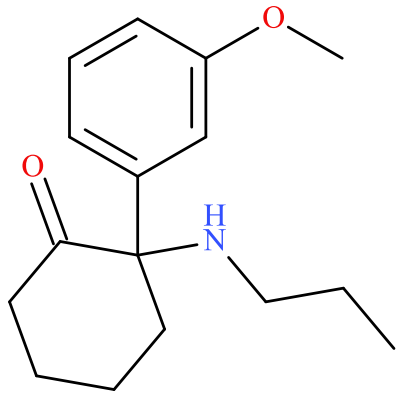
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

Methoxpropamine (MXPr)

Sample Type: **Seized Material**



Latest Revision: **April 13, 2020**

Date Received: **November 13, 2019**

Date of Report: **April 13, 2020**

1. GENERAL INFORMATION

IUPAC Name:	2-(3-methoxyphenyl)-2-(propylamino)cyclohexanone
InChI String:	InChI=1S/C16H23NO2/c1-3-11-17-16(10-5-4-9-15(16)18)13-7-6-8-14(12-13)19-2/h6-8,12,17H,3-5,9-11H2,1-2H3
CFR:	Not Scheduled (04/2020)
CAS#	Not Available
Synonyms:	MXPr, 3-methoxy-2-oxo-PCPr, 3-MeO-2'-OxO-PCPr
Source:	Department of Homeland Security
Appearance:	White Solid Material

***Important Note**: All identifications were made based on evaluation of analytical data (GC-MS, LC-QTOF-MS, and NMR), as no standard reference material was available at the time of testing. Delay between date of receipt and date of report may be due to the requirement of complex analytical testing for confirmation.*

***Prepared By:** Alex J. Krotulski, PhD, Melissa F. Fogarty, MSFS, D-ABFT-FT, and Barry K. Logan, PhD, F-ABFT*

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
Base	$C_{16}H_{23}NO_2$	261.4	261	262.1802

3. BRIEF DESCRIPTION

Methoxpropamine (MXPr) is classified as a novel hallucinogen, with subclassification as an arylcyclohexylamine. Novel hallucinogens have been reported to cause effects similar to ketamine and phencyclidine (PCP). Novel hallucinogens have caused adverse events, including deaths, as described in the literature. Structurally similar arylcyclohexylamines include methoxetamine (MXE) and methoxmetamine (MXM). Analogues in this series are not scheduled in the United States.

4. ADDITIONAL RESOURCES

https://www.wikiwand.com/en/Arylcyclohexylamine

No other resources available at this time.

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

Testing Performed At: NMS Labs (Willow Grove, PA)

Sample Preparation: Acid/Base extraction

Instrument: Agilent 5975 Series GC/MSD System

Column: Zebron™ Inferno™ ZB-35HT (15 m x 250 µm x 0.25 µm)

Carrier Gas: Helium (Flow: 1 mL/min)

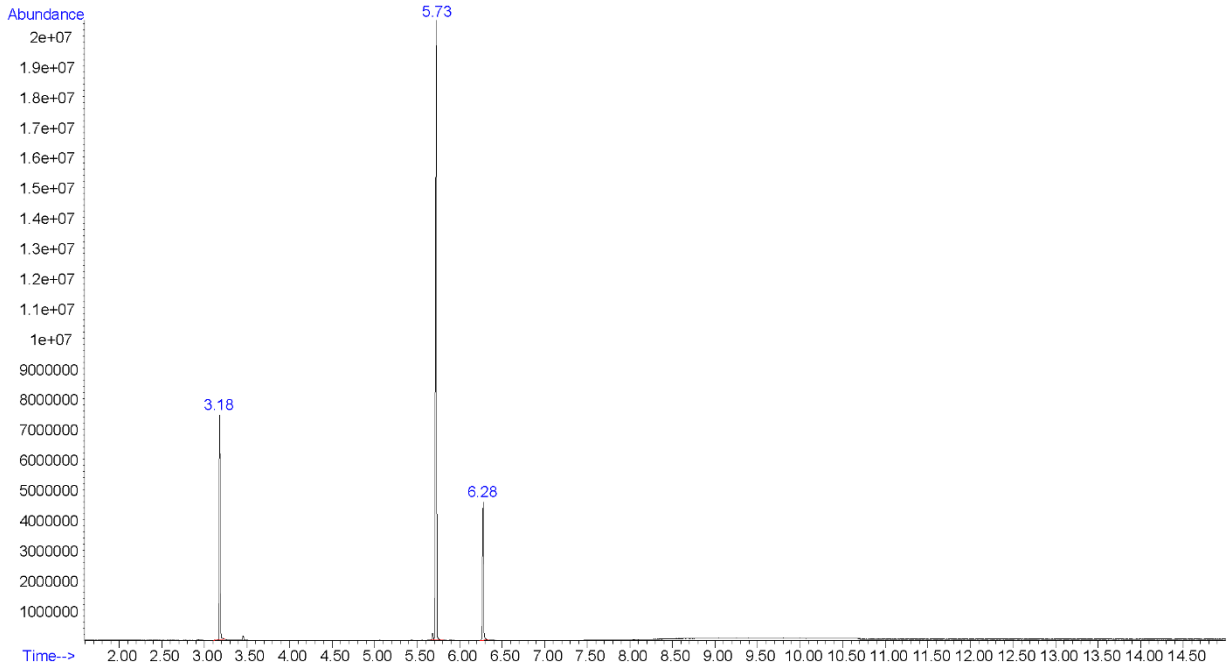
Temperatures: Injection Port: 265 °C

Transfer Line: 300 °C

MS Source: 230 °C

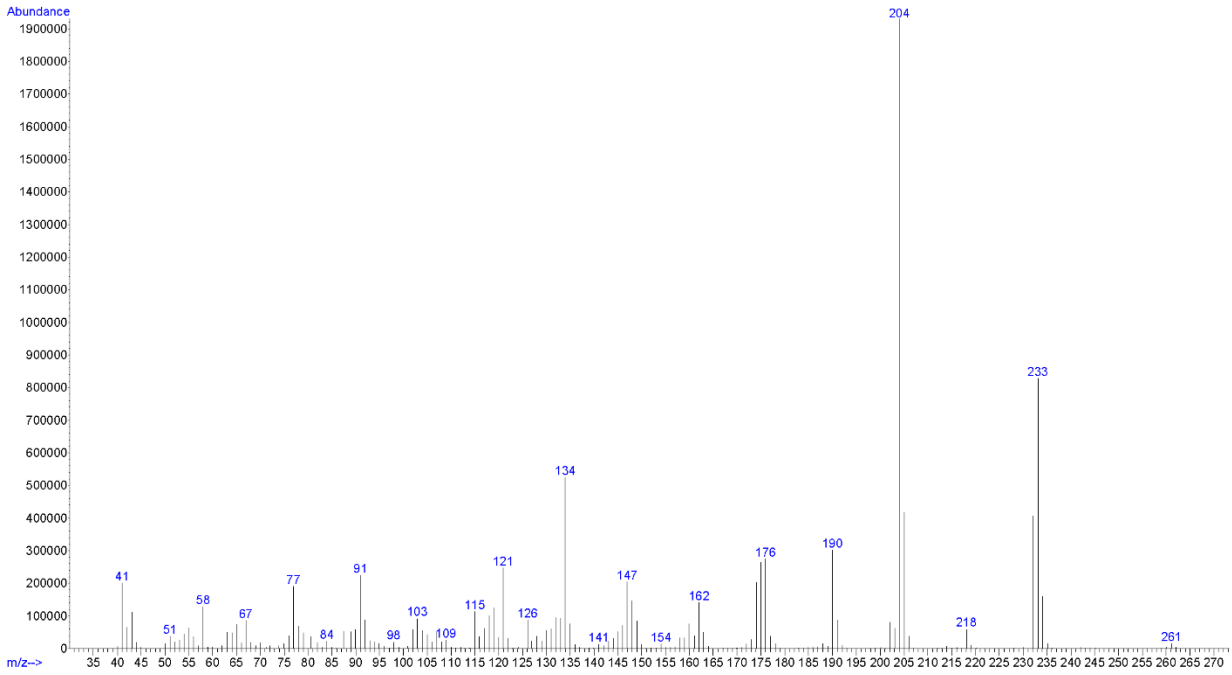
	MS Quad: 150 °C
	Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	5.73 min

