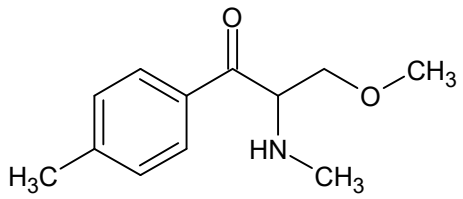
Mexedrone

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 (^{o}C)
Base	$C_{12}H_{17}NO_2$	207	Not Determined
HCl	$C_{12}H_{17}NO_2$ HCl	243	193.0-194.1

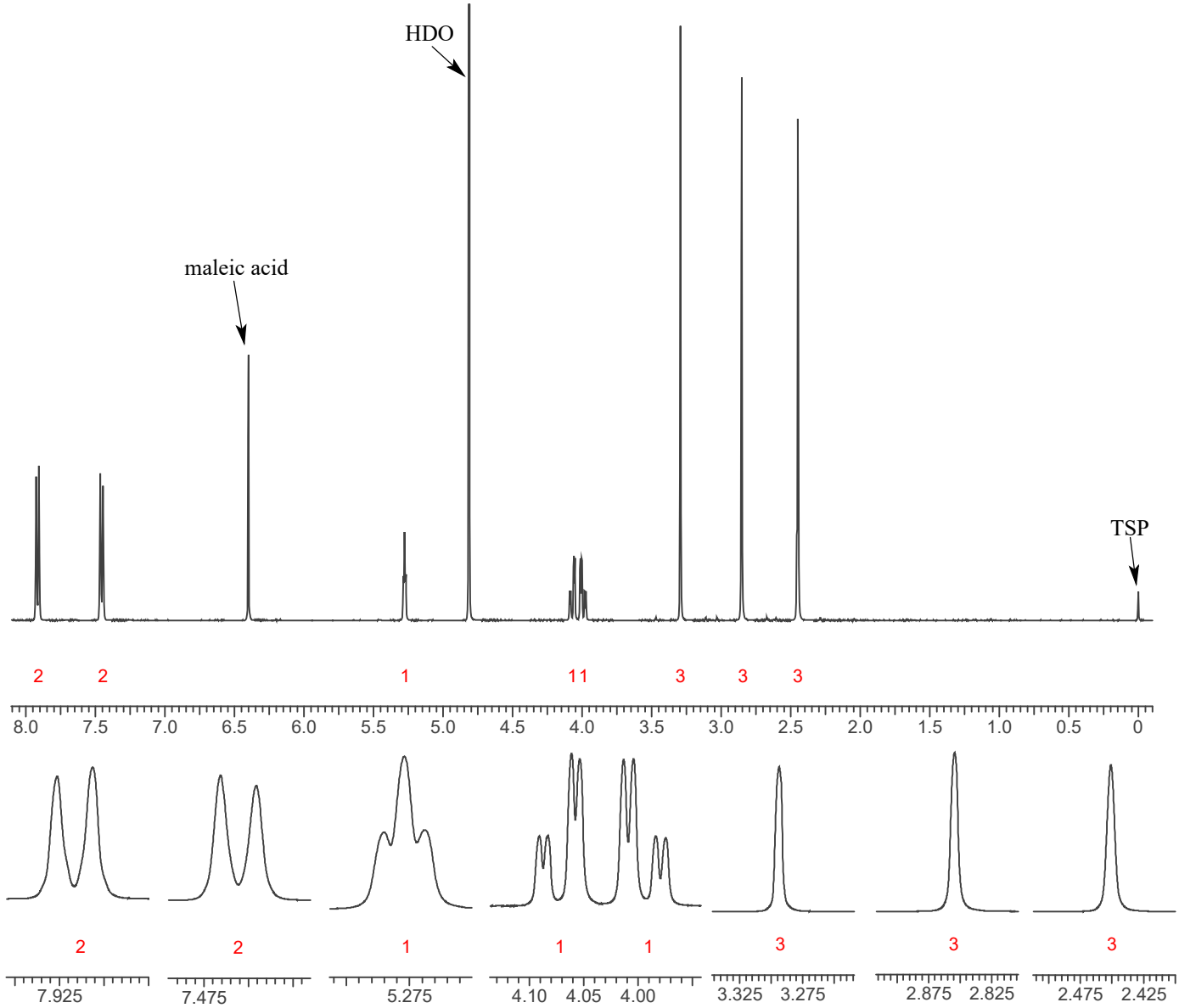
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~26 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

