

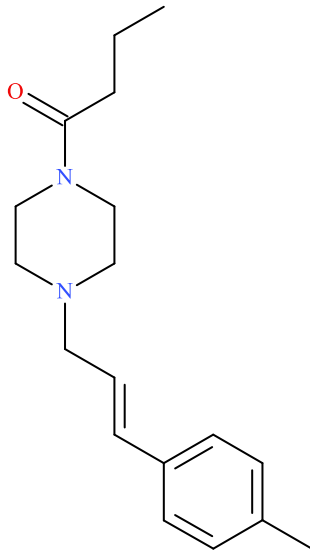
***para*-Methyl AP-237**

Sample Type: **Seized Material**

Latest Revision: **April 13, 2020**

Date Received: **November 29, 2019**

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



1. GENERAL INFORMATION

IUPAC Name:	1-[4-[(E)-3-(p-tolyl)allyl]piperazin-1-yl]butan-1-one
InChI String:	InChI=1S/C18H26N2O/c1-3-5-18(21)20-14-12-19(13-15-20)11-4-6-17-9-7-16(2)8-10-17/h4,6-10H,3,5,11-15H2,1-2H3/b6-4+
CFR:	Not Scheduled (04/2020)
CAS#	Not Available
Synonyms:	<i>para</i> -Methyl Bucinnazine
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.

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2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion [M ⁺]	Exact Mass [M+H] ⁺
Base	C ₁₈ H ₂₆ N ₂ O	286.4	286	287.2118

3. BRIEF DESCRIPTION

para-Methyl AP-237 is classified as a synthetic opioid; however, *para*-methyl AP-237 is structurally distinct from fentanyl and its analogues. *para*-Methyl AP-237 is an analogue of bucinnazine (AP-237), an opioid used therapeutically, although bucinnazine is not prescribed within the United States. 2-Methyl AP-237 is an additional structurally similar analogue. *para*-Methyl AP-237 is the third analogue in this series to be reported by NPS Discovery. Analogues in this series are not scheduled substances in the United States.

4. ADDITIONAL RESOURCES

No additional resources are 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

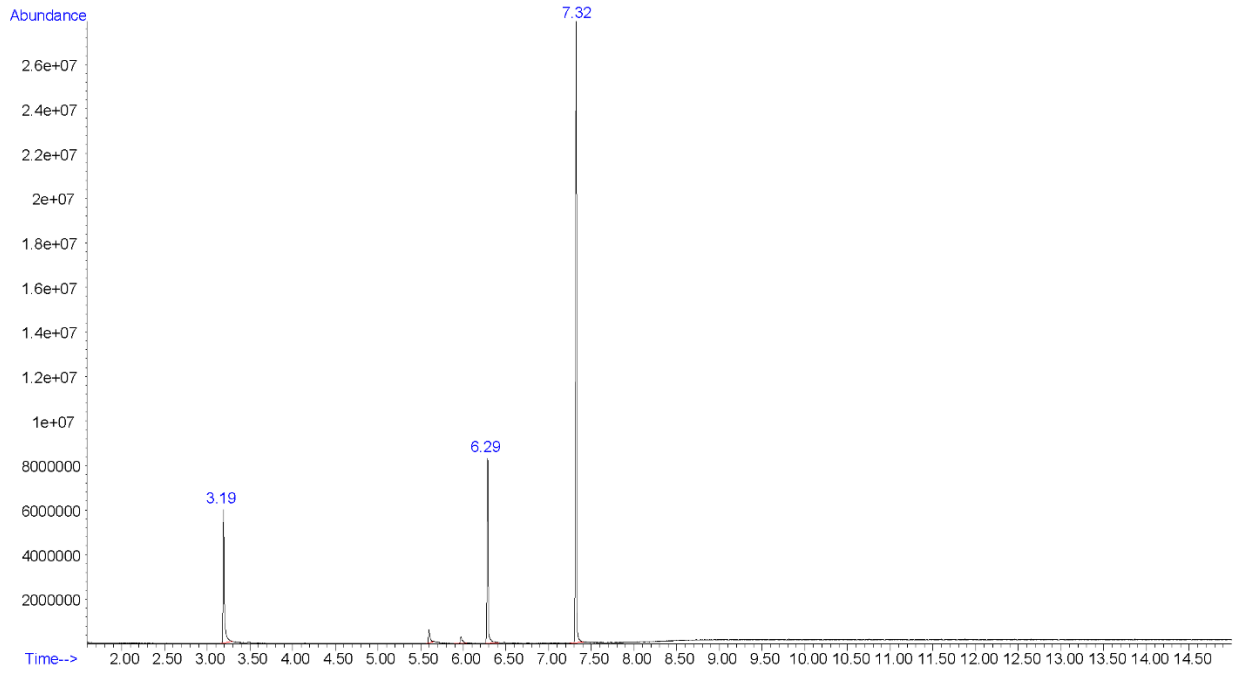
Injection Volume: 1 µL

MS Parameters: Mass Scan Range: 40-550 m/z

Threshold: 250

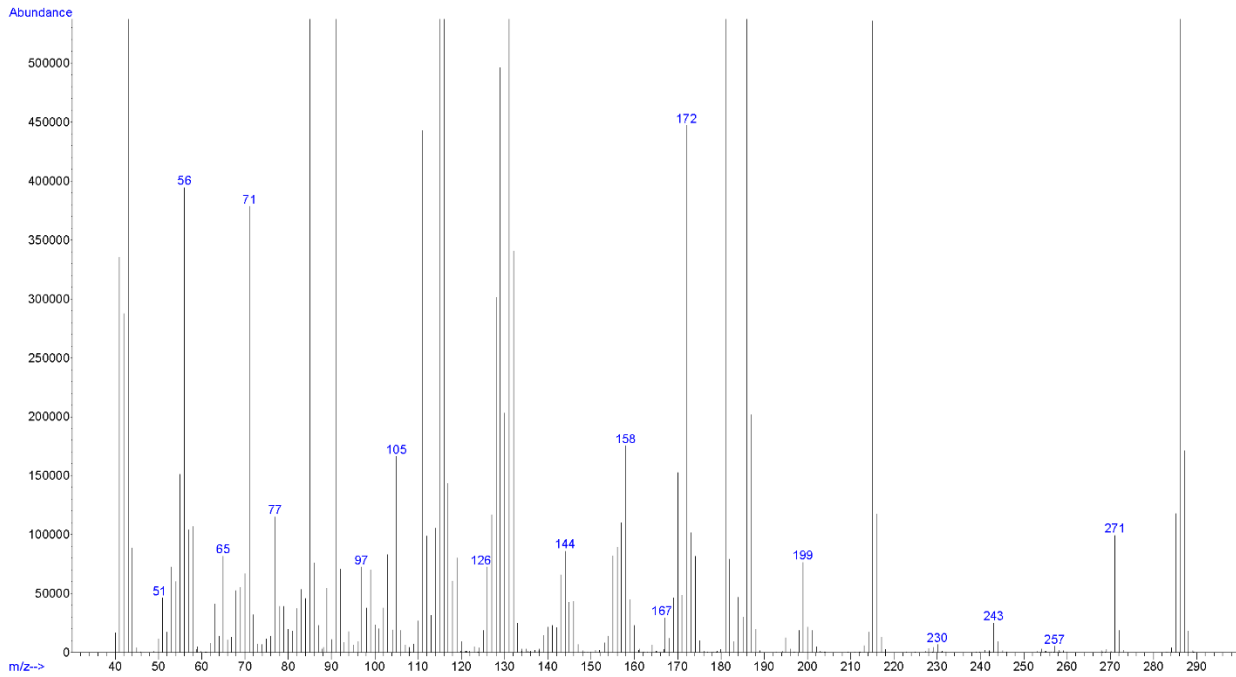
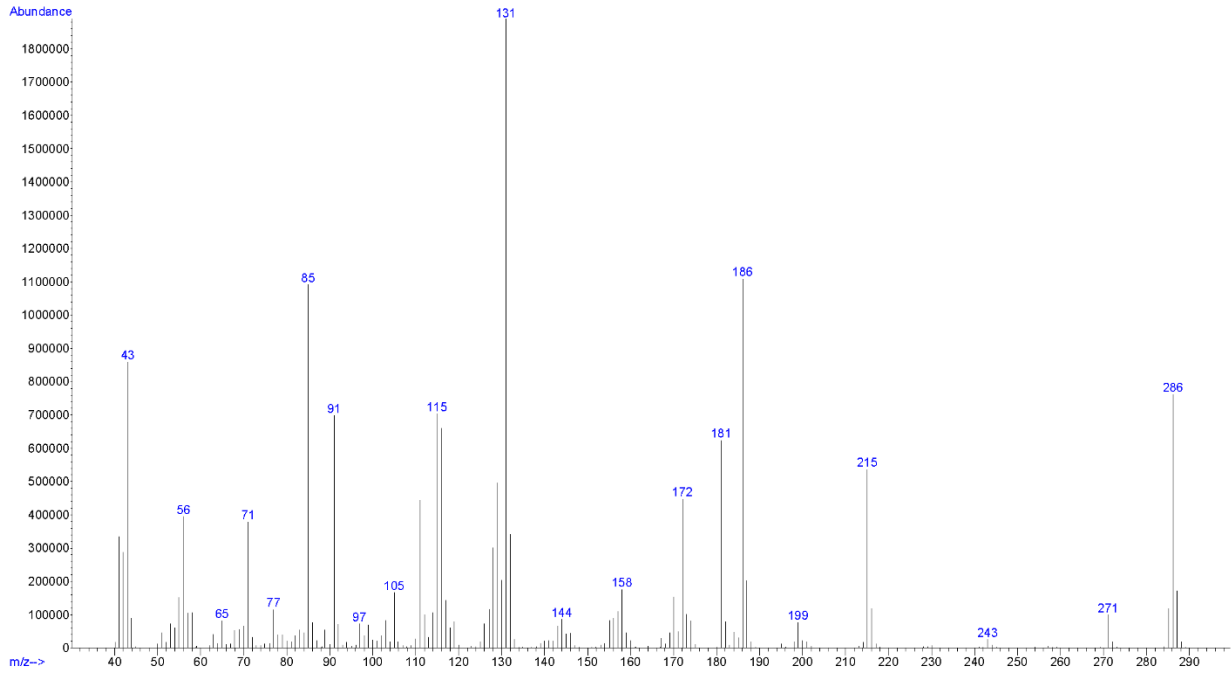
Retention Time: 7.32 min

Chromatogram: *para*-Methyl AP-237



Additional peaks present in chromatogram: internal standards (3.19 and 6.29 min)

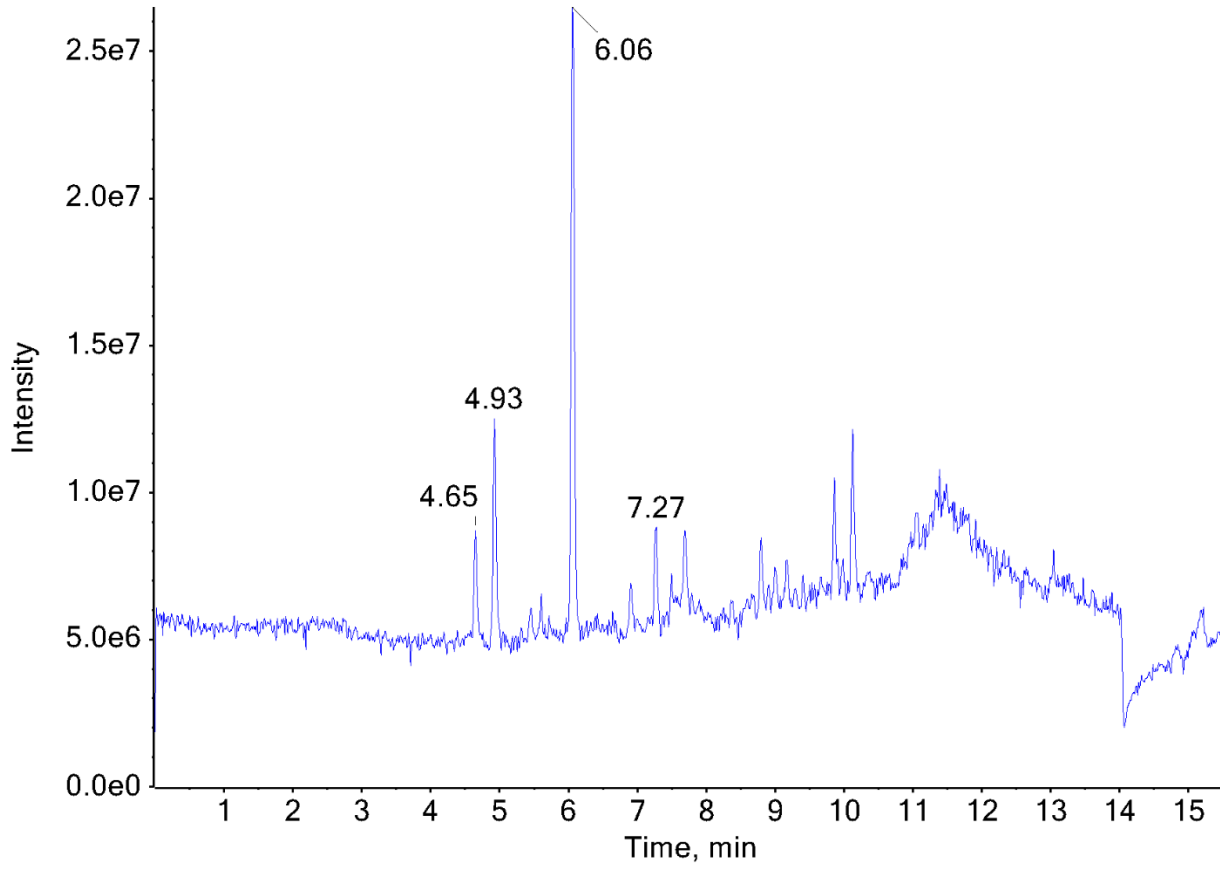
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): *para*-Methyl AP-237



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

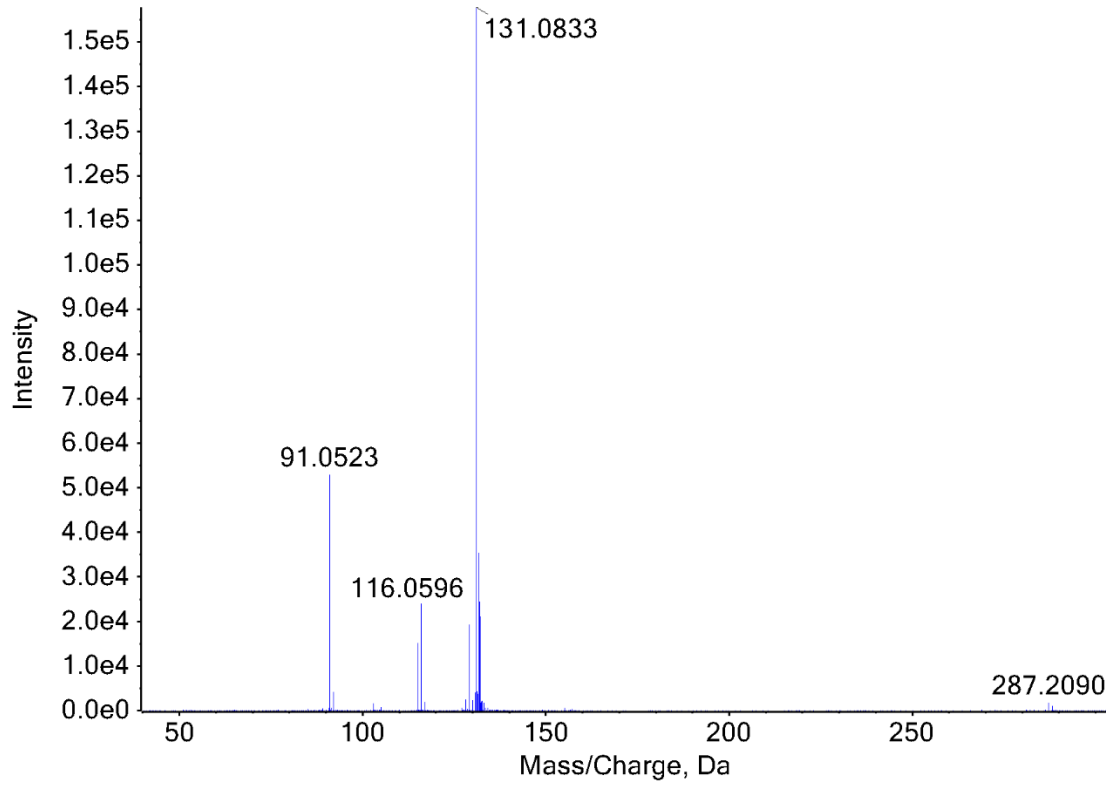
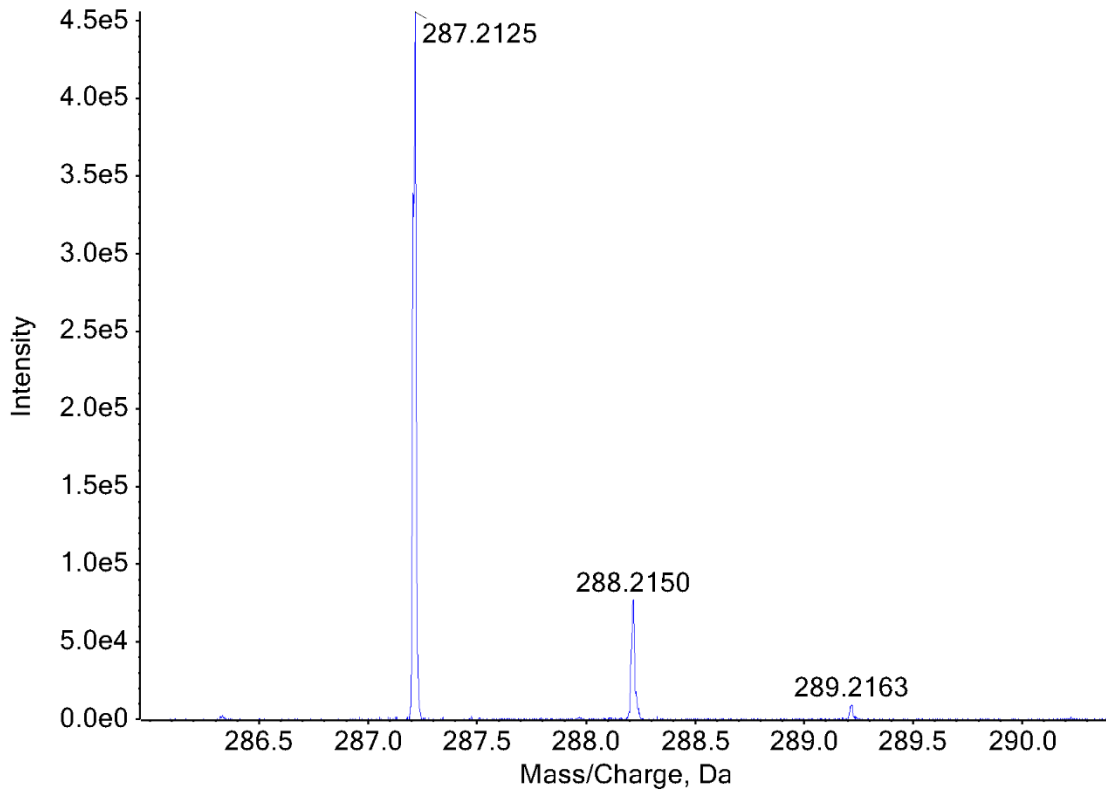
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extract in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex C18 (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: Collision Energy Spread (35±15 eV) MS/MS Scan Range: 50-510 Da
Retention Time:	6.06 min

Chromatogram: *para*-Methyl AP-237



*Additional peaks present in chromatogram: not a controlled substance (4.65 min)
and internal standards (4.93 min and 7.27 min)*

TOF MS (Top) and MS/MS (Bottom) Spectra: *para*-Methyl AP-237



5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Powder dissolved in CDCl₃

Instrument: 600 MHz Bruker AVANCE™ III Spectrometer

Parameters: Pulse Sequence: Proton

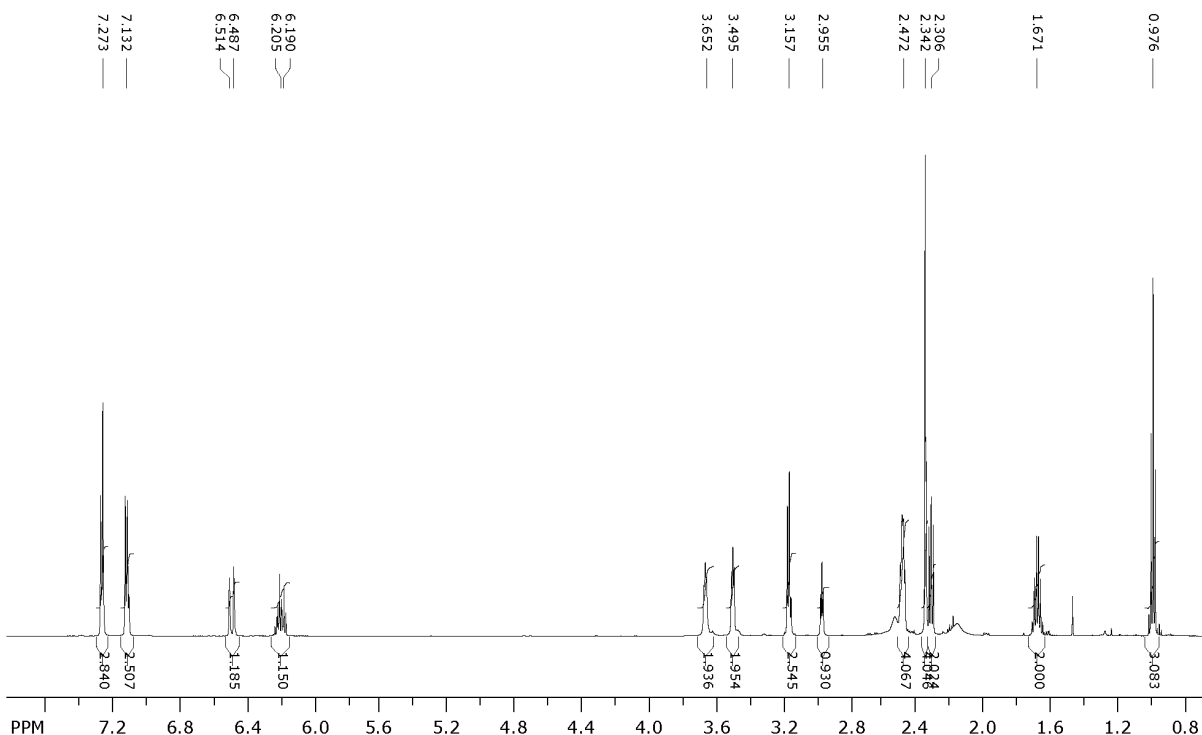
Solvent: CDCl₃

Spectral Width: 12019.23 Hz = 20.0276 ppm = 0.183399 Hz/pt for ¹H; 36231.88 Hz = 240.0768 ppm = 0.552855 Hz/pt for ¹³C; 5241.09 Hz = 8.7332 ppm = 2.5591 Hz/pt for COSY; 5241.09 Hz = 8.7332 ppm = 2.5591 Hz/pt for HSQC; 5241.09 Hz = 8.7332 ppm = 1.7061 Hz/pt for HSQC

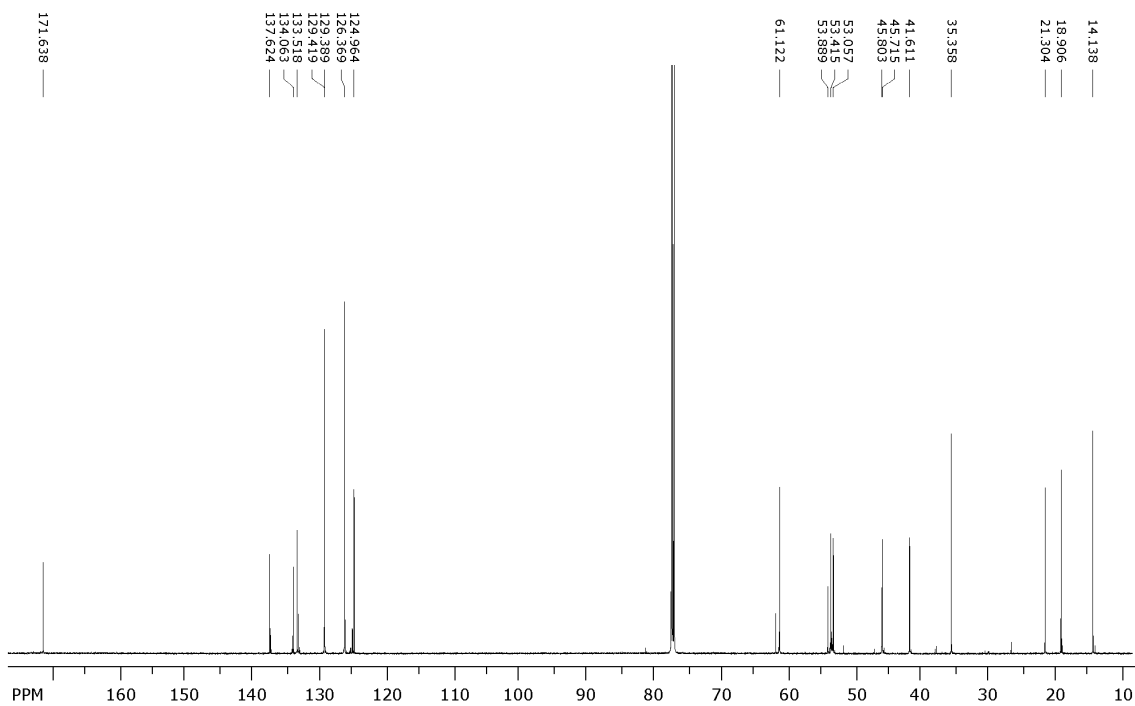
Number of Scans: 4 for ¹H; 1024 for ¹³C; 2 for COSY; 2 for HSQC; 6 for HMBC

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

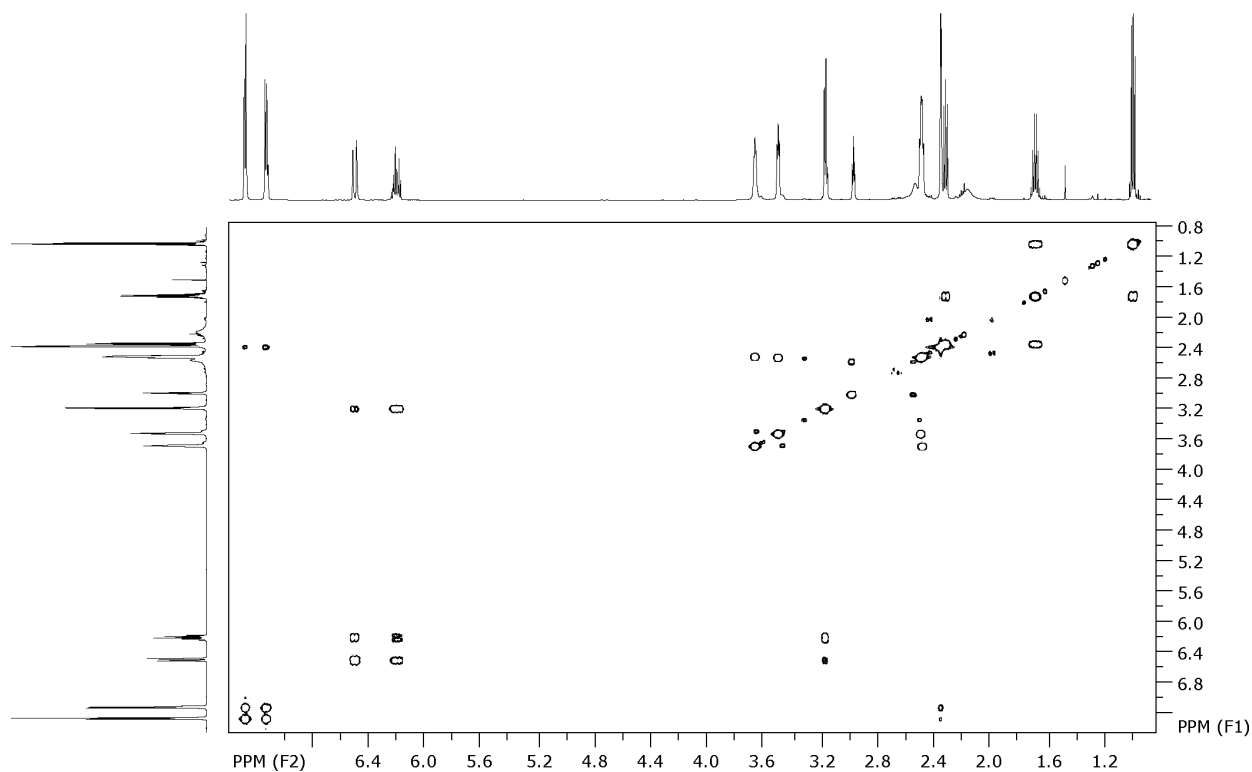
¹H NMR: *para*-Methyl AP-237



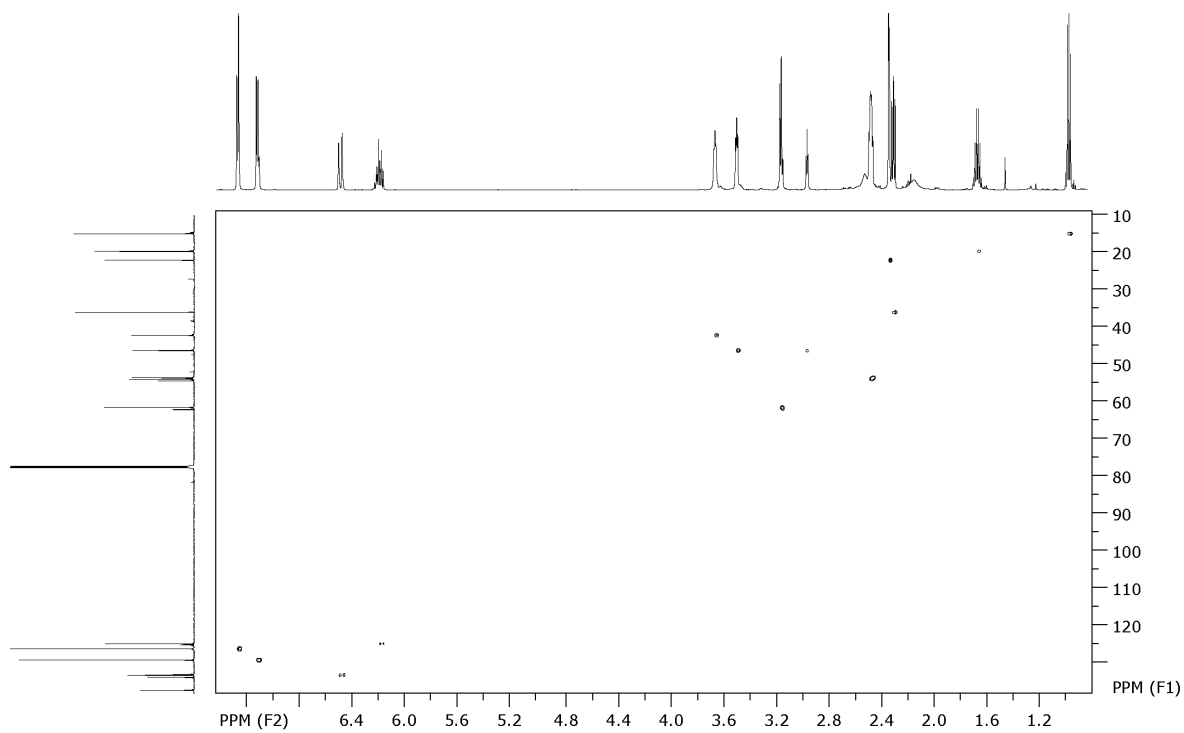
¹³C NMR: *para*-Methyl AP-237



COSY NMR: *para*-Methyl AP-237



HSQC NMR: *para*-Methyl AP-237



HMBC NMR: *para*-Methyl AP-237

