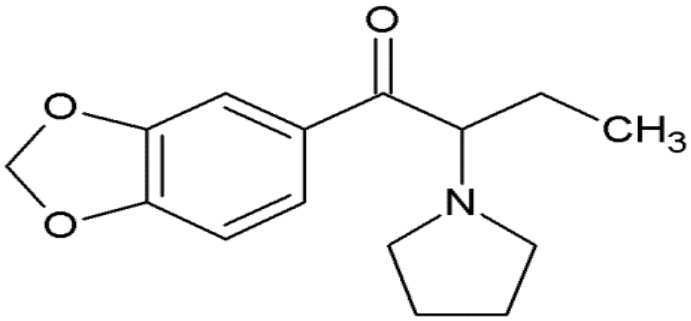
MDPBP

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



1. GENERAL INFORMATION

IUPAC Name:	1-(1,3-benzodioxol-5-yl)-2-(1-pyrrolidinyl)-1-butanone
CAS #:	24622-60-4
Synonyms:	3,4-methylenedioxy-α-pyrrolidinobutiophenone; 3,4-MD-α-PBP; 3,4-MDPBP
Source:	DEA Reference Material Collection
Appearance:	White powder (HCl)
UV_{max}:	Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{15}H_{19}NO_3$	261	Not Determined
HCl	$C_{15}H_{19}NO_3 \cdot HCl$	297	241.9

3. QUALITATIVE DATA

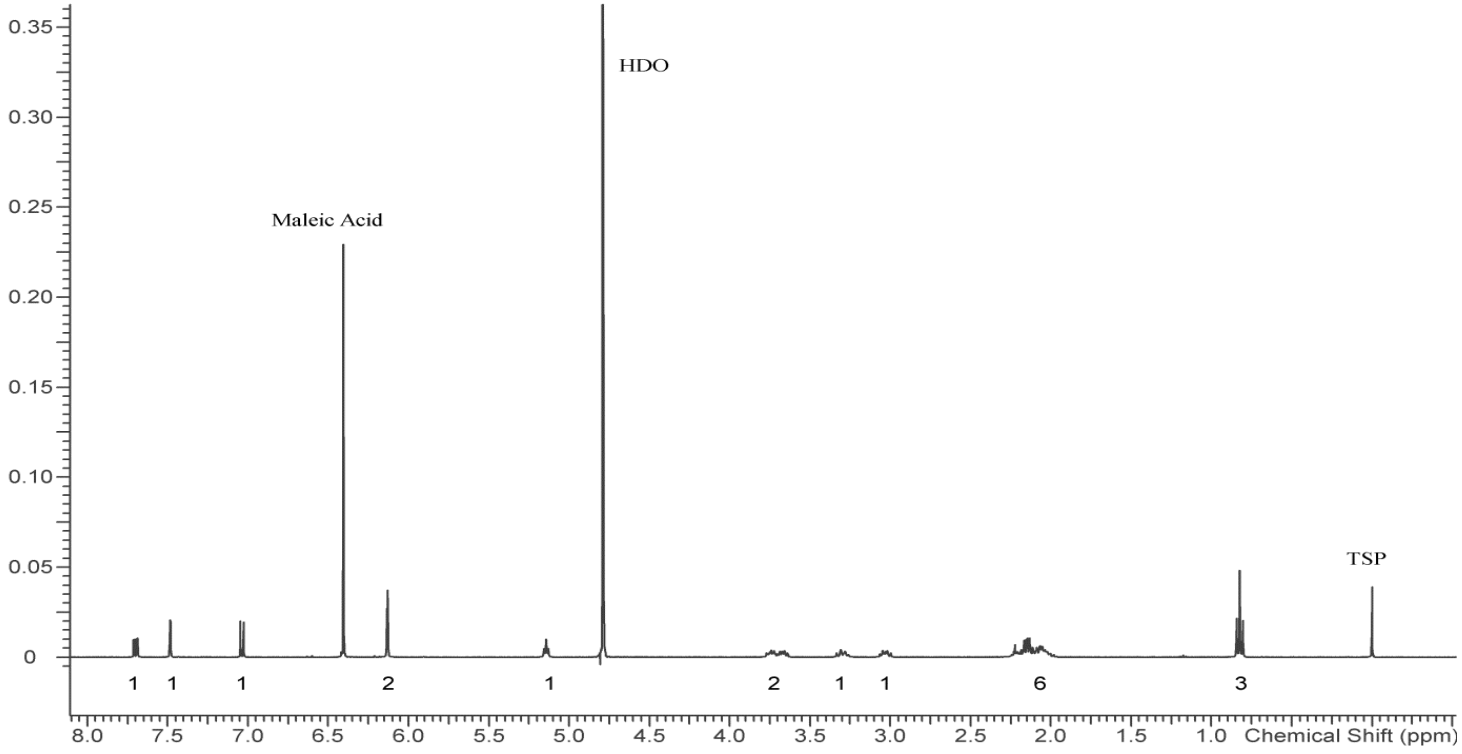
3.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D_2O

