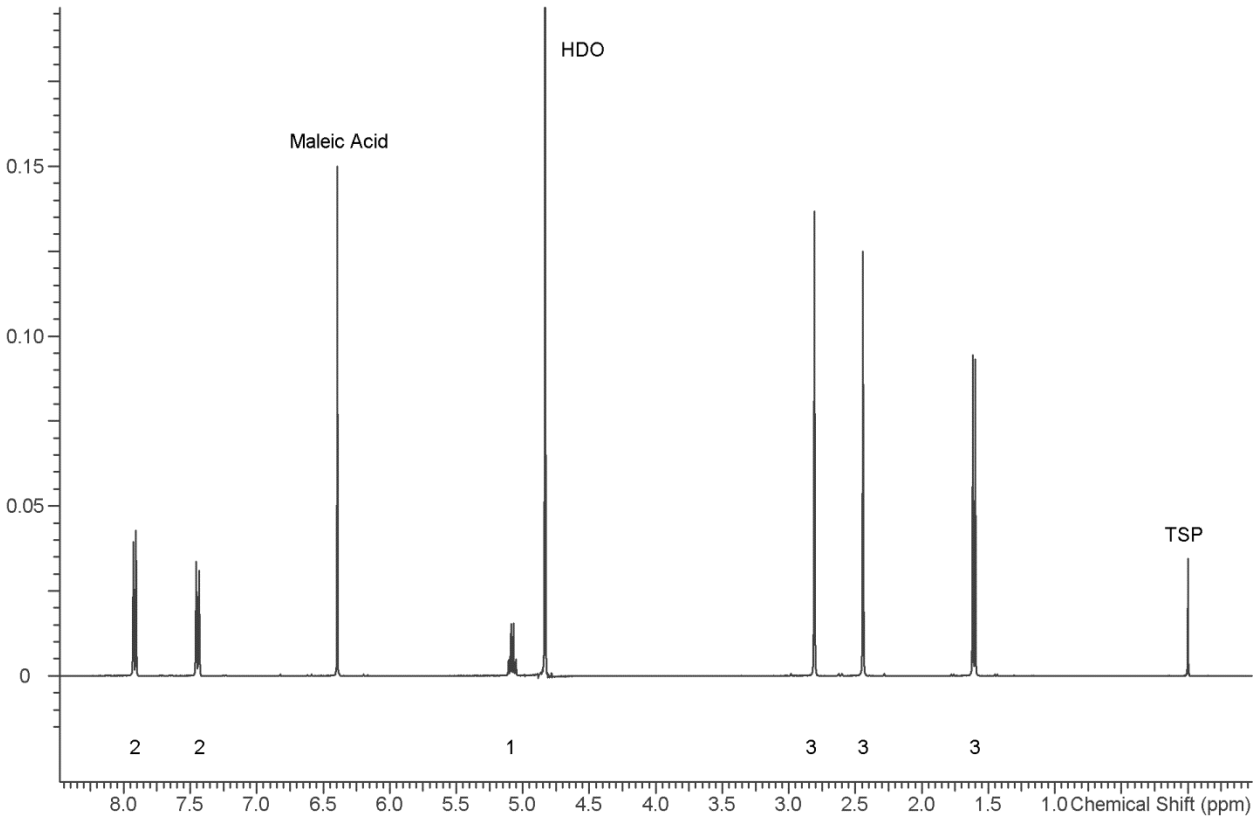
4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D_2O

