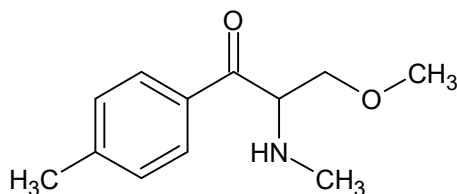




Mexedrone

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



1. GENERAL INFORMATION

IUPAC Name: 3-methoxy-2-(methylamino)-1-(4-methylphenyl)propan-1-one

CAS#: NA

Synonyms: NA

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 ₁₂ H ₁₇ NO ₂	207	Not Determined
HCl	C ₁₂ H ₁₇ NO ₂ HCl	243	193.0-194.1



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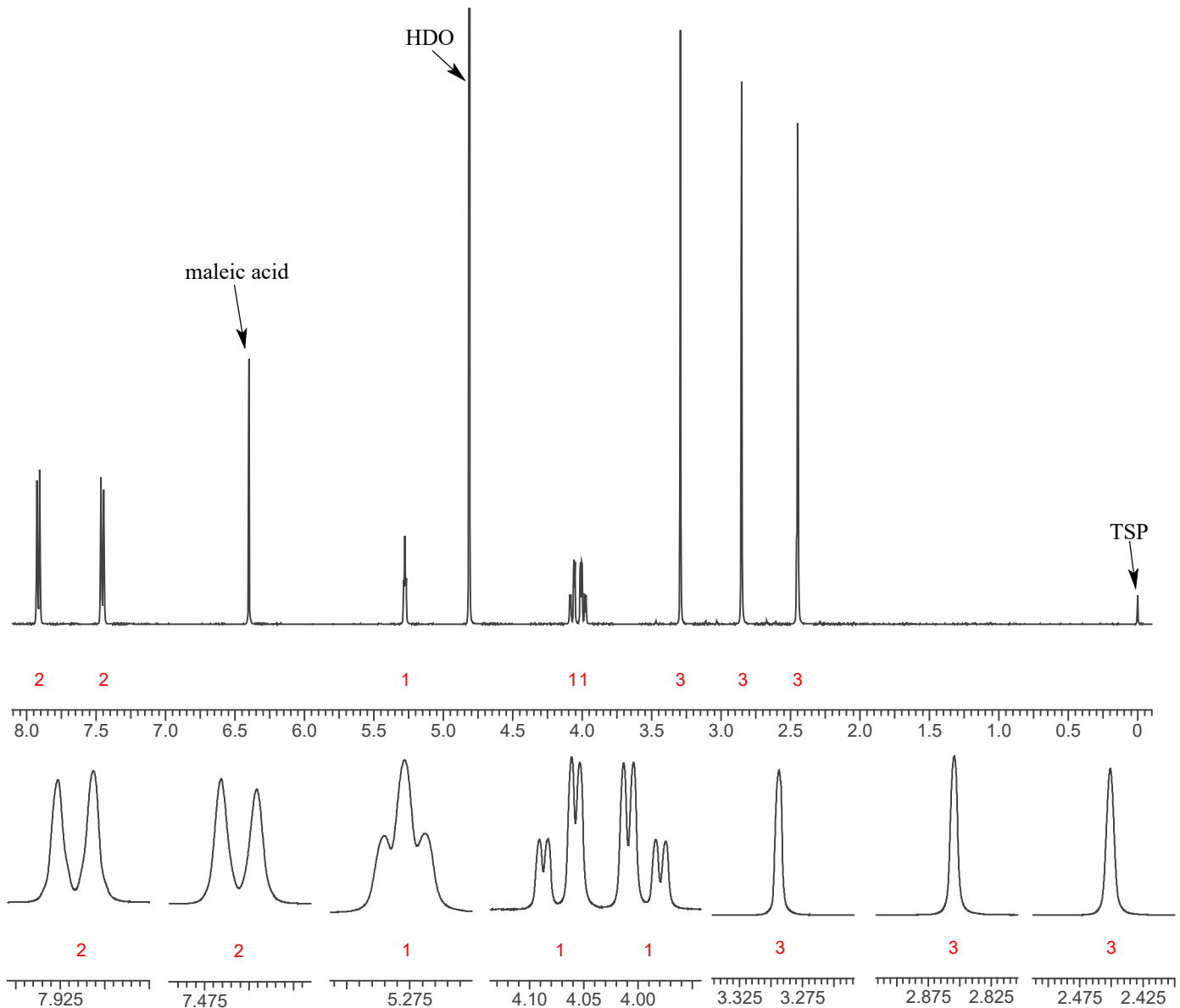
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~26 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

¹HNMR: Mexedrone HCl; Lot# RM-160203-01; D₂O; 400MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in CHCl₃

