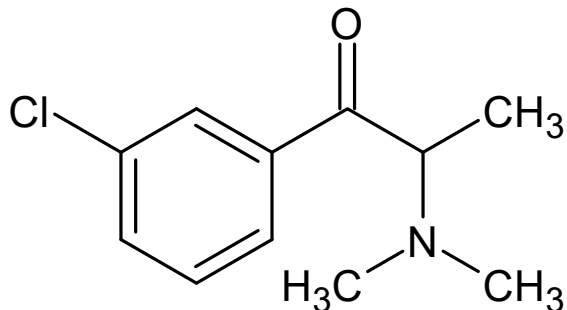




3-Chloro-N,N-Dimethylcathinone

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



1. GENERAL INFORMATION

IUPAC Name: 1-(3-chlorophenyl)-2-(dimethylamino)propan-1-one

CAS#: 514168-22-0 (HCl)

Synonyms: 3-Cl-N,N-DMC, 3-Chloro-N,N-DMC

Source: Cayman Chemical

Appearance: White powder

UV_{max}(nm): Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₁ H ₁₄ ClNO	211.69	N/A
Hydrochloride	C ₁₁ H ₁₄ ClNO HCl	248.15	N/A



3-Chloro-N,N-Dimethylcathinone

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



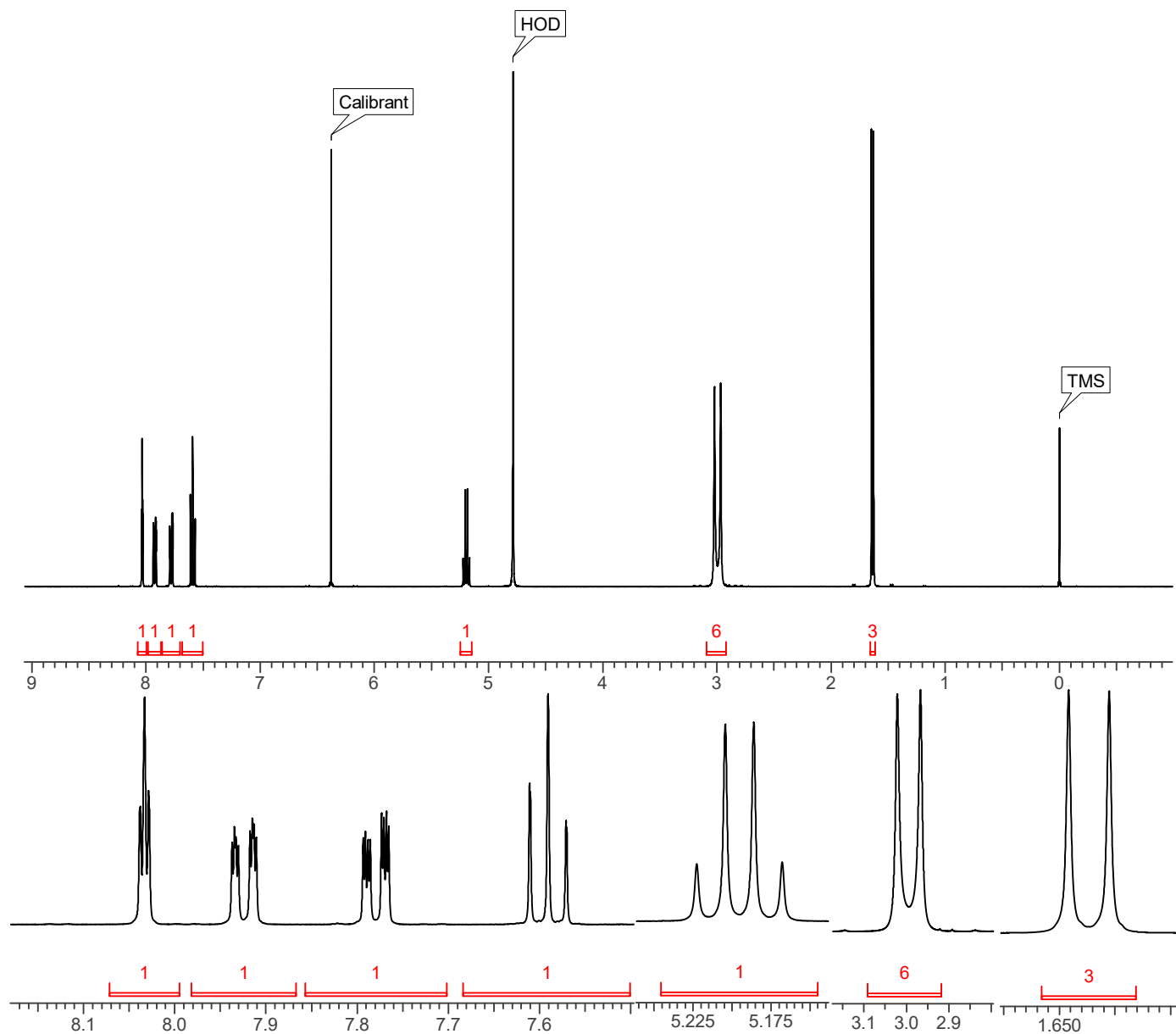
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~15 mg/mL in CDCl₃ containing TMS for 0 ppm reference and dimethyl sulfone 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

¹HNMR: 3-Chloro-N,N-Dimethylcathinone HCl; Lot 0533202-18; D₂O; 400 MHz





3-Chloro-N,N-Dimethylcathinone

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 ~3mg/mL in CHCl₃, base extracted.