Sample Preparation: Dilute analyte to ~5 mg/mL in D_2O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

Instrument:	Varian Mercury 400 MHz NMR spectrometer with proton detection probe
Parameters:	Spectral width: at least containing -3 ppm through 13 ppm Pulse angle: 90° Delay between pulses: 45 seconds Number of scans (NT): 8 Number of steady state scans: 0 Oversampling: 4 or more Shimming: automatic gradient shimming of Z1-4 shims Phasing, Drift Correction: automatic or manual

1H NMR: MDPBP HCl Lot #0435471-8, D_2O, 400MHz



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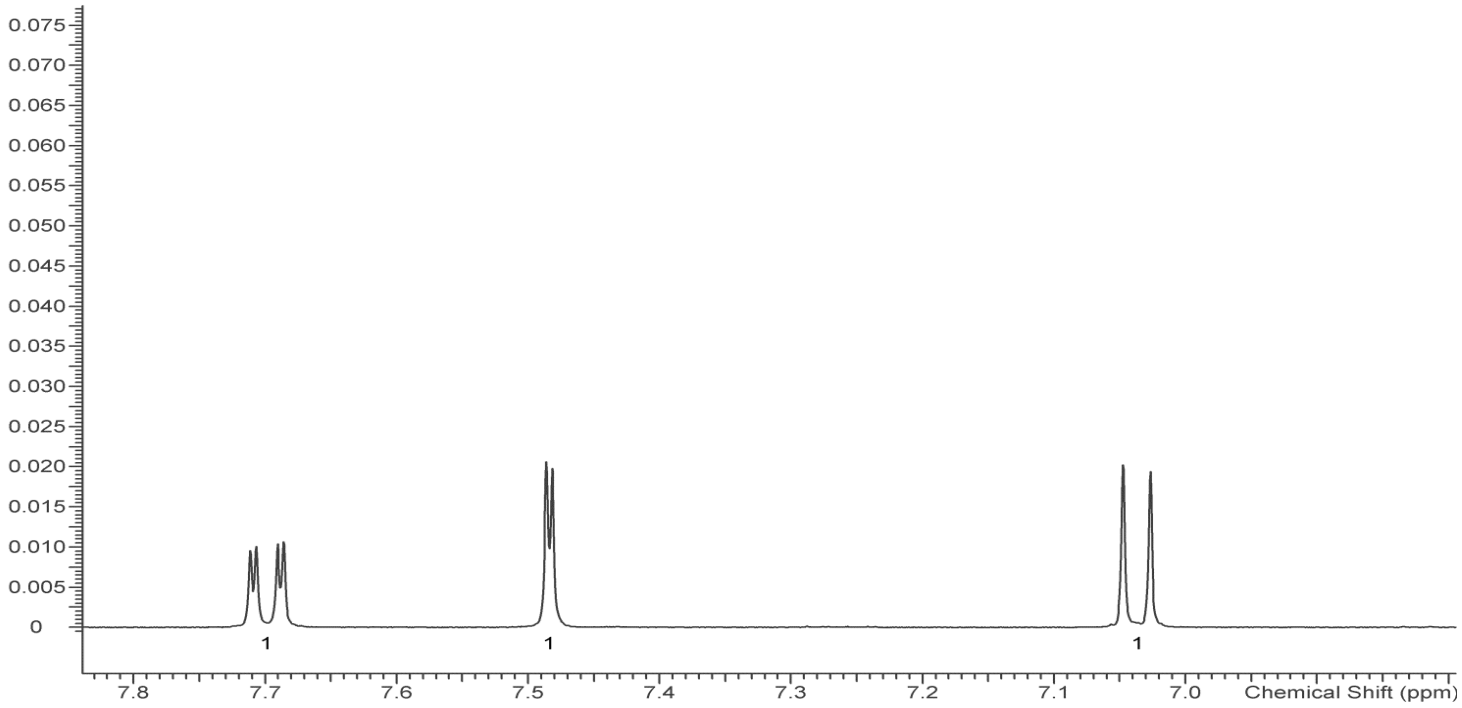

