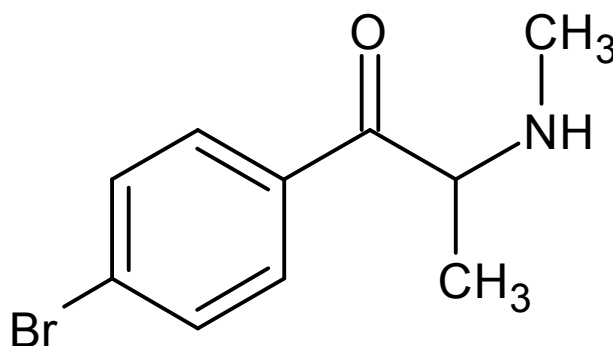




4-Bromomethcathinone

The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.



1. GENERAL INFORMATION

IUPAC Name:	1-(4-bromophenyl)-2-(methylamino)propan-1-one
CAS#:	486459-03-4 (base); 135333-27-6 (HCl)
Synonyms:	4-bromo-N-methylcathinone, 4-BMC, brephedrone
Source:	DEA Reference Material Collection
Appearance:	White powder (HCl)
UV_{max}(nm):	Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₀ H ₁₂ BrNO	242	Not Determined
HCl	C ₁₀ H ₁₂ BrNO · HCl	278	97.6



4-Bromomethcathinone

The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.



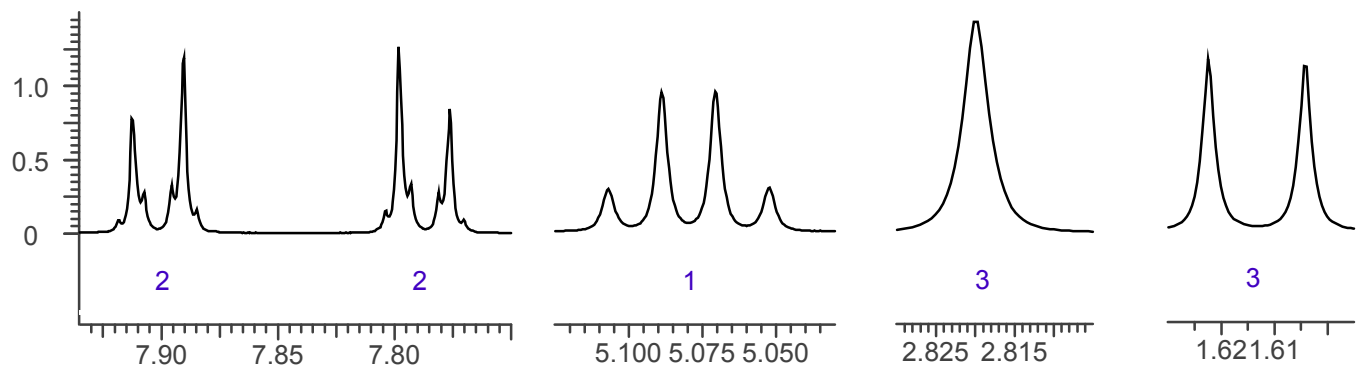
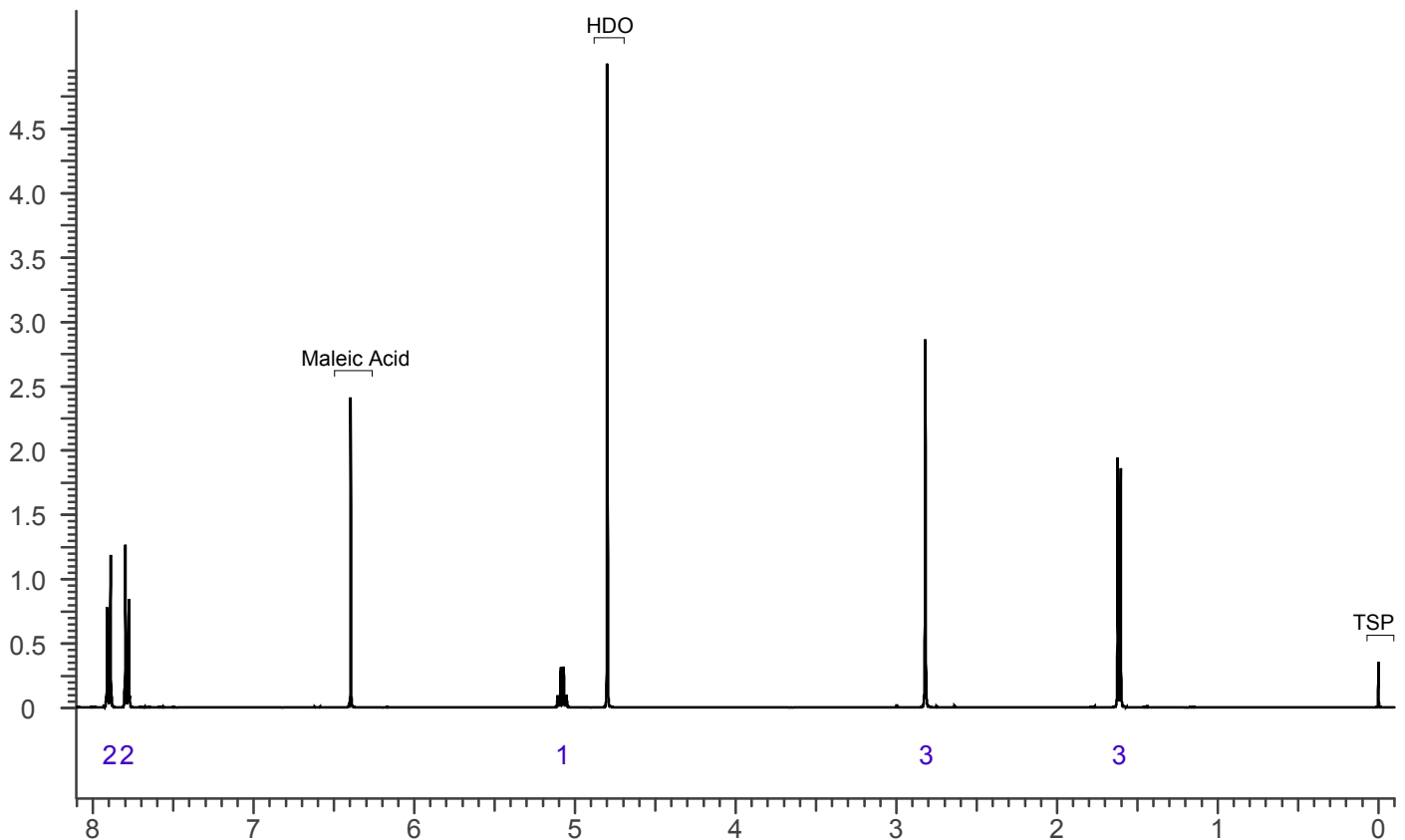
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~25 mg/mL in D₂O 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-bromomethcathinone HCl Lot RM-140723-07; D₂O; 400MHz