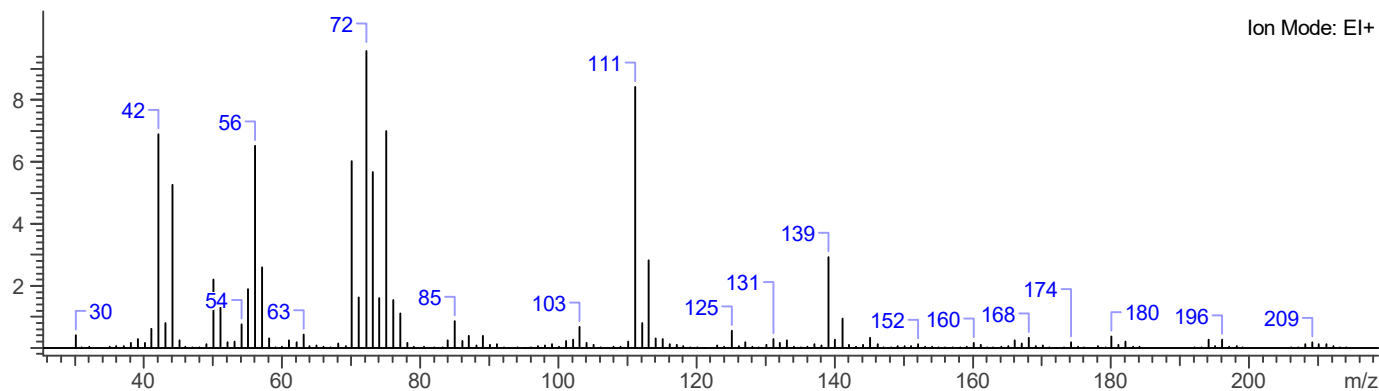
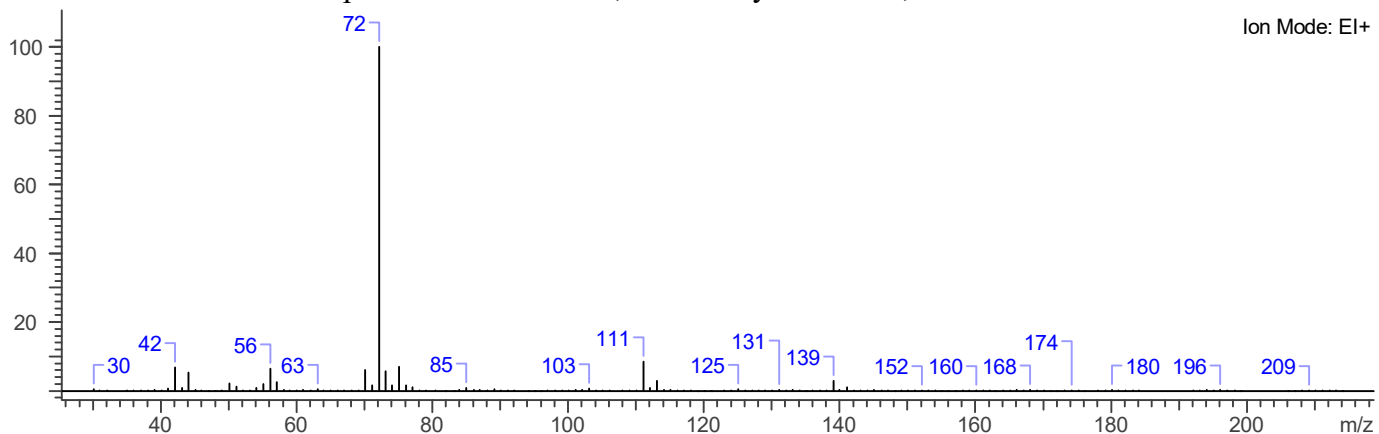
Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: HP-5 MS (or equivalent); 30m x 0.25 mm x 0.25 μm
Carrier Gas: Helium at 1.5 mL/min
Temperatures: Injector: 280°C
 MSD transfer line: 280°C
 MS Source: 230°C
 MS Quad: 150°C
 Oven program:
 1) 100°C initial temperature for 1.0 min
 2) Ramp to 280°C at 12 °C/min
 3) Hold final temperature for 9.0 min

Injection Parameters: Split Ratio = 25:1, 1 μL injected

MS Parameters: Mass scan range: 30-550 amu
 Threshold: 100
 Tune file: stune.u
 Acquisition mode: scan

Retention Time: 6.904 min

EI Mass Spectrum: 3-Chloro-N,N-Dimethylcathinone; Lot#0533202-18





3-Chloro-N,N-Dimethylcathinone

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



3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: Scan FTIR with diamond ATR attachment (1 bounce)
Parameters: Number of scans: 32
Number of background scans: 32
Resolution: 4 cm⁻¹
Sample gain: 4.0
Aperture: 150

FTIR ATR (Diamond 1 Bounce): 3-Chloro-N,N-Dimethylcathinone; Lot# 0533202-18