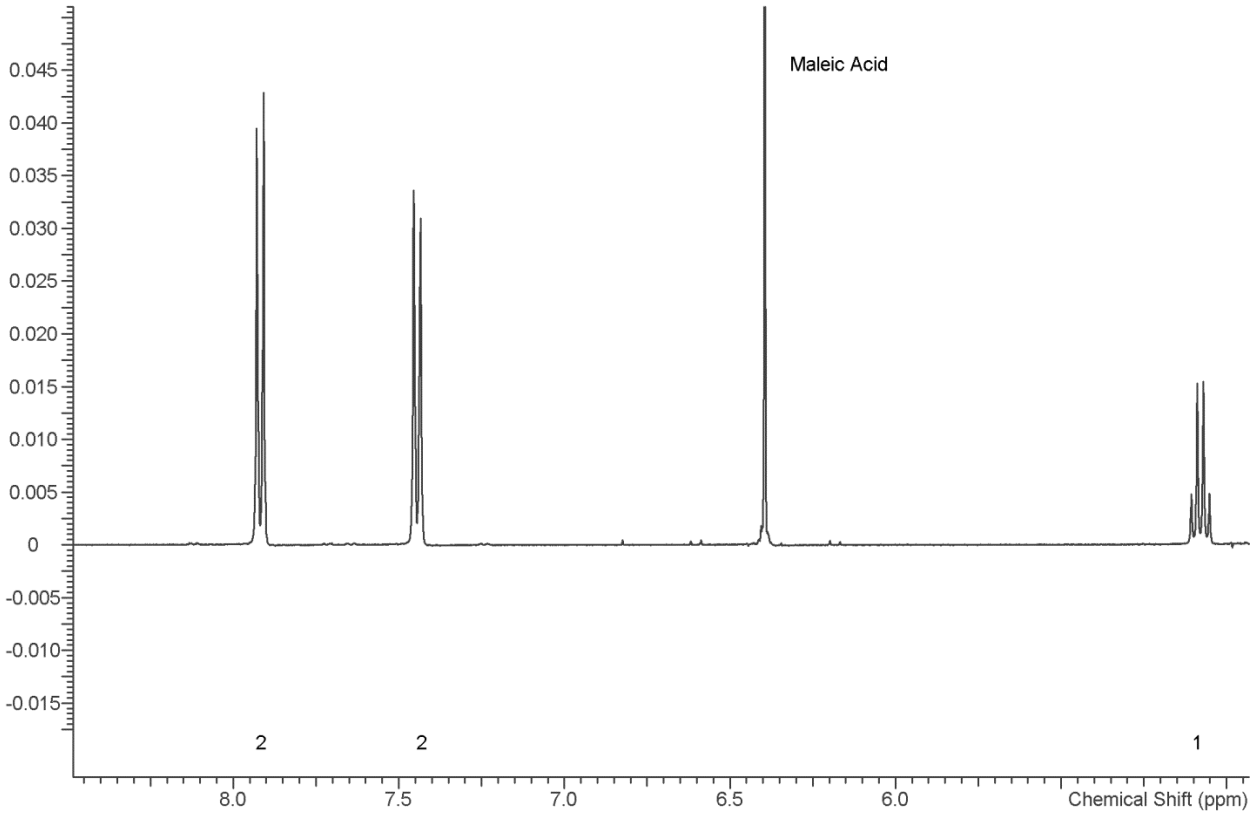
Sample Preparation: Dilute analyte to ~20 mg/mL in D_2O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

Instrument:	400 MHz NMR spectrometer
Parameters:	Spectral width: at least containing -3 ppm through 13 ppm Pulse angle: 90° Delay between pulses: 45 seconds