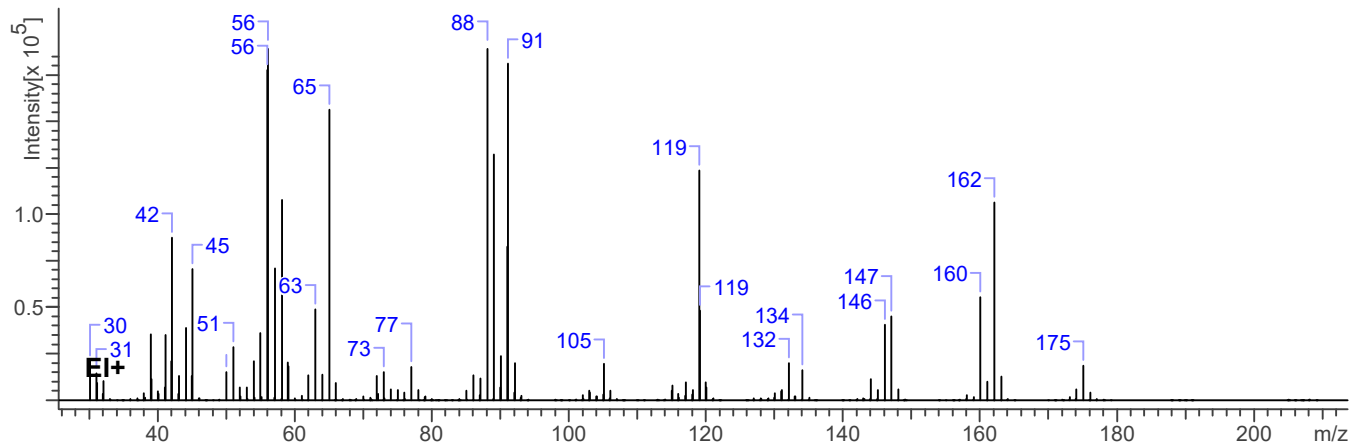
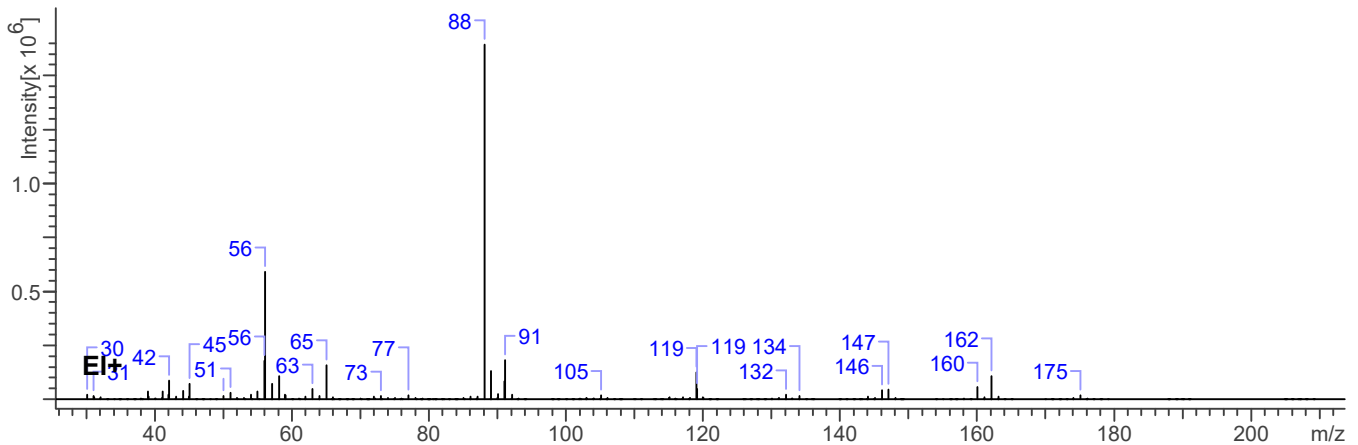
Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: DB-5 MS (or equivalent); 15m x 0.25 mm x 0.25 μm
Carrier Gas: Helium at 1.5 mL/min
Temperatures: Injector: 280°C MSD transfer line: 280°C
MS Source: 250°C MS Quad: 150°C
Oven program:
1) 100°C initial temperature for 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: 150
Tune file: stune.u Acquisition mode: scan