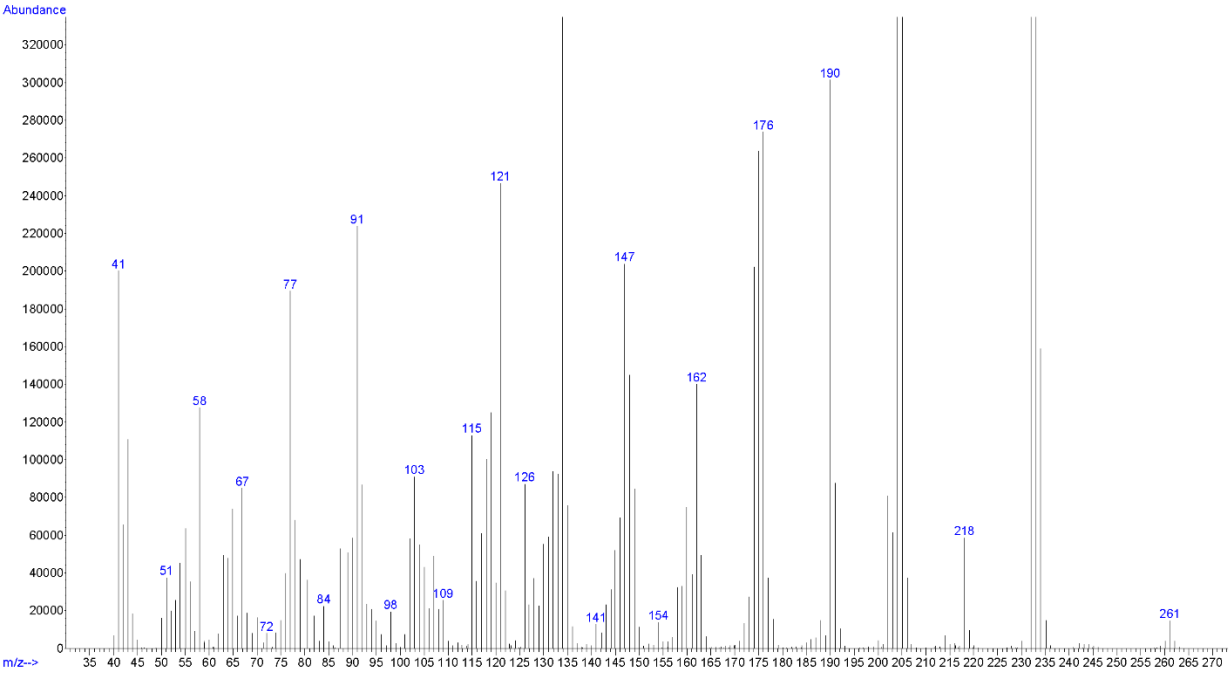
Chromatogram: Methoxpropamine



Additional peaks present in chromatogram: internal standards (3.18 and 6.28 min)

EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Methoxpropamine

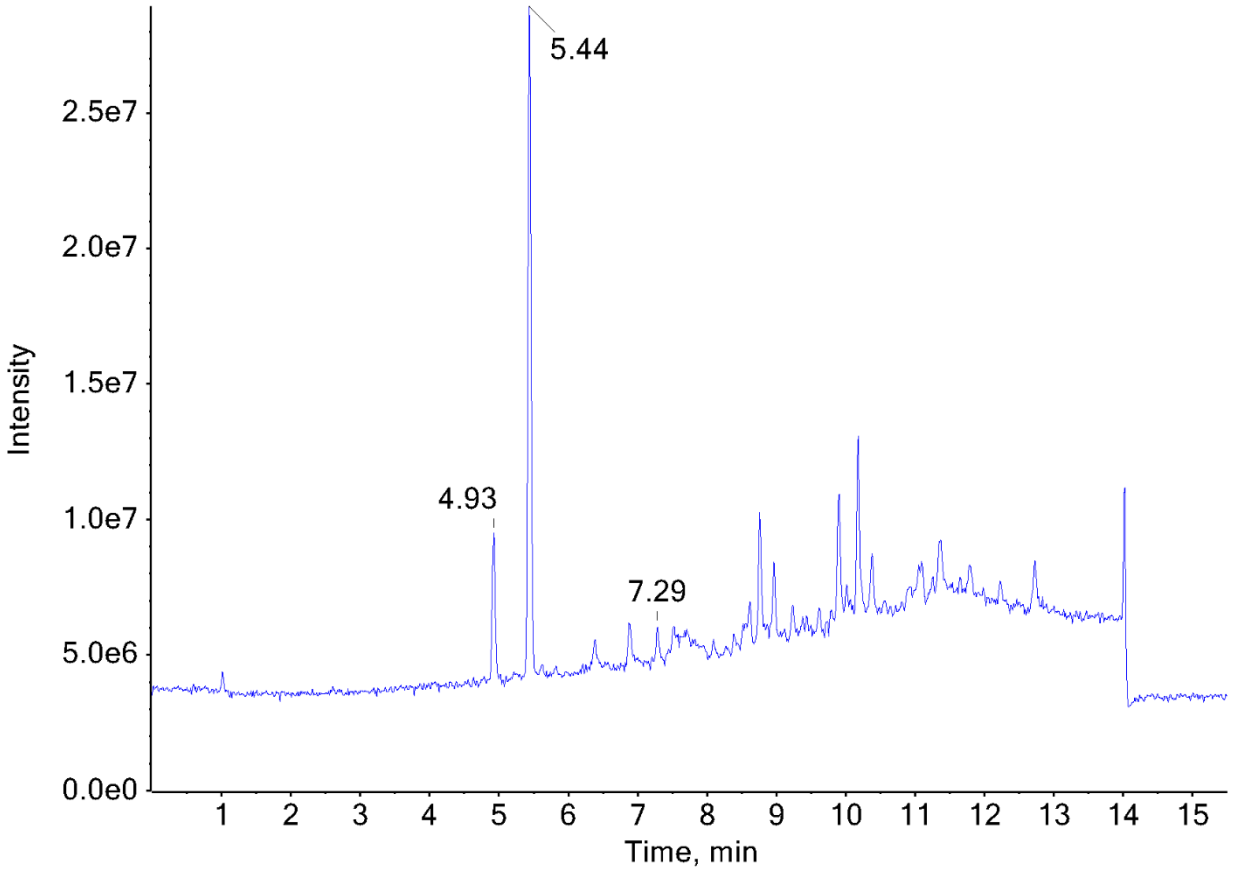




5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

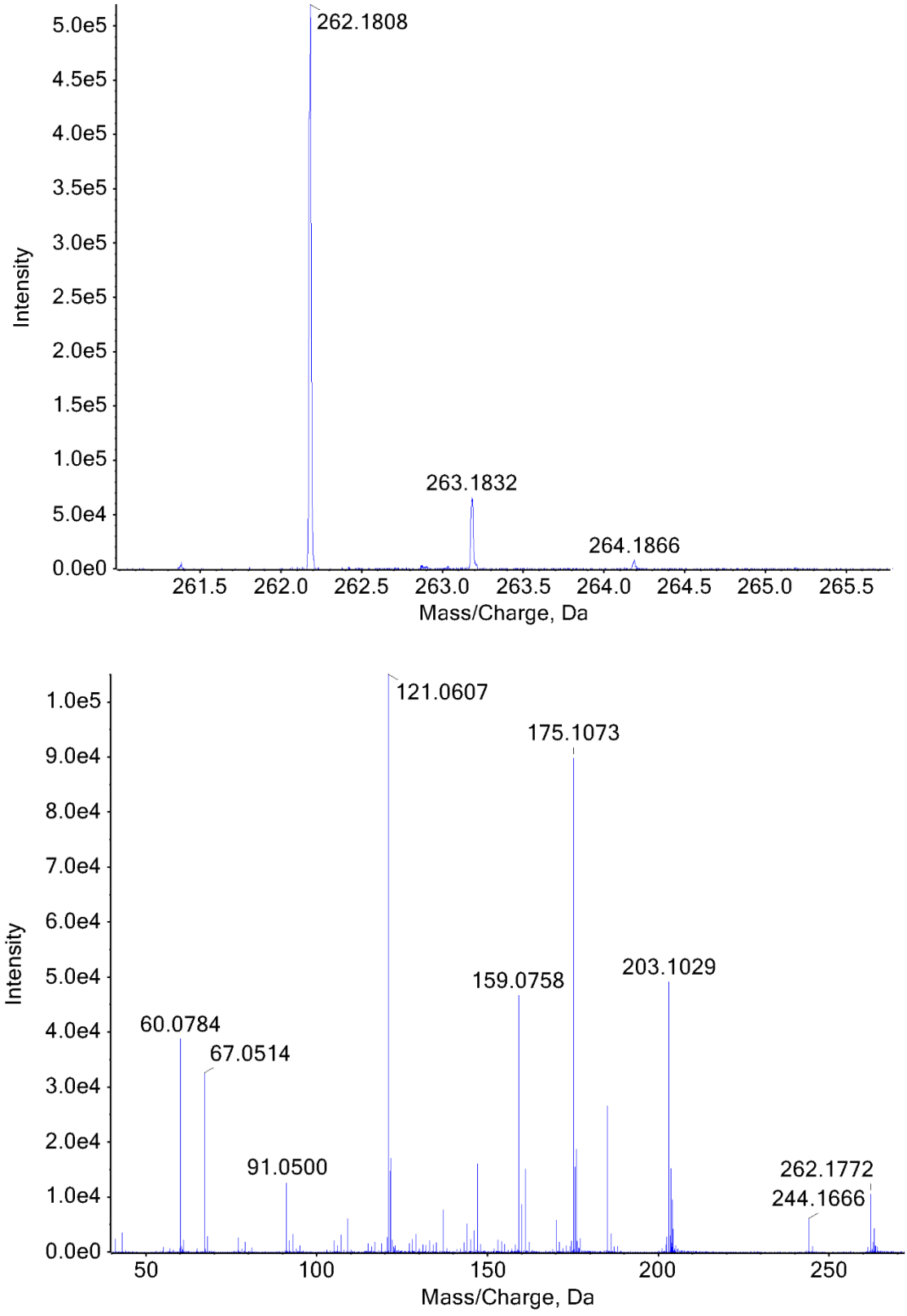
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extract in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6 µm)
Mobile Phase:	A: Ammonium formate (10 mM, pH 3.0)
	B: Methanol/acetonitrile (50:50)
	Flow rate: 0.4 mL/min
Gradient:	Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min
Temperatures:	Autosampler: 15 °C
	Column Oven: 30 °C
	Source Heater: 600 °C
Injection Parameters:	Injection Volume: 10 µL
QTOF Parameters:	TOF MS Scan Range: 100-510 Da
	Precursor Isolation: SWATH® acquisition (27 windows)
	Fragmentation: Collison Energy Spread (35±15 eV)
	MS/MS Scan Range: 50-510 Da
Retention Time:	5.44 min

Chromatogram: Methoxpropamine



Additional peaks present in chromatogram: internal standards (4.93 min and 7.29 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: Methoxpropamine



5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Powder dissolved in CD_3OD

Instrument: 600 MHz Bruker AVANCE™ III Spectrometer

Parameters: Pulse Sequence: Proton

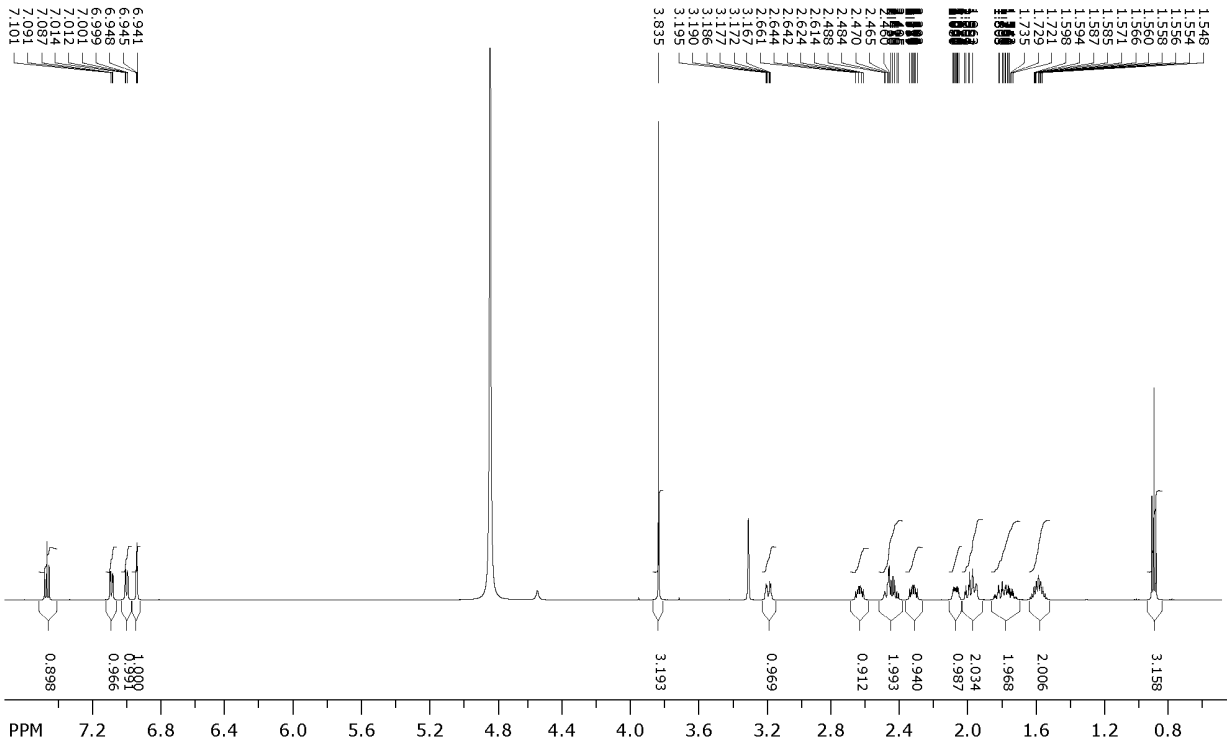
Solvent: CD_3OD

Spectral Width: 12019.23 Hz = 20.0276 ppm = 0.183399 Hz/pt for ^{1}H; 36231.88 Hz = 240.0768 ppm = 0.552855 Hz/pt for ^{13}C; 5319.15 Hz = 8.8633 ppm = 2.5972 Hz/pt for COSY; 5319.15 Hz = 8.8633 ppm = 2.5972 Hz/pt for HSQC; 5319.15 Hz = 8.8633 ppm = 1.7315 Hz/pt for HMBC

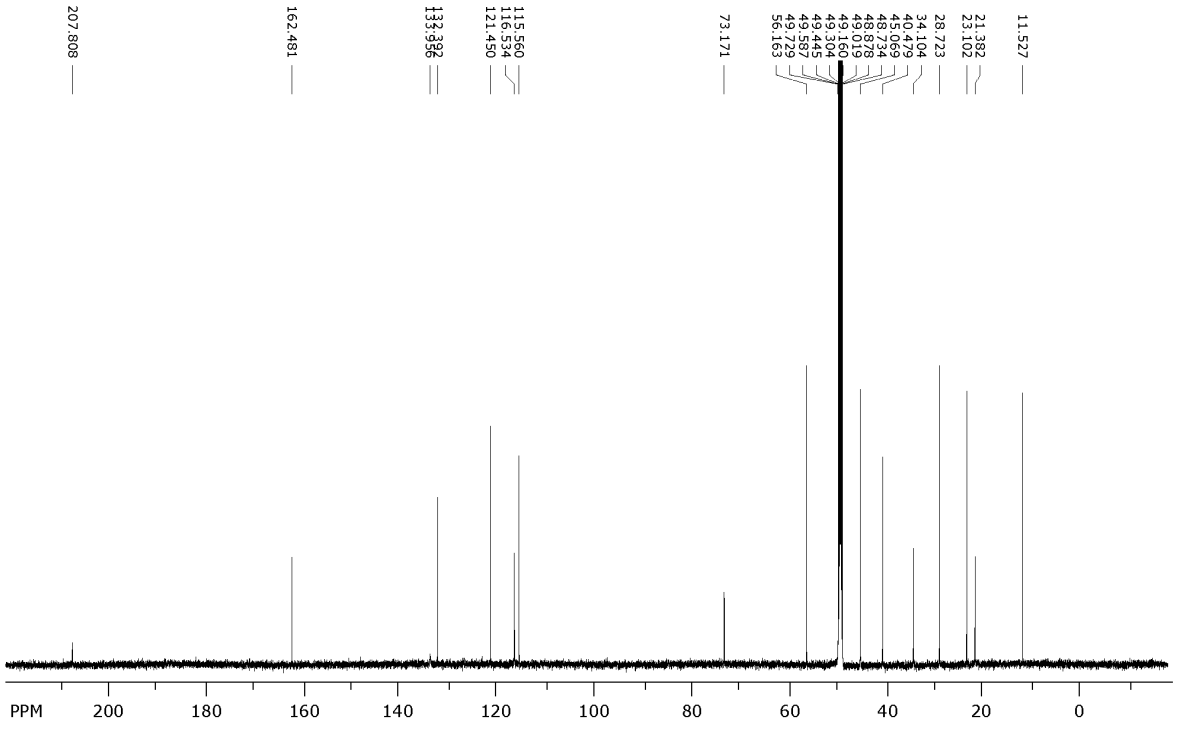
Number of Scans: 8 for ^{1}H; 2987 for ^{13}C; 4 for COSY; 8 for HSQC; 20 for HMBC

Delay Between Pulses: 1.000 second for ^{1}H, 2.000 seconds for ^{13}C

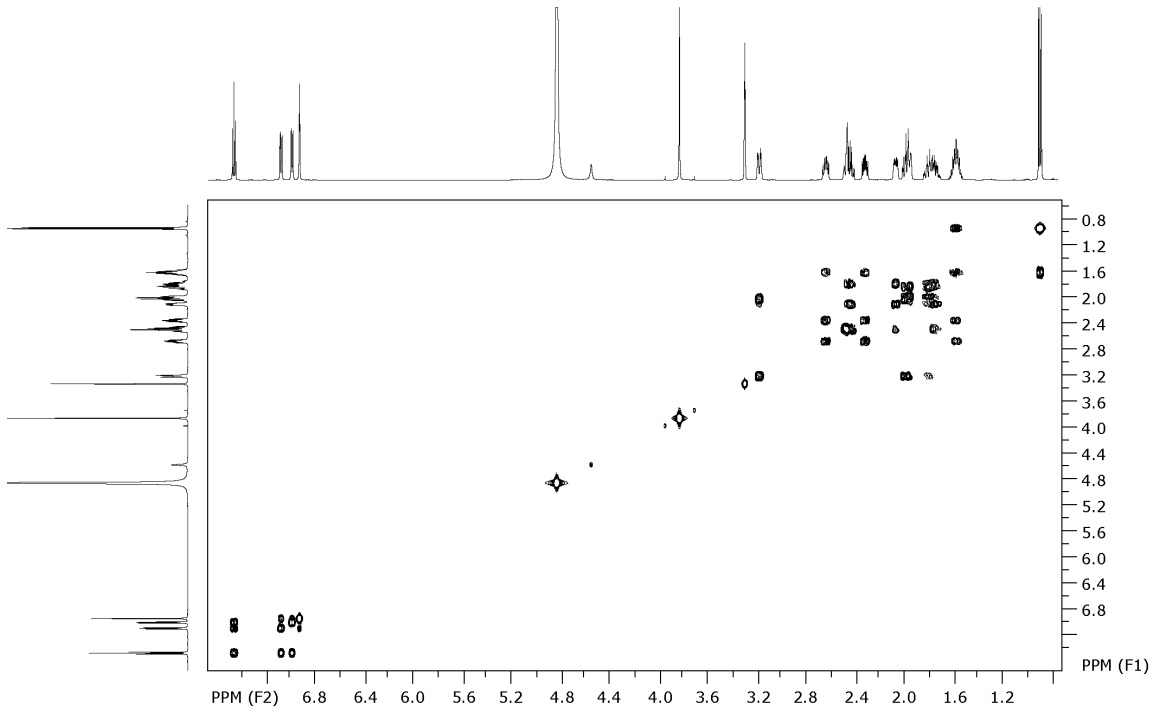
^{1}H NMR: Methoxpropamine



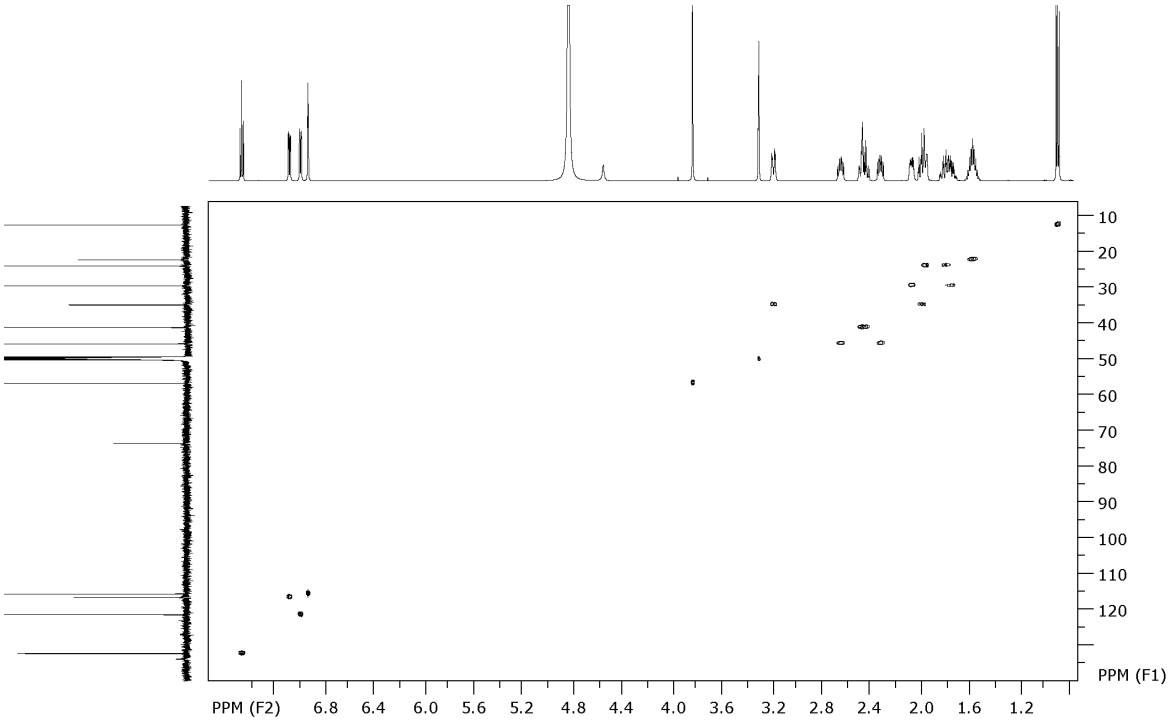
^{13}C NMR: Methoxpropamine



COSY NMR: Methoxpropamine



HSQC NMR: Methoxpropamine



HMBC NMR: Methoxpropamine