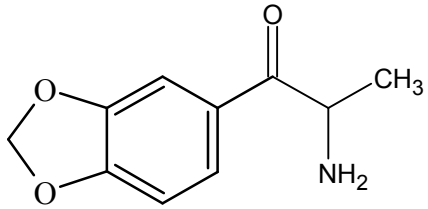
3,4-Methylenedioxycathinone

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



1. GENERAL INFORMATION

IUPAC Name: 2-amino-1-(1,3-benzodioxol-5-yl)propan-1-one

CAS#: Not Available

Synonyms: MDC, MDCATH, Bk-MDA, Amylone

Source: DEA Reference Materials Collection

Appearance: White powder (HCl)

UV_{max} (nm): 280.4 , 316.0

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (^{o}C)
Base	$C_{10}H_{11}NO_3$	193	Not Determined
HCl	$C_{10}H_{11}NO_3 \cdot HCl$	229	210.8

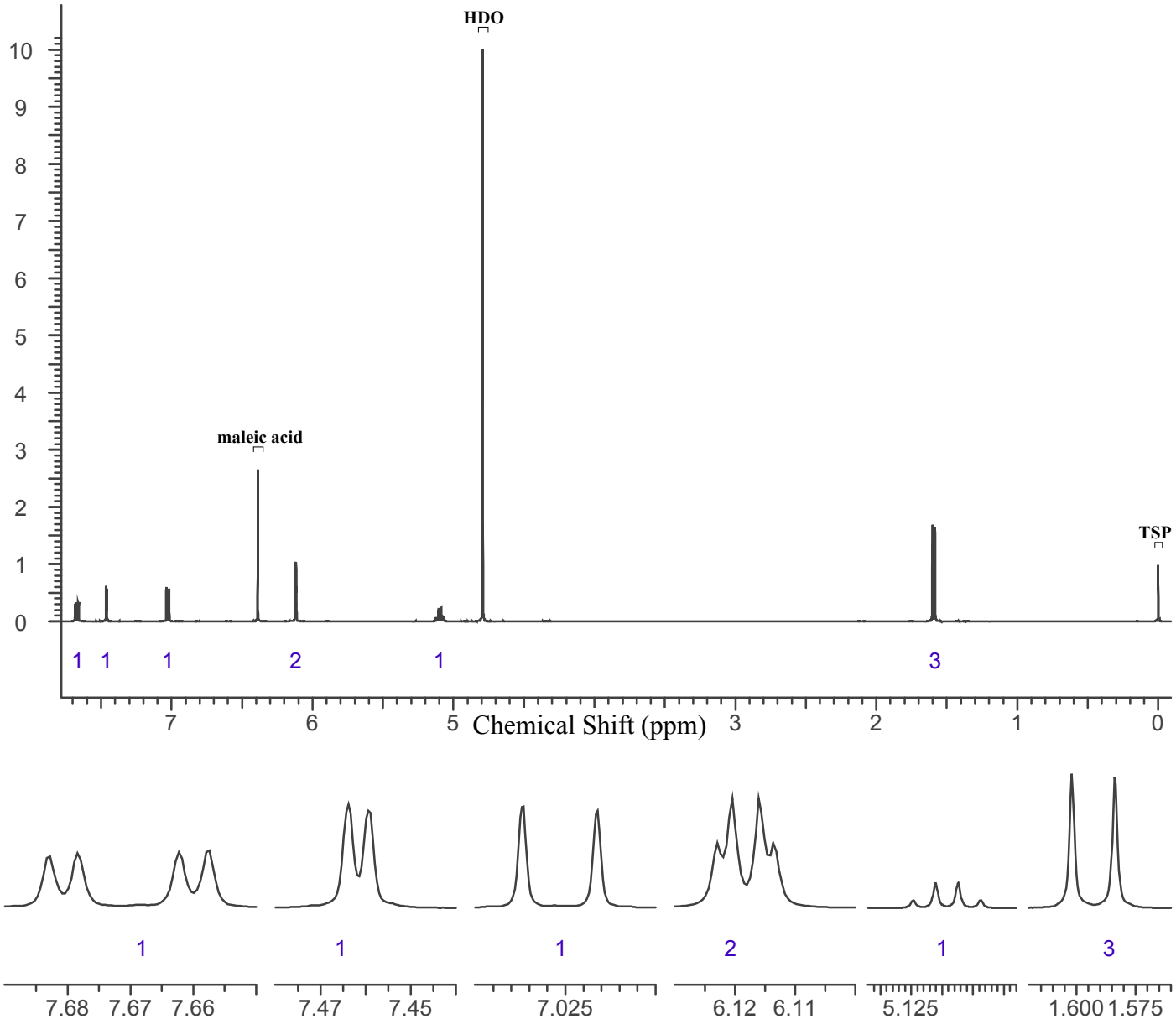
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 mg/mL in deuterium oxide (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: 3,4-Methylenedioxycathinone HCl; Lot TAD21OCT93C; D_2O 400MHz