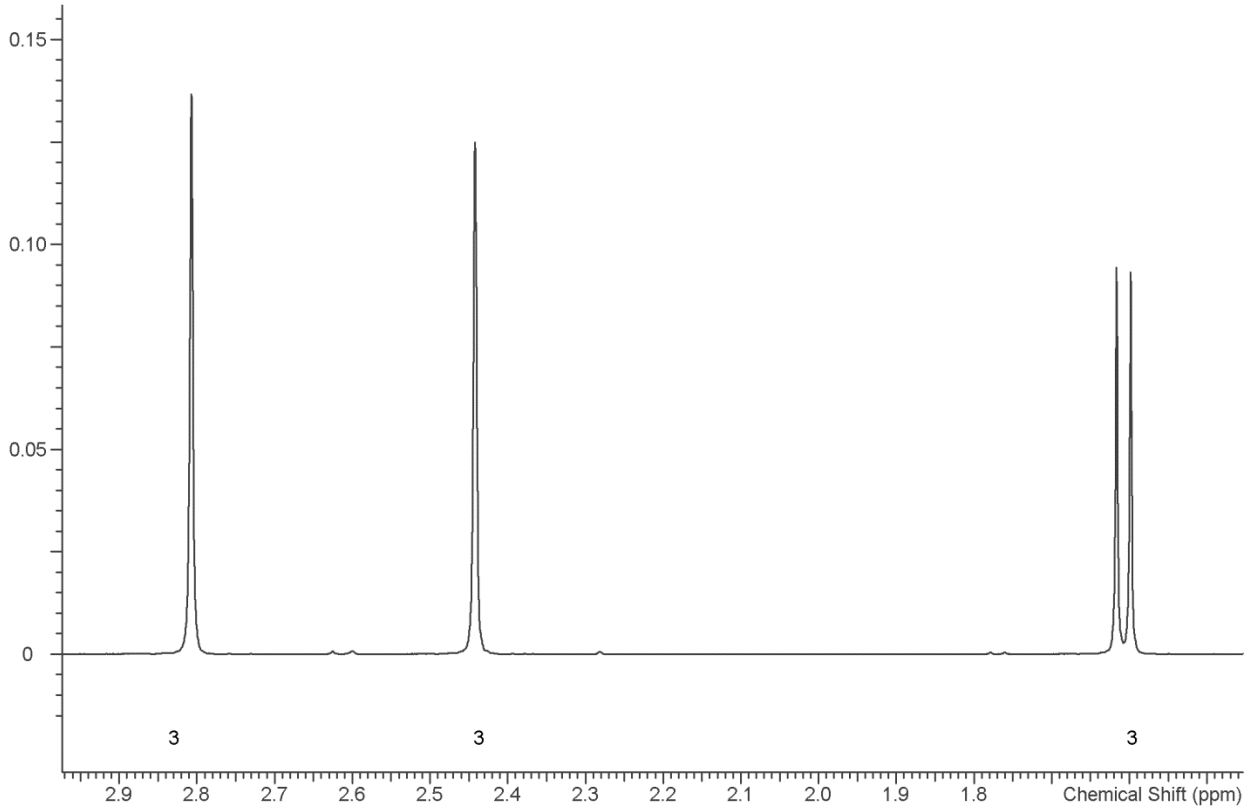
1H NMR: 4-Methylmethcathinone HCl Lot # SF0002; D_2O; 400MHz