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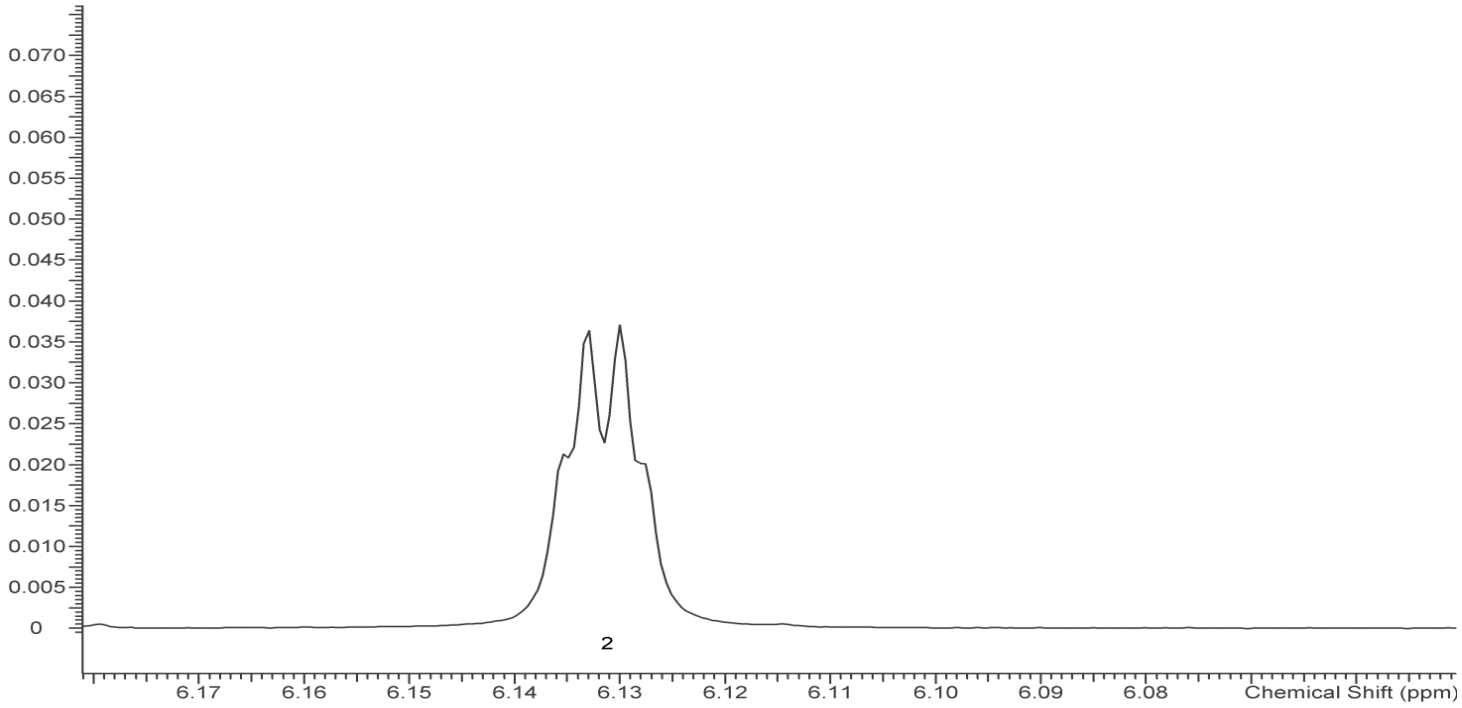