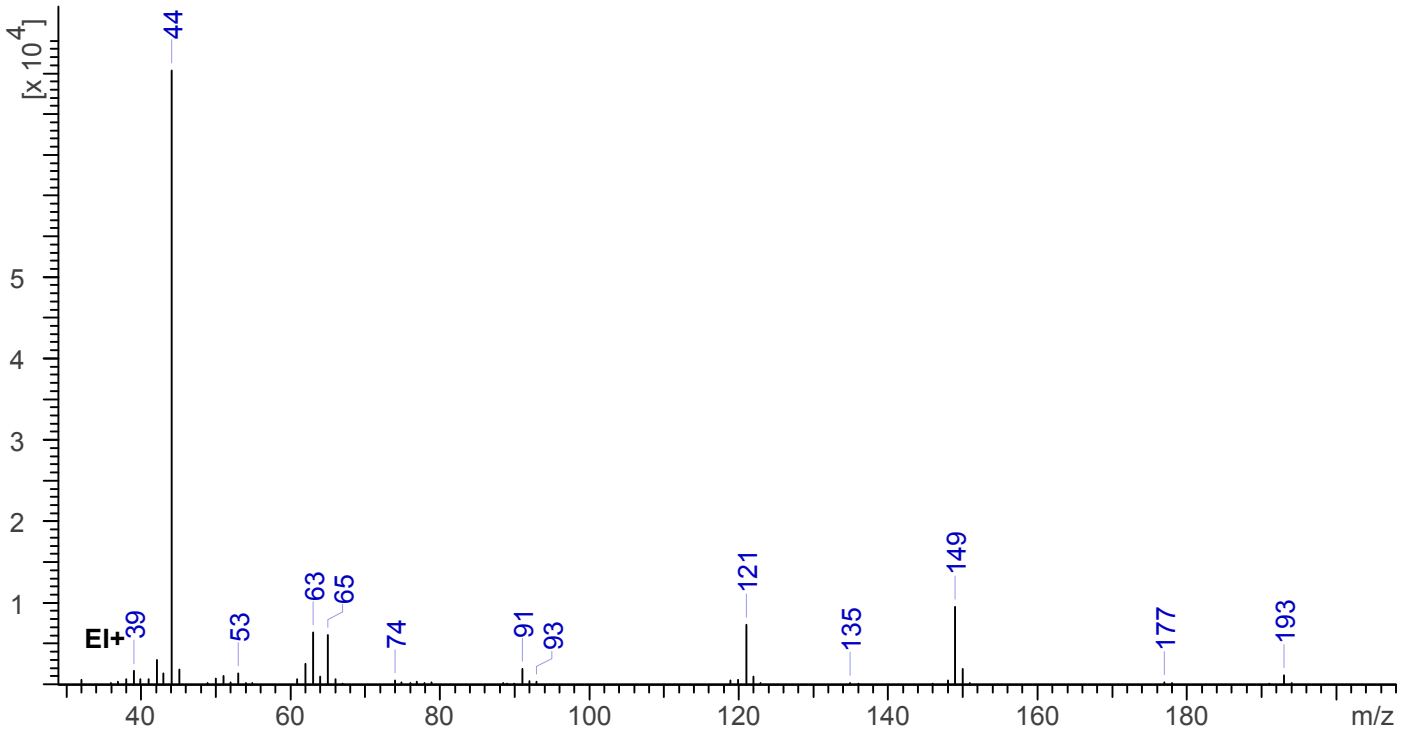


3.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~ 1 mg/mL base extracted into chloroform

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 µm
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:	9.145 min