4-Bromomethcathinone

The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.



3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

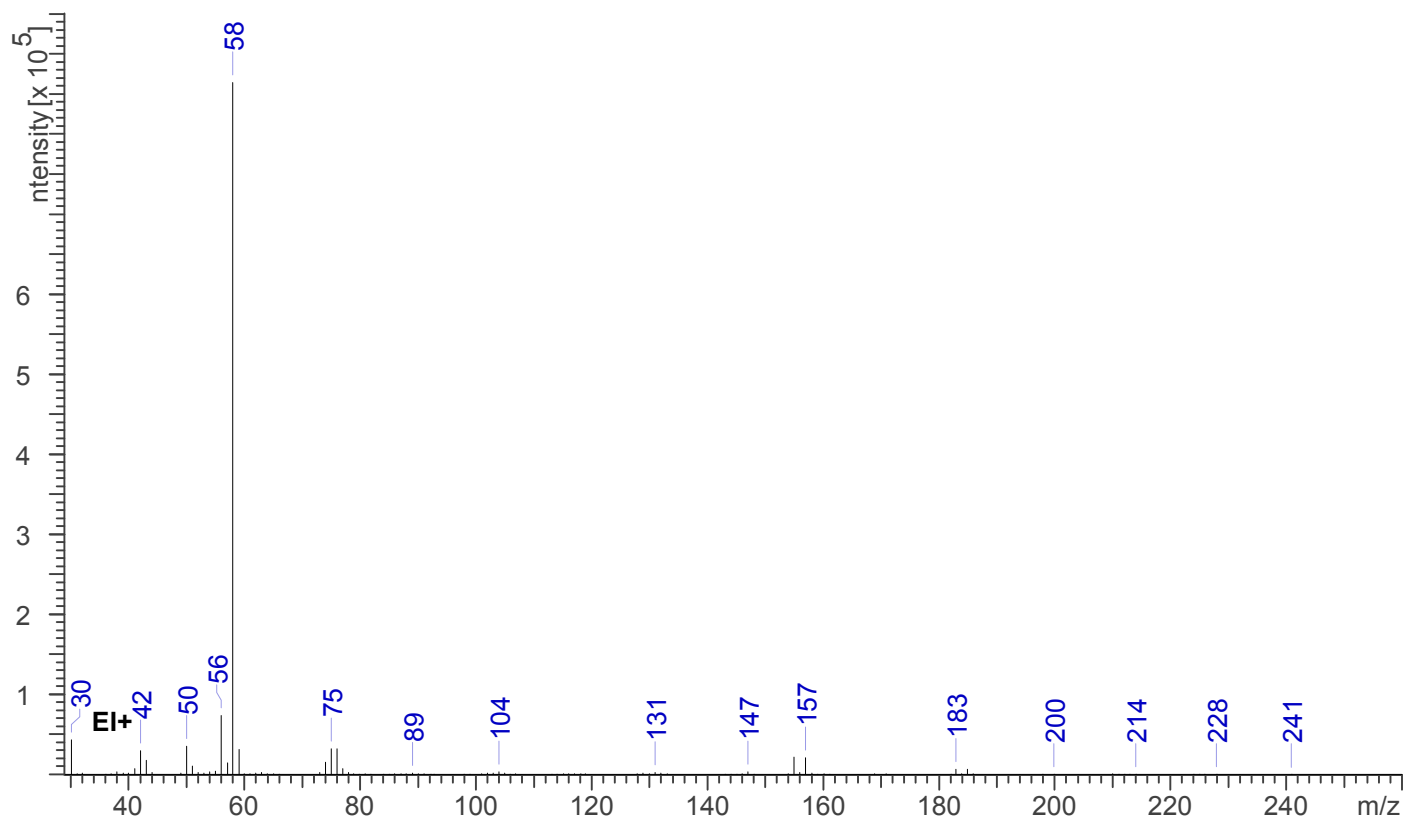
Sample Preparation: Dilute analyte ~4 mg/mL in 1:1 chloroform:methanol.

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 μ m
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 μ L injected
MS Parameters: Mass scan range: 30-550 amu
Threshold: 100
Tune file: stune.u
Acquisition mode: scan