^{1}HNMR: Mexedrone HCl; Lot# RM-160203-01; D_2O; 400MHz

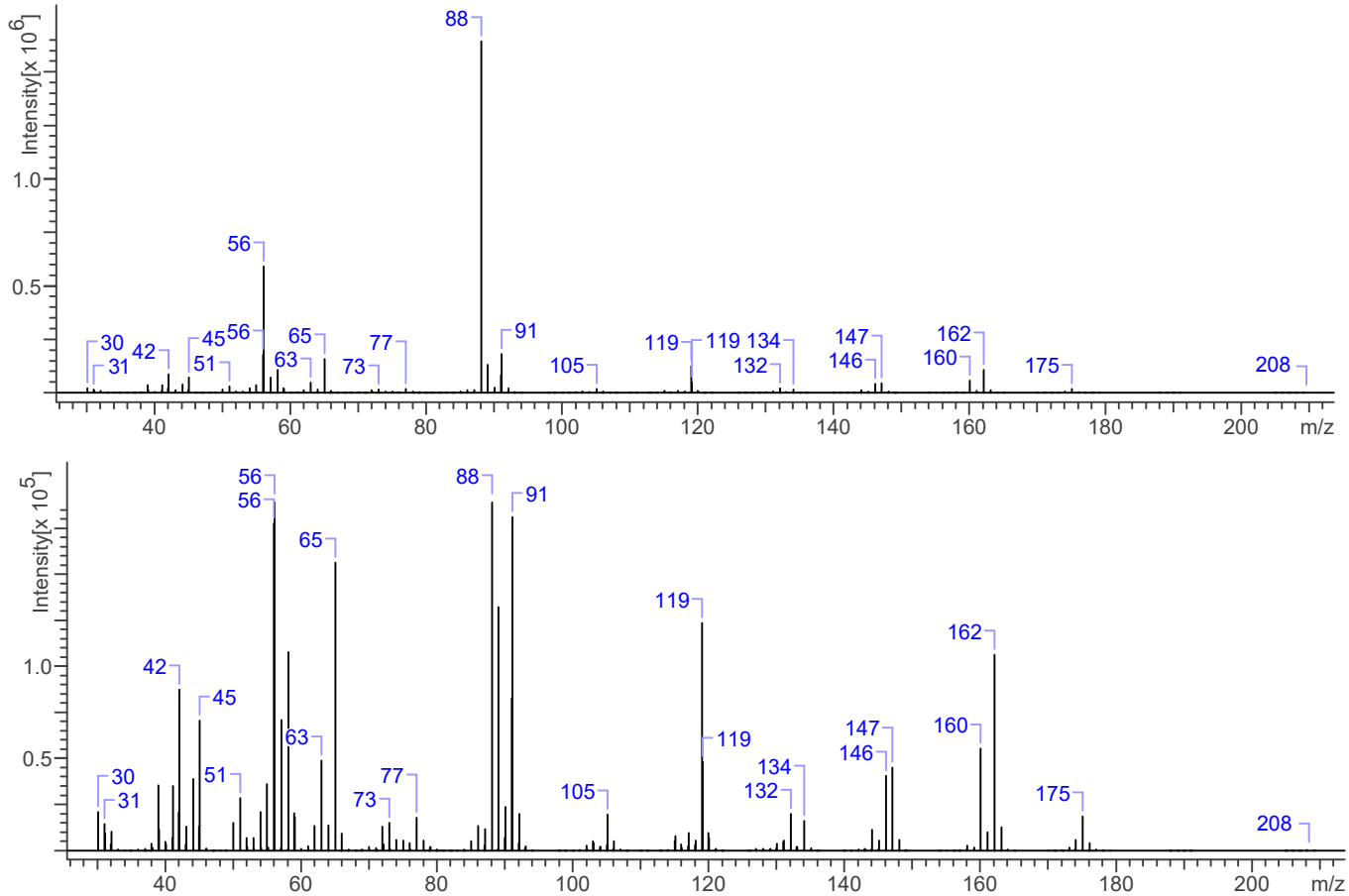


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in $CHCl_3$ (sample base extracted)