1H NMR: 4-Methylmethcathinone HCl Lot # SF0002; D_2O; 400MHz



1H NMR: 4-Methylmethcathinone HCl Lot # SF0002; D_2O; 400MHz

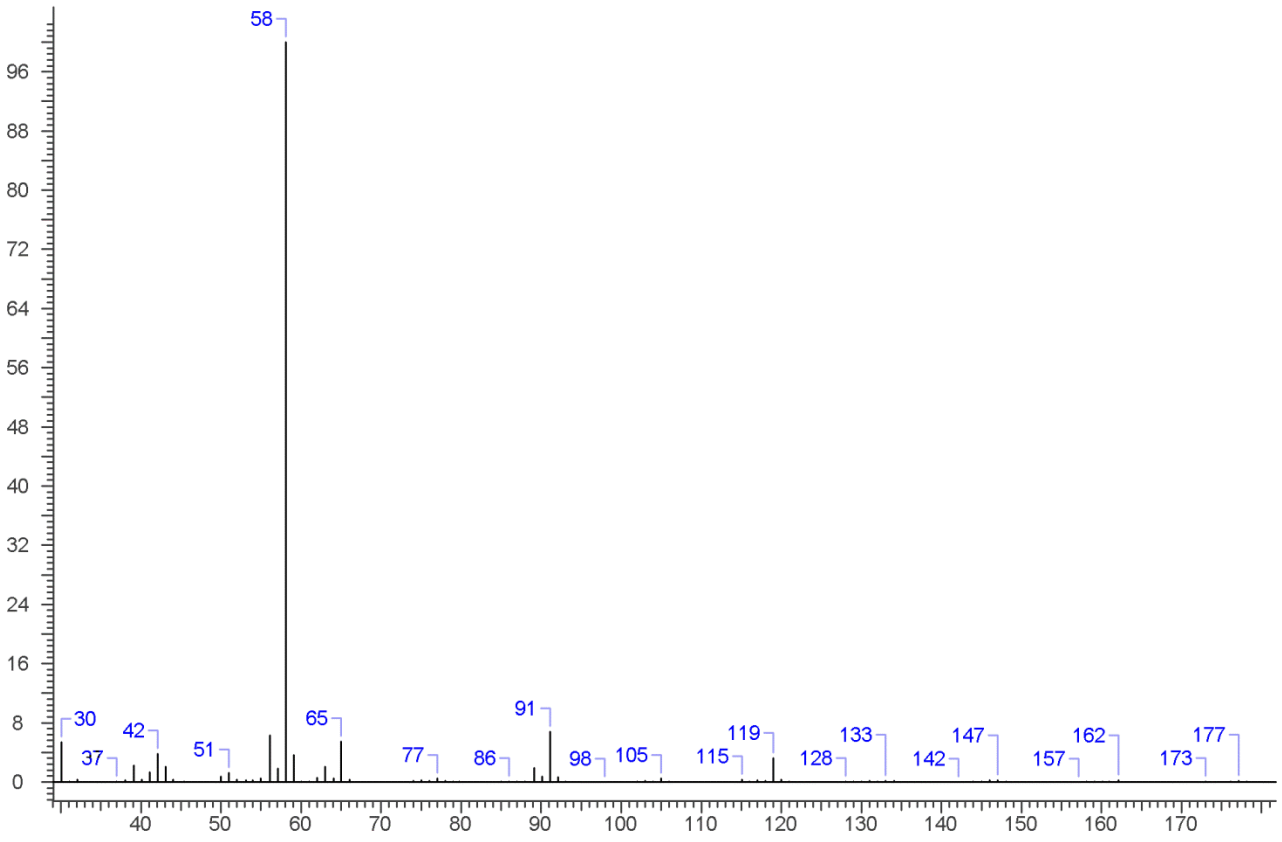


4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~1 mg/mL base extracted in $CHCl_3$.

Instrument:	Agilent gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS or equivalent; 30m x .25mm x .25µm
Carrier Gas:	Helium at 1 mL/min
Temperatures:	Injector: 280°C MSD transfer line: 280°C MS Source: 230°C MS Quad: 150°C Oven program: 1) 100°C initial temperature for 1.0 min 2) Ramp to 300°C at 12°C/min 3) Hold final temperature for 9.0 min
Injection Parameters:	Split Ratio = 20:1, 1 µL injected
MS Parameters:	Mass scan range: 30-550 amu Threshold: 100 Tune file: stune.u Acquisition mode: scan
Retention Time:	7.145 minutes