Retention Time: 7.584 min

EI Mass Spectrum: 4-bromomethcathinone HCl Lot RM-140723-07





4-Bromomethcathinone



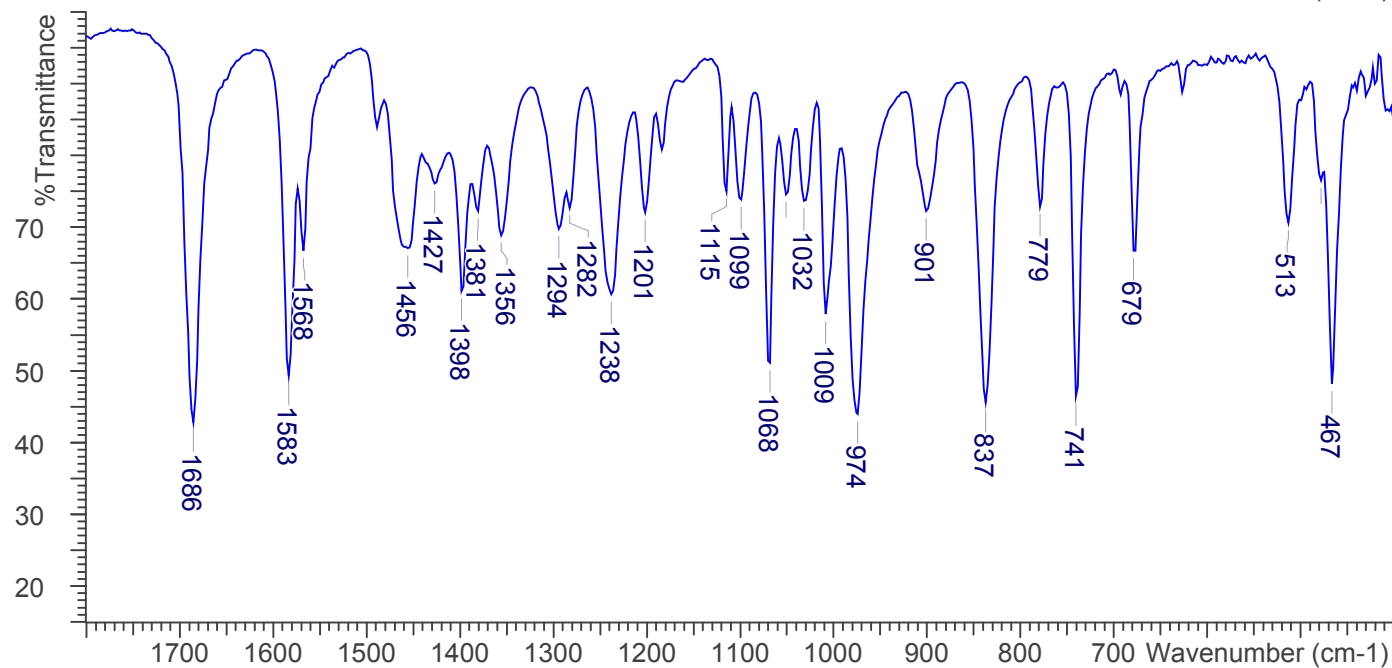
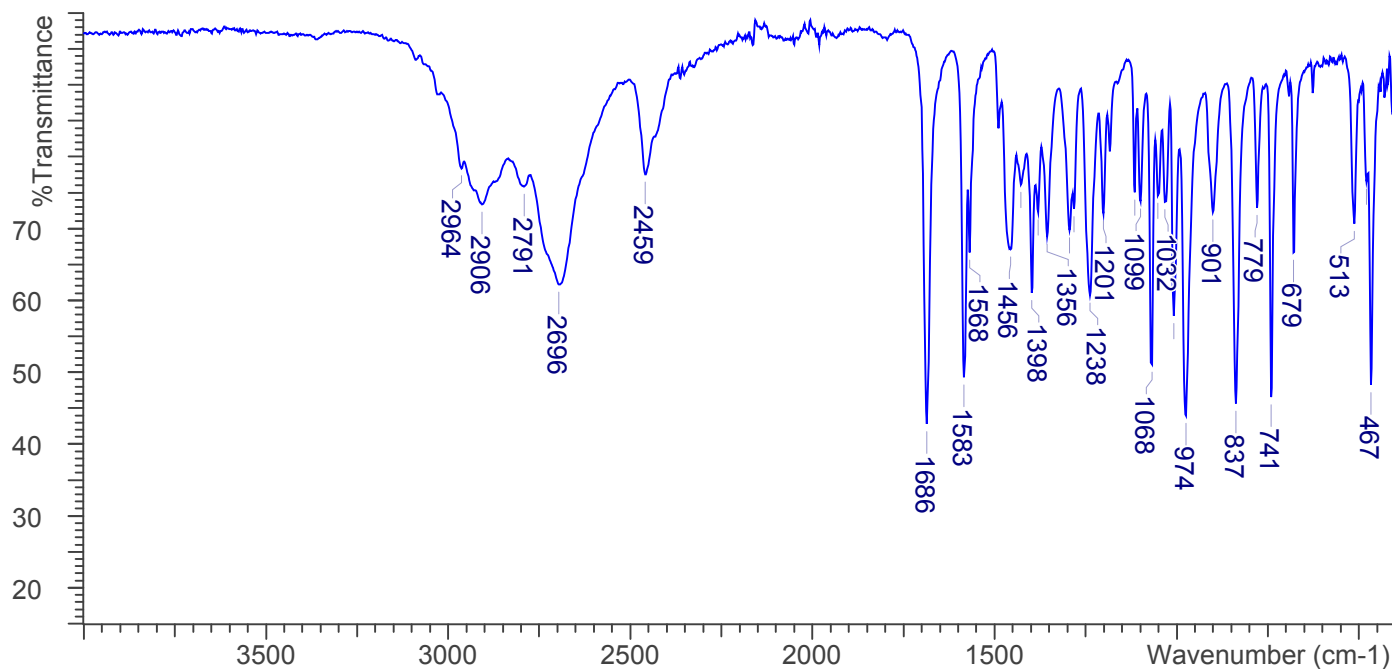
The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.

3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (1 bounce)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4 cm⁻¹
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 1 Bounce): 4-bromomethcathinone HCl Lot RM-140723-07





4-Bromomethcathinone

The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.



4. ADDITIONAL RESOURCES

[Wikipedia](#)