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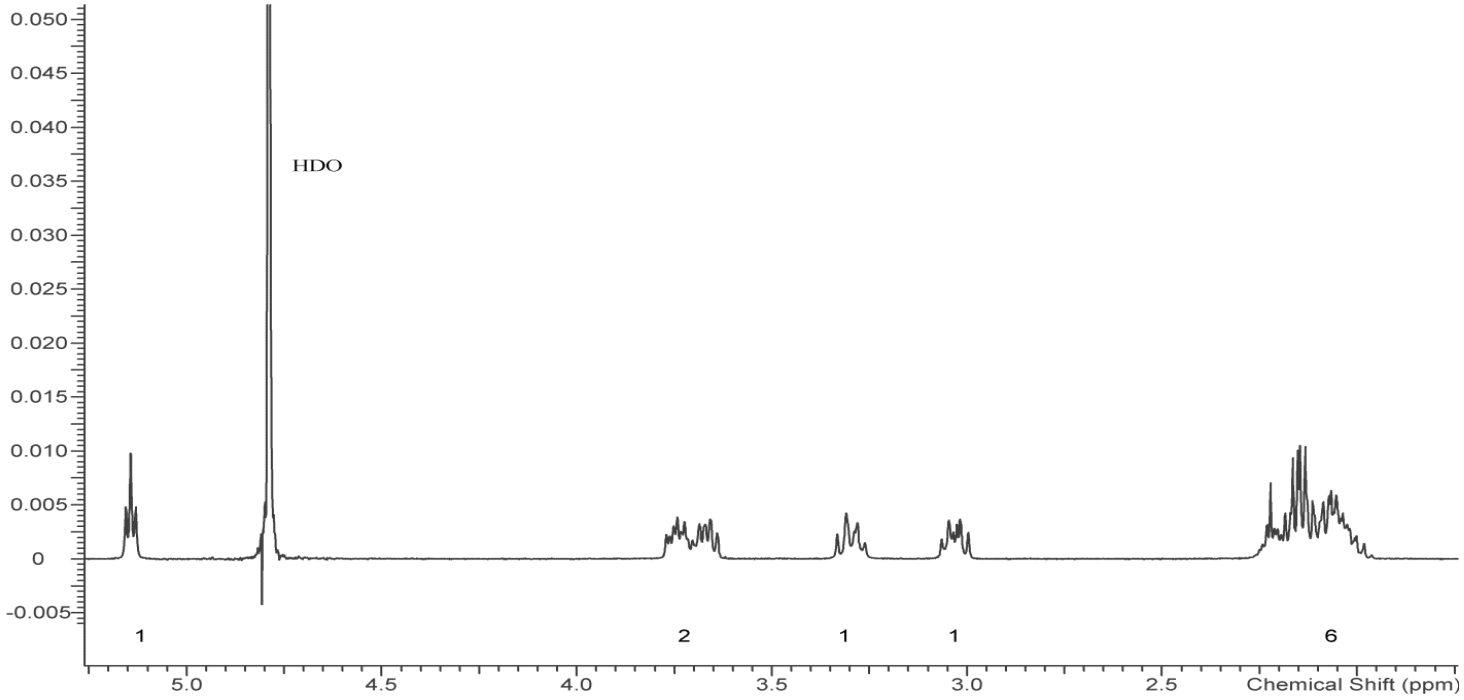
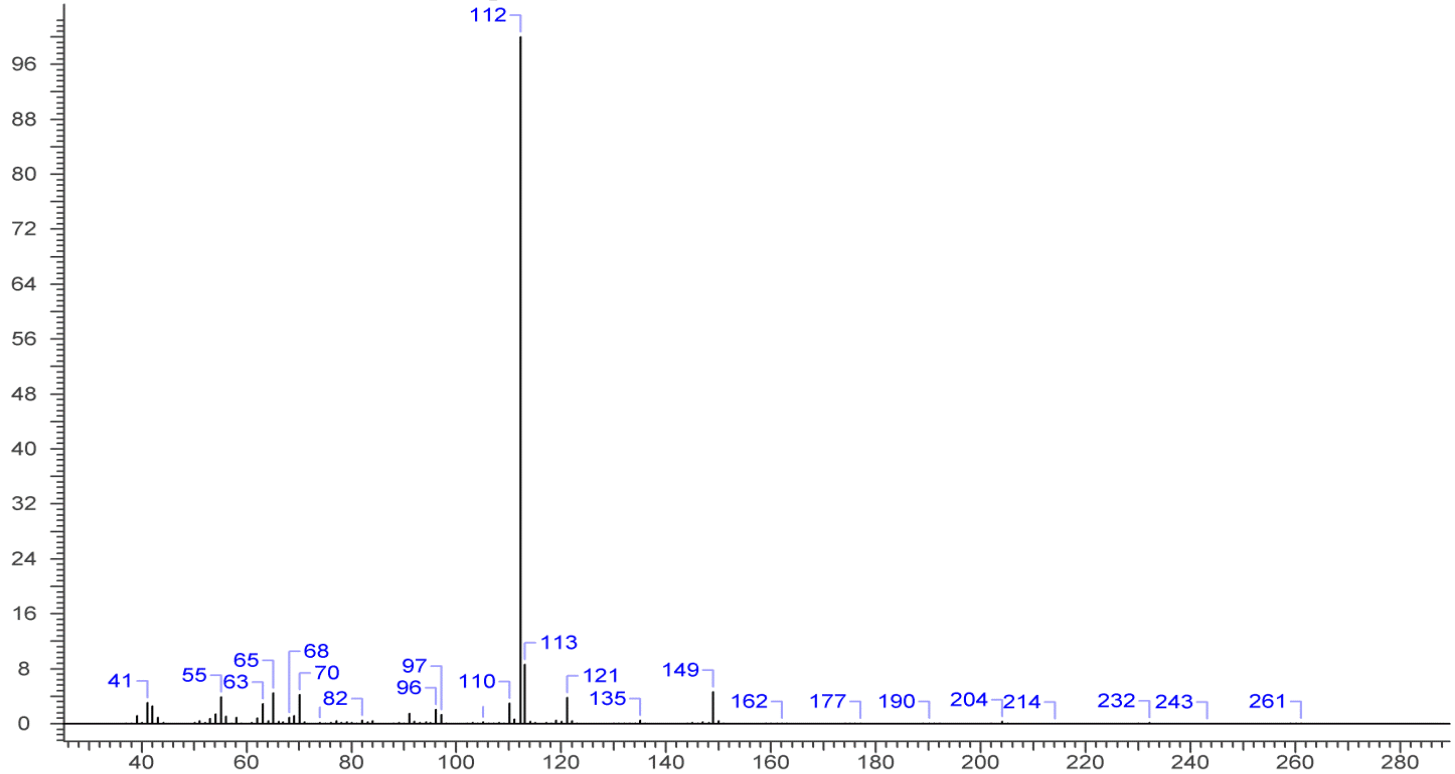