EI Mass Spectrum: 4-Methylmethcathinone HCl Lot # SF0002

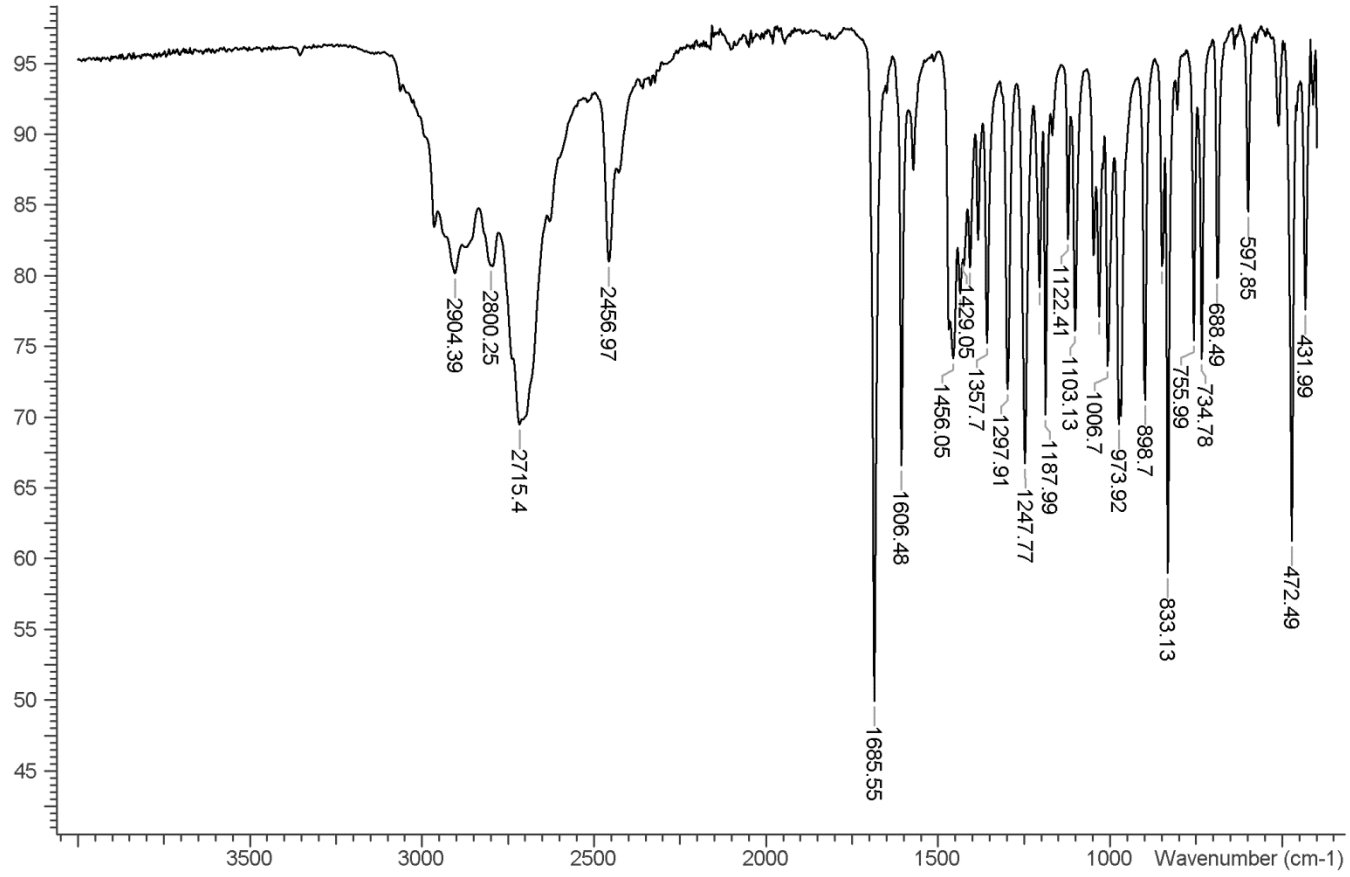


4.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (3 bounce)

Scan Parameters: Number of scans: 32
Number of background scans: 32
Resolution: 4cm^{-1}
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): 4-Methylmethcathinone HCl Lot # SF0002



FTIR ATR (Diamond, 3 Bounce): 4-Methylmethcathinone HCl Lot # SF0002