Analytical Profile of 30C-NBOMe

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Table of contents:

Part 1: Cayman Chemical Data:

Figure 1. 30C-NBOMe GC/MS Data

Figure 2. 30C-NBOMe 1H NMR Data

Figure 3. 30C-NBOMe 1H NMR Data, Enlarged

Figure 4. 30C-NBOMe ESI-MS Data

Part 2: Georgia Bureau of Investigation Data:

Figure 5. 30C-NBOMe GC/MS Data

Figure 6. 30C-NBOMe Expanded GC/MS Data

Figure 7. 30C-NBOMe FTIR Data

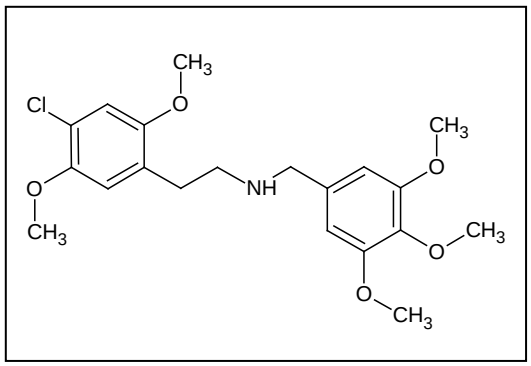
Figure 8. 30C-NBOMe Expanded FTIR Data

Figure 9. 30C-NBOMe HPLC Data

Figure 10. 30C-NBOMe UV Data

Part 3: External Link

Part 1. Cayman Chemical Company Data



Name: 30C-NBOMe

Synonyms: 2-(4-chloro-2,5-dimethoxyphenyl)-N-(3,4,5-trimethoxybenzyl)ethanamine

CAS#: N/A

Molecular Formula: $C_{20}H_{26}ClNO_5$

Molecular Weight: 395.5 g/mol

SMILES: COc2cc(CCNCc1cc(OC)c(OC)c(OC)c1)c(cc2Cl)OC

InChl Key: ZQYYVTABADQBTJ-UHFFFAOYAT

InChl: InChI=1/C20H26ClNO5/c1-23-16-11-15(21)17(24-2)10-14(16)6-7-22-12-13-8-18(25-3)20(27-5)19(9-13)26-4/h8-11,22H,6-7,12H2,1-5H3

Background:

30C-NBOMe is a N-alkylated analogue of the phenethylamine 2C-C, a known hallucinogen that stimulates monoamine receptor activity and inhibits the reuptake of serotonin (IC50 = 31uM) and norepinephrine (IC50 = 63uM) in rat brain synaptosomes.[1,2] 30C-NBOMe exhibits a 3,4,5 tri-methoxy benzyl group bridged by the nitrogen to the 2C-C core. The aryl benzyl moiety has been shown to increase affinity and selectivity for the 5-HT_{2A} receptor in the non-chlorinated 2C-H phenethylamine series[3]. Moreover, the 3,4,5 tri-methoxy benzyl group resembles the hallucinogenic alkaloid mescaline, less one carbon in the alkyl chain. The physiological and toxicological properties of this compound are not known.

1. Nagai, F., Nonaka, R., Satoh Hisashi Kamimura, K.*Eur. J. Pharmacol.* **2007**. 559(2-3), 132-137.

2. Nonaka, R., Nagai, R., Ogata, A., *et al. Biol. Pharm. Bull*. **2007**. 30(12), 2328-2333.

3. Braden, M.R., Parrish, J.C., Naylor, J.C., Nichols, D.E. *Mol Pharm*. **2006**. 70(6), 1956-1964.

Gas chromatography/Mass spectrometry:

Experiment Parameters:

Instrument: Agilent 6890 GC / 5973 MSD

Column: 30mx0.32mm, 0.5um Rtx-5MS

Carrier Gas: Helium Flow: 2mL/min

Inlet temp: 300 ^{o}C, 15:1 split

Oven Program: Initial temp: 240 ^{o}C, Ramp to 300 ^{o}C at 30C/min, Hold at 300 ^{o}C for 27 minutes

Transfer Line Temp: 300 ^{o}C

MS Source: 230^{o}C

MS Quad: 150^{o}C

Mass Scan Range: 40-600 amu

Threshold: 150

Tune File: stune.u

Figure 1: Gas Chromatography/Mass Spectrometry of 30C-NBOMe (hydrochloride)