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~4 mg/mL in $CHCl_3$.

Instrument:	Gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS or equivalent; 30m x 0.25mm x 0.25µm
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:	12.799 minutes

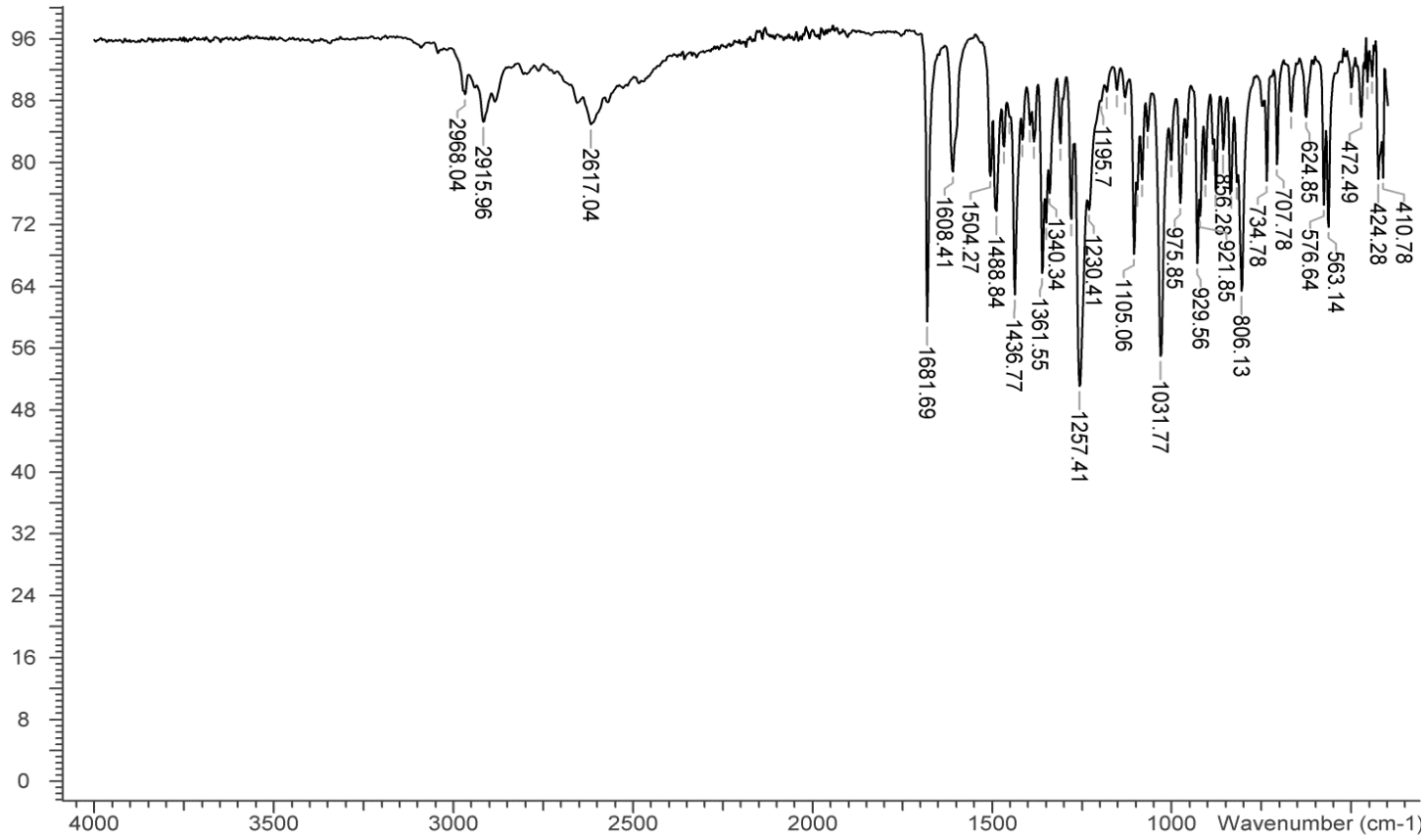
EI Mass Spectrum: MDPBP HCl Lot # 0435471-8