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

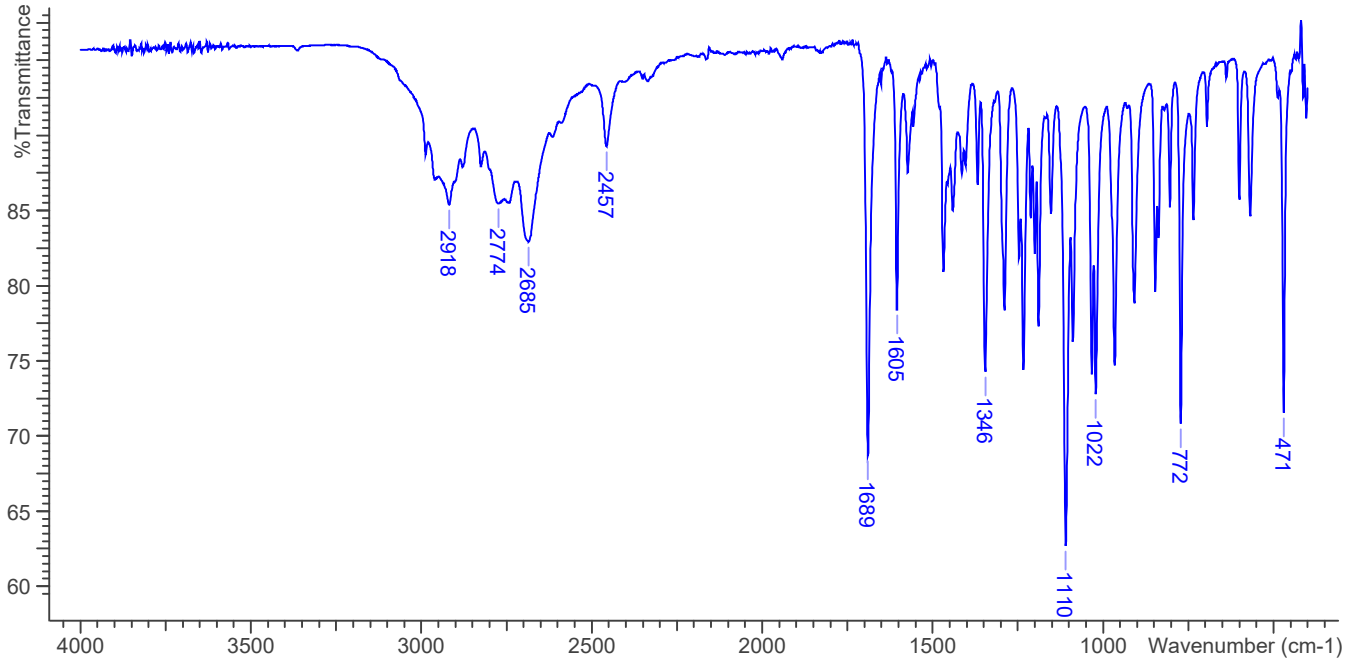


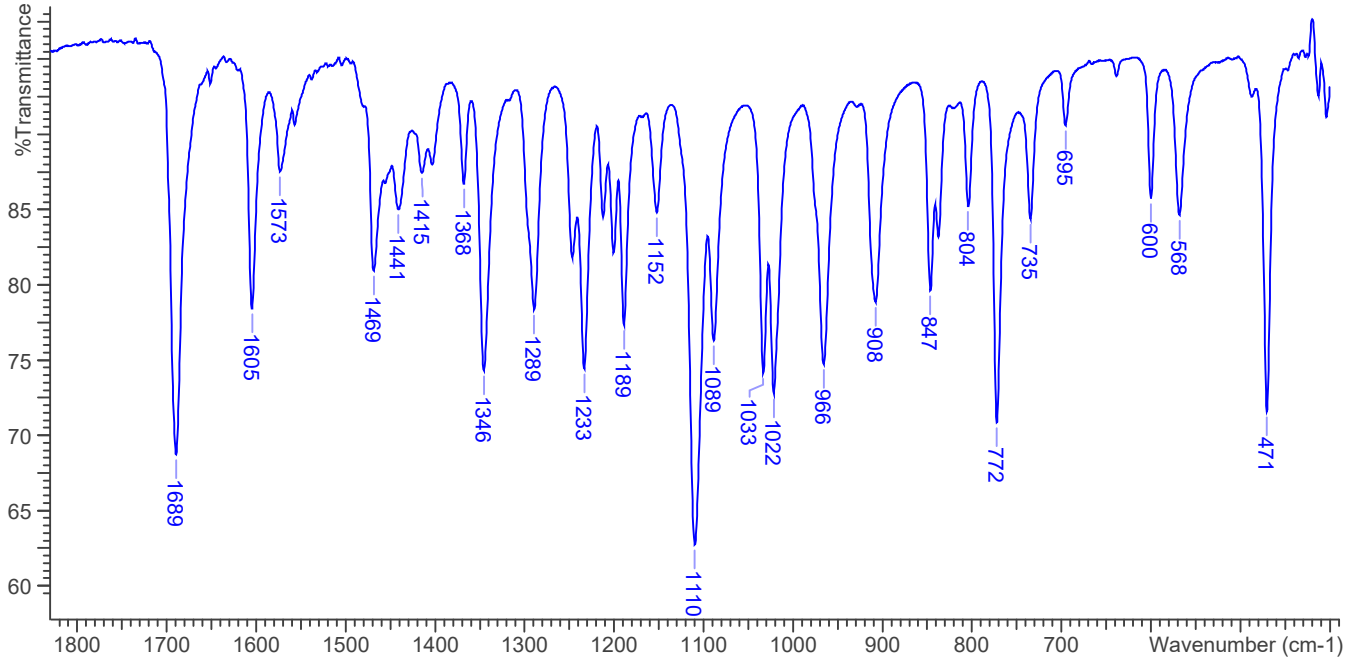
3.3 INFRARED SPECTROSCOPY (FTIR)

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





4. ADDITIONAL RESOURCES

Wikipedia

Forendex