EI Mass Spectrum: 3,4-Methylenedioxycathinone HCl; Lot TAD21OCT93C

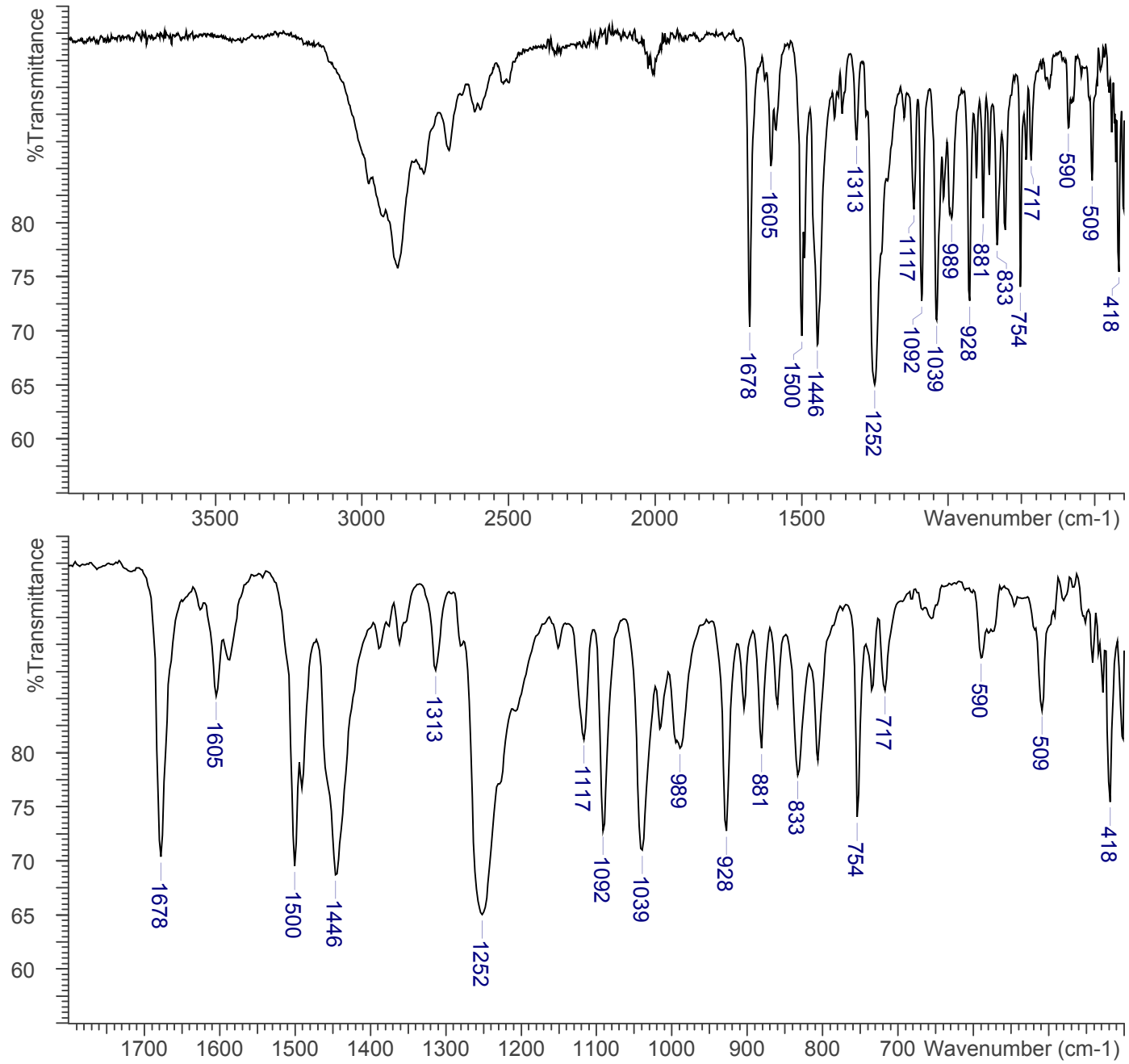


3.3 INFRARED SPECTROSCOPY (FTIR)

Insrument: FTIR with diamond ATR attachment (3 bounce)

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

FTIR ATR (Diamond, 3 Bounce): 3,4-Methylenedioxycathinone HCl; Lot TAD21OCT93C



4. ADDITIONAL RESOURCES

Dal Cason, T. The characterization of some 3,4-methylenedioxycathinone (MDCATH) homologs. Forensic Science International 87(1997) 9-53

Wikipedia