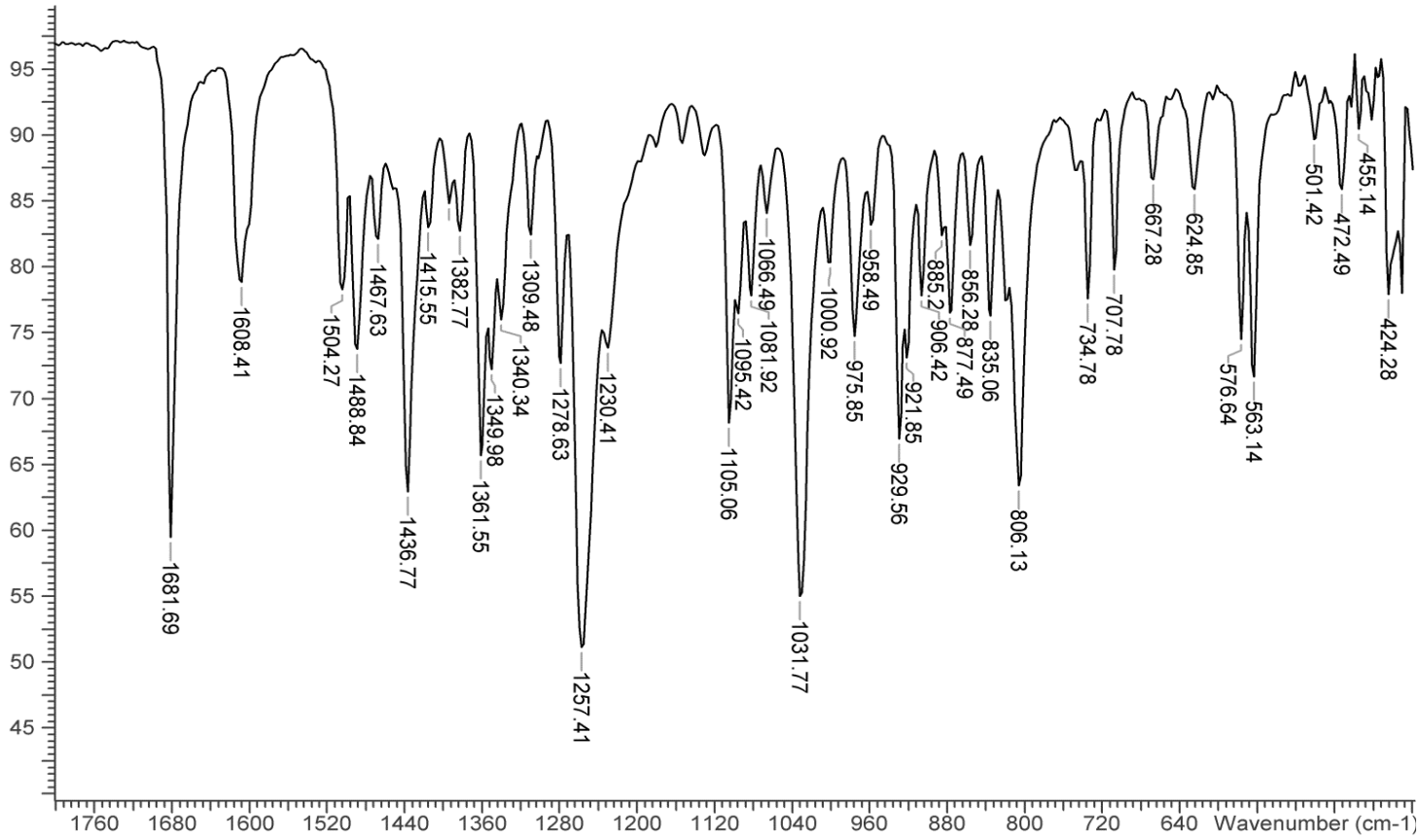
3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (3 bounce)
Scan Parameters: Number of scans: 32
Number of background scans: 32
Resolution: 4cm^{-1}
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): MDPBP HCl Lot # 0435471-8



FTIR ATR (Diamond, 3 Bounce): MDPBP HCl Lot # 0435471-8



4. ADDITIONAL RESOURCES

Forendex

Wikipedia

F. Westphal, T. Junge, B. Klein, G. Fritschi, U. Girreser. Spectroscopic characterization of 3,4-methylenedioxypyrrolidinobutyrophenone: A new designer drug with α-pyrrolidinophenone structure. Forensic Science International 209 (2011) 126-132.