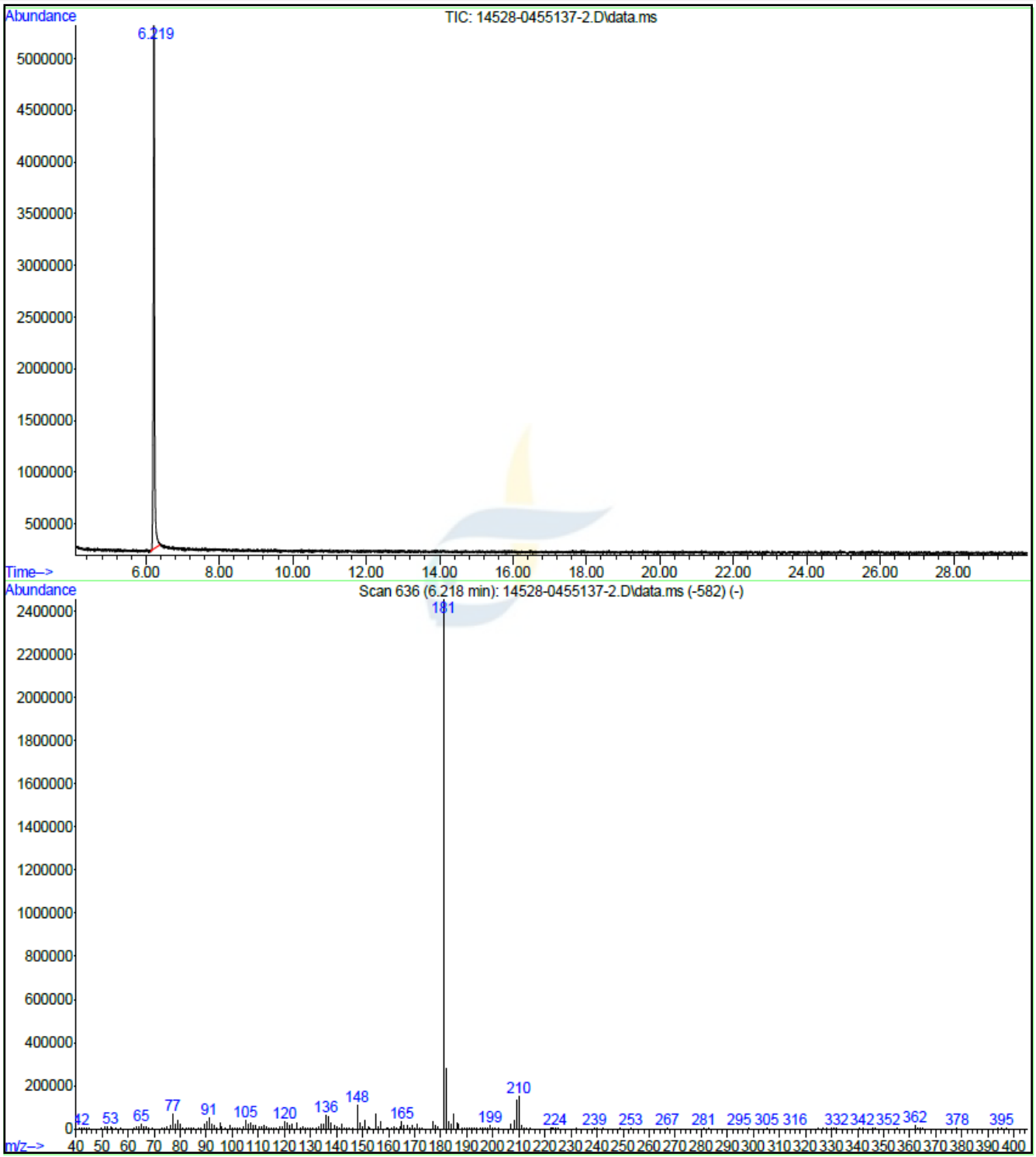


Figure 2. 1H Nuclear Magnetic Resonance Spectroscopy of 30C-NBOMe (hydrochloride)

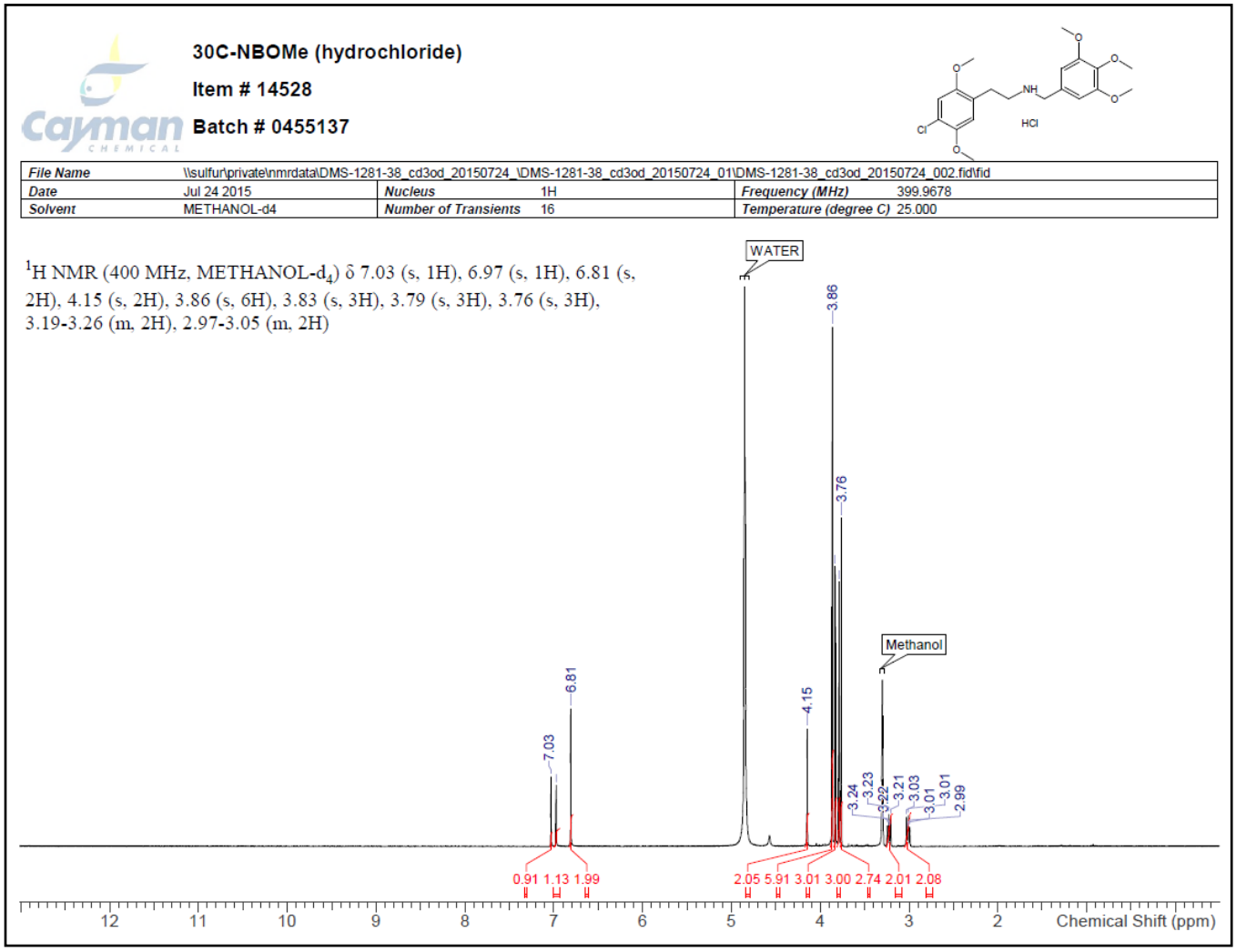


Figure 3. 1H Nuclear Magnetic Resonance Spectroscopy of 30C-NBOMe (hydrochloride), Enhanced for Detail

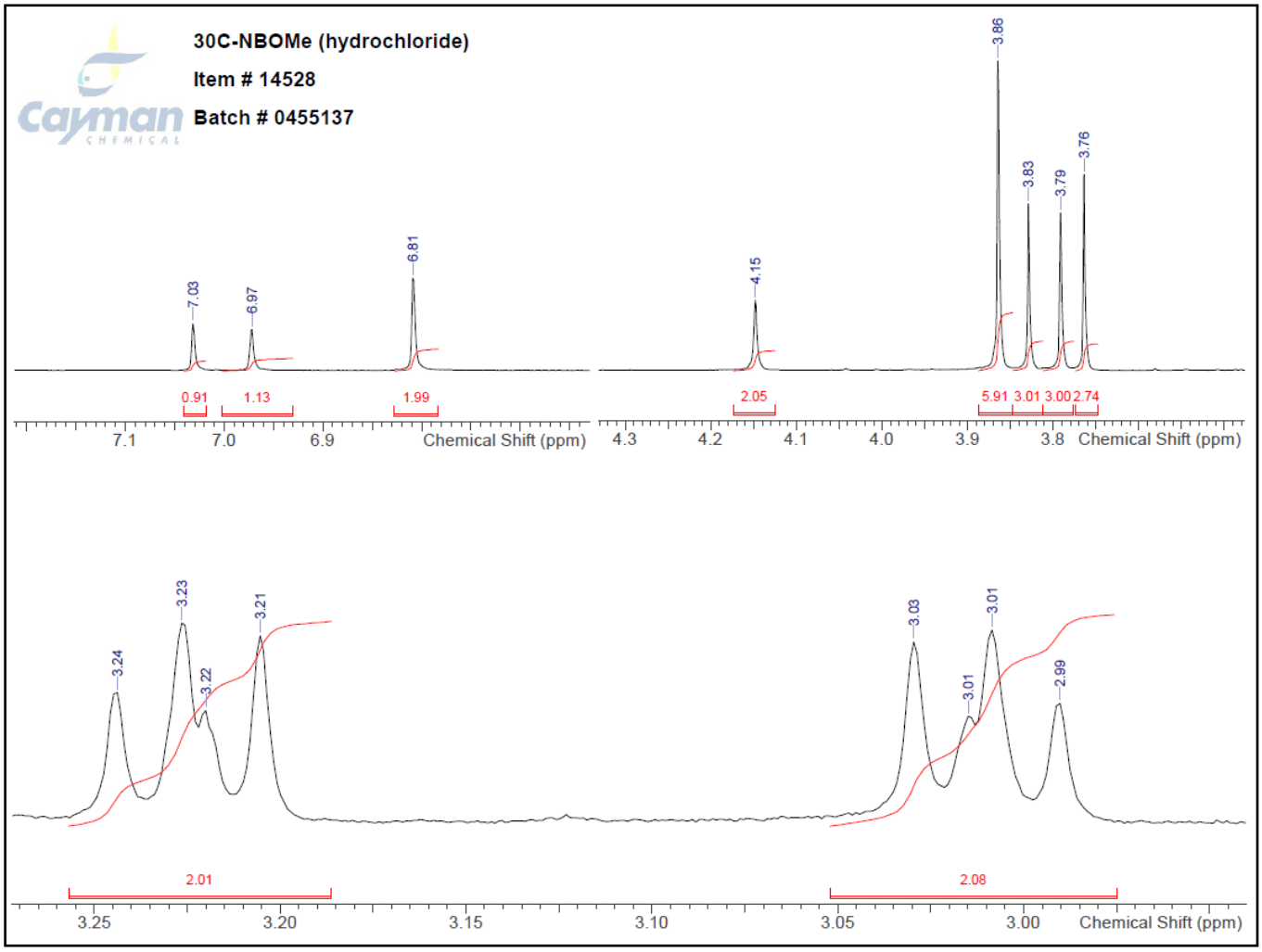
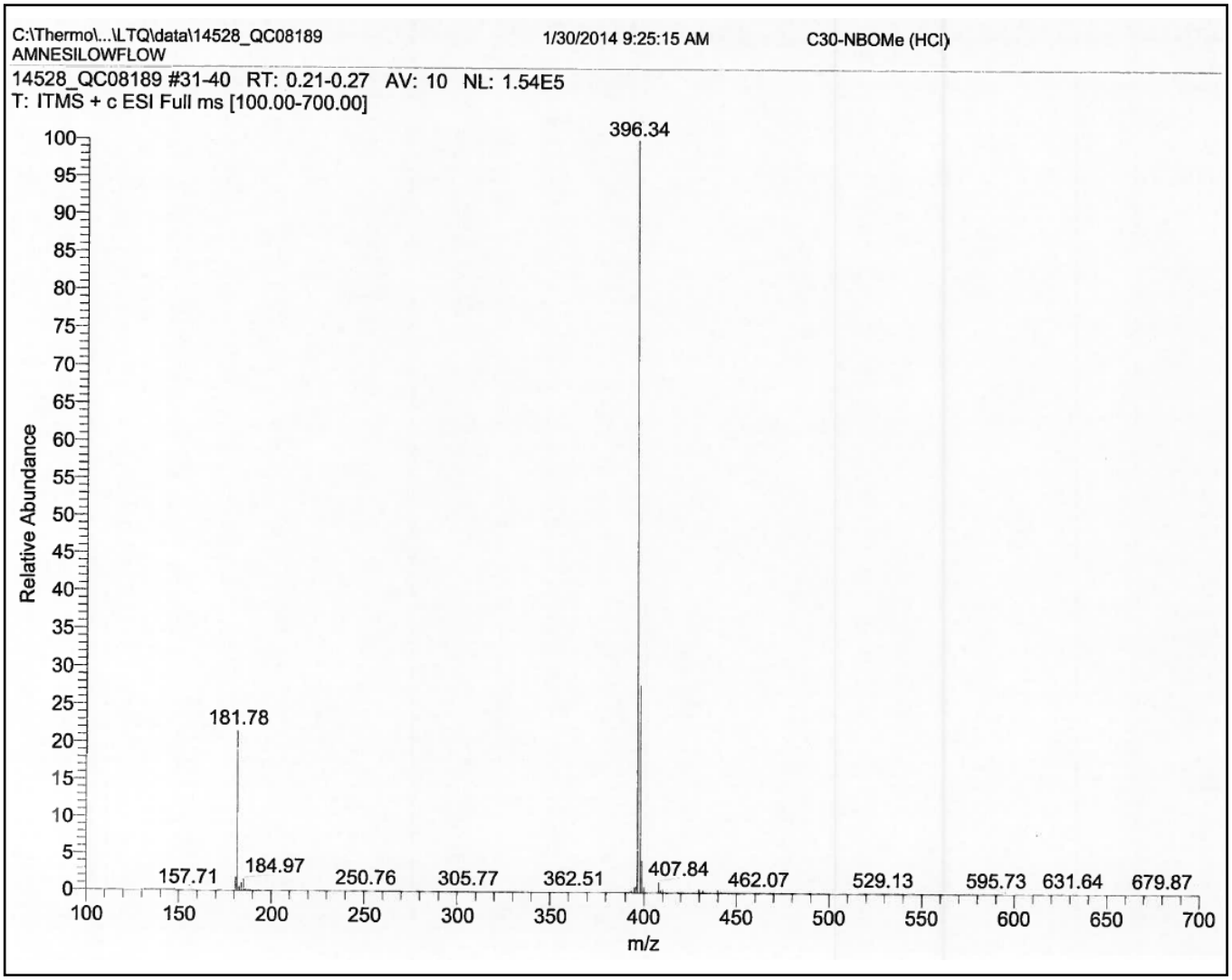
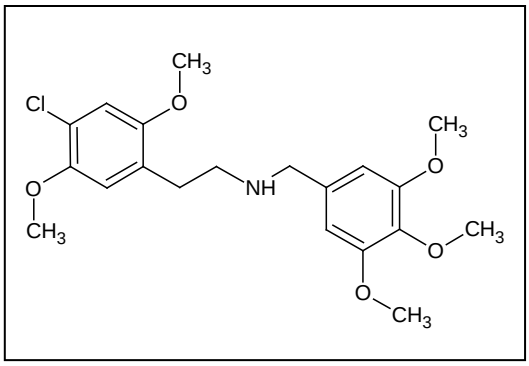


Figure 4. ESI-MS of 30C-NBOMe (hydrochloride)

Experiment Parameters:
Instrument: Thermo LCQ Ion Trap MS
Sample Infusion: 500 µl/min
Mode: +ESI
Mass range: 100-700 amu
Capillary Temperature: 275 C



Part 2. Georgia Bureau of Investigation Data



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CAS#: N/A

Molecular Formula: $C_{20}H_{26}ClNO_5$

Molecular Weight: 395.5 g/mol

Source: Cayman Chemicals lot # 0455137-3

Appearance: white, crystalline solid

SMILES: COc2cc(CCNCc1cc(OC)c(OC)c(OC)c1)c(cc2Cl)OC

InChl Key: ZQYYVTABADQBTJ-UHFFFAOYAT

InChl: InChI=1/C20H26ClNO5/c1-23-16-11-15(21)17(24-2)10-14(16)6-7-22-12-13-8-18(25-3)20(27-5)19(9-13)26-4/h8-11,22H,6-7,12H2,1-5H3

Gas Chromatography/Mass Spectrometry (GCMS):

Sample Preparation: ~ 2mg/mL in EtOH

Instrument: Agilent 7890A gas chromatograph / 5975C mass spectrometer

GC Parameters

Column: HP Ultra-1 12m × 200µm × 0.33µm

Carrier gas: Helium

Oven program:
1) initial temperature 60ºC for 2 min.
2) ramp to 275ºC at 35ºC/min.
3) hold at 275ºC for 12 min.

Injection parameters: 1µL injection; pulsed splitless

Inlet temperature: 270ºC

Constant Pressure: 8 psi

MS Parameters

Transfer Line temperature: 280ºC

Source temperature: 230ºC

Quad temperature: 150ºC

Mass scan range: 40-500 amu

Tune file: stune

Figure 5: Gas Chromatography/Mass Spectrometry of 30C-NBOMe (hydrochloride)

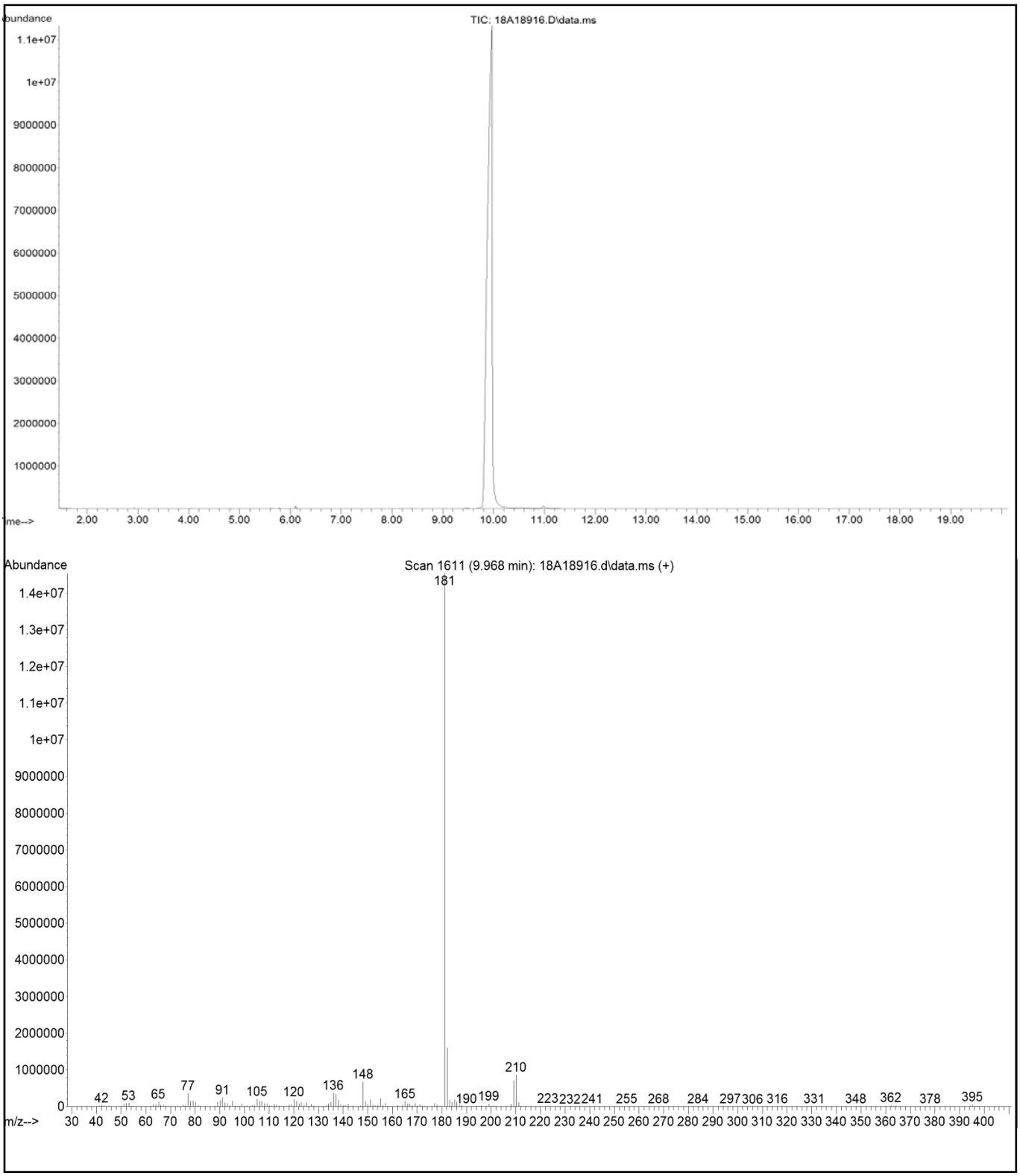
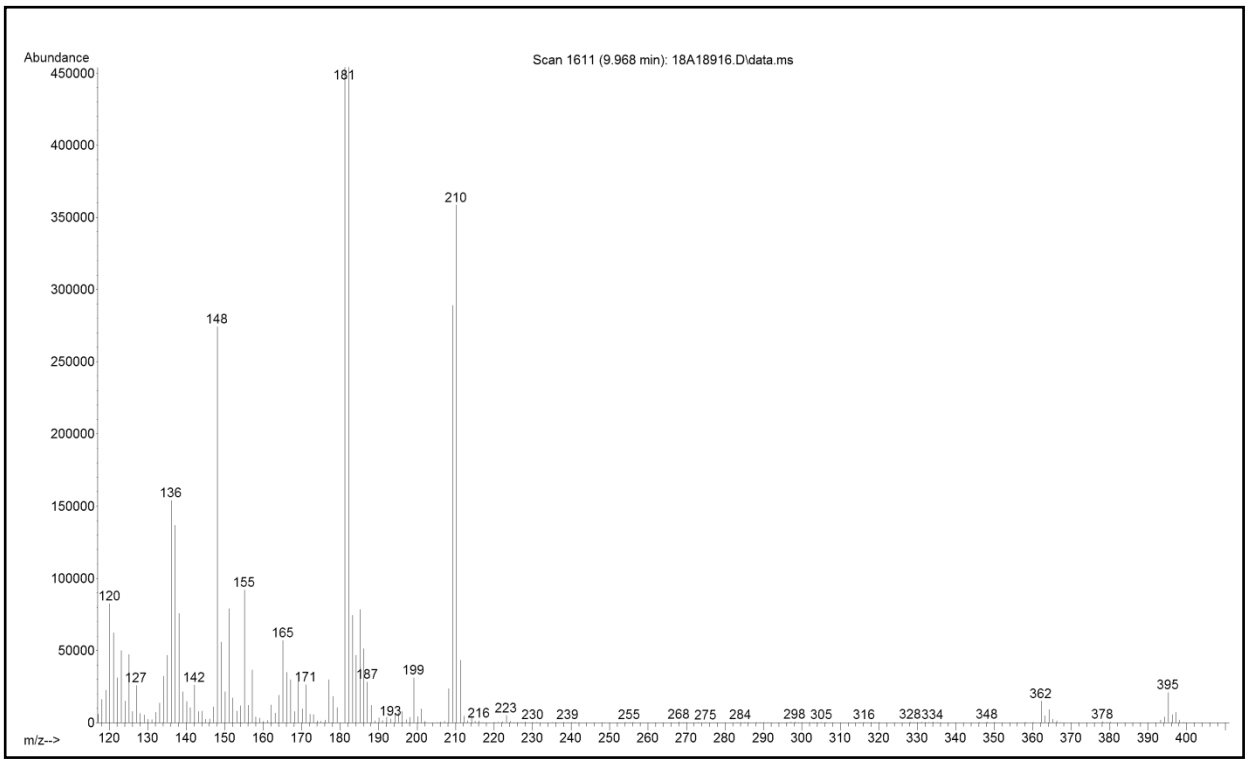


Figure 6: Expanded Gas Chromatography/Mass Spectrometry of 30C-NBOMe (hydrochloride)



Infrared Spectroscopy (FTIR):

Instrument: Nicolet 4700 with diamond ATR attachment (3 bounce)

Scan Parameters: **Number of scans:** 32

Number of background scans: 32

Resolution: 4 cm^{-1}

Sample gain: 8

Figure 7: Infrared Spectroscopy of 30C-NBOMe (hydrochloride)