Retention Time: 6.14 min

EI Mass Spectrum: Mexedrone HCl; Lot# RM-160203-01





Mexedrone

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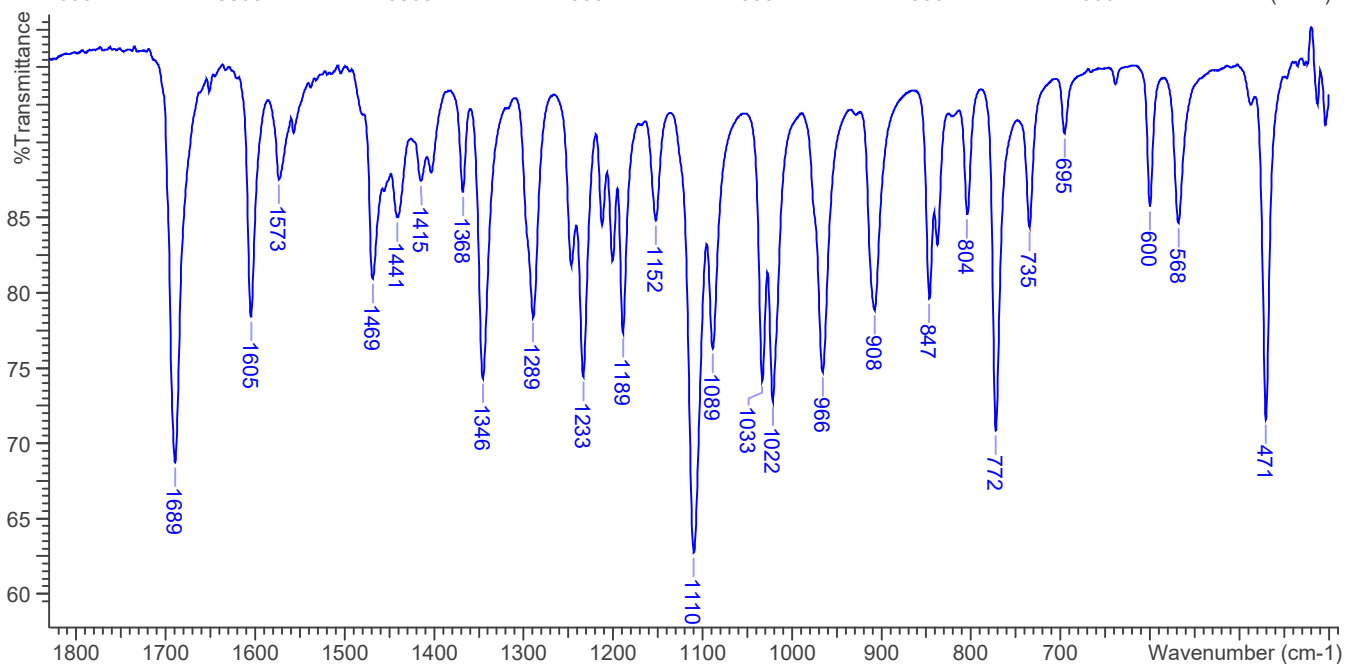
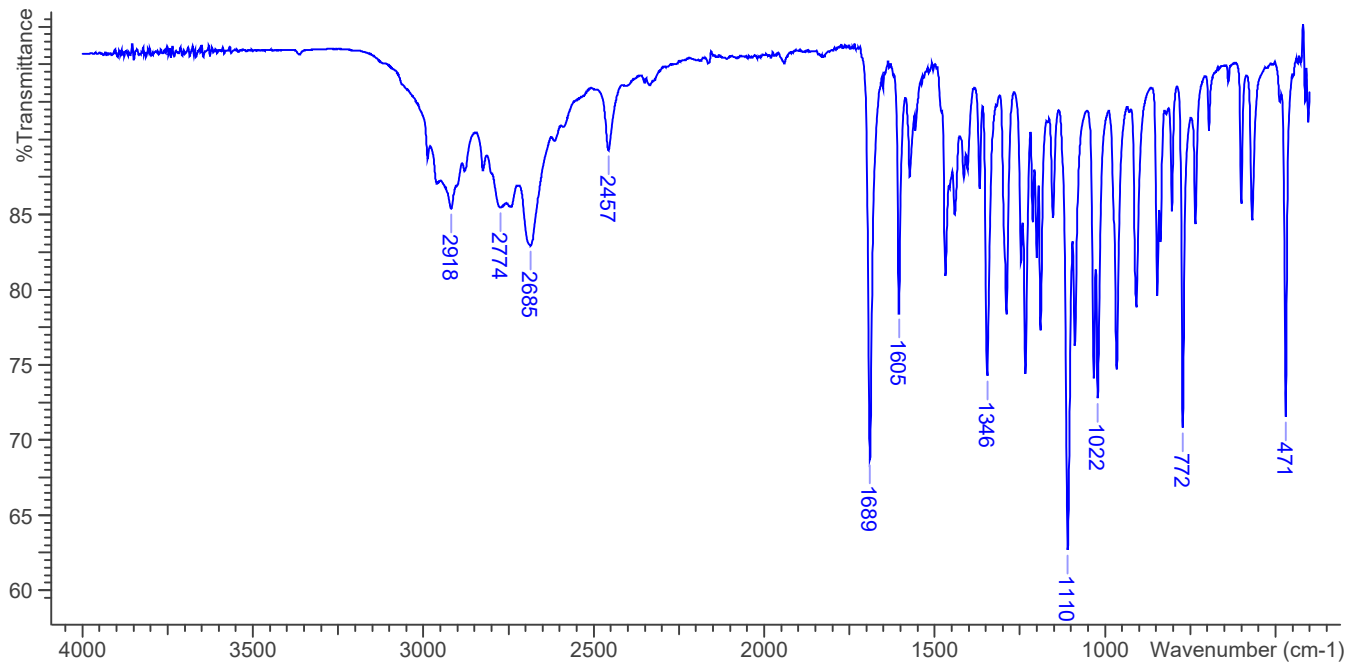


3.3 INFRARED SPECTROSCOPY (FTIR)

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: 1
Aperture: 150

FTIR ATR (Diamond 1 Bounce): Mexedrone HCl; Lot# RM-160203-01





Mexedrone

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4. ADDITIONAL RESOURCES

[*Wikipedia*](#)

[*Forendex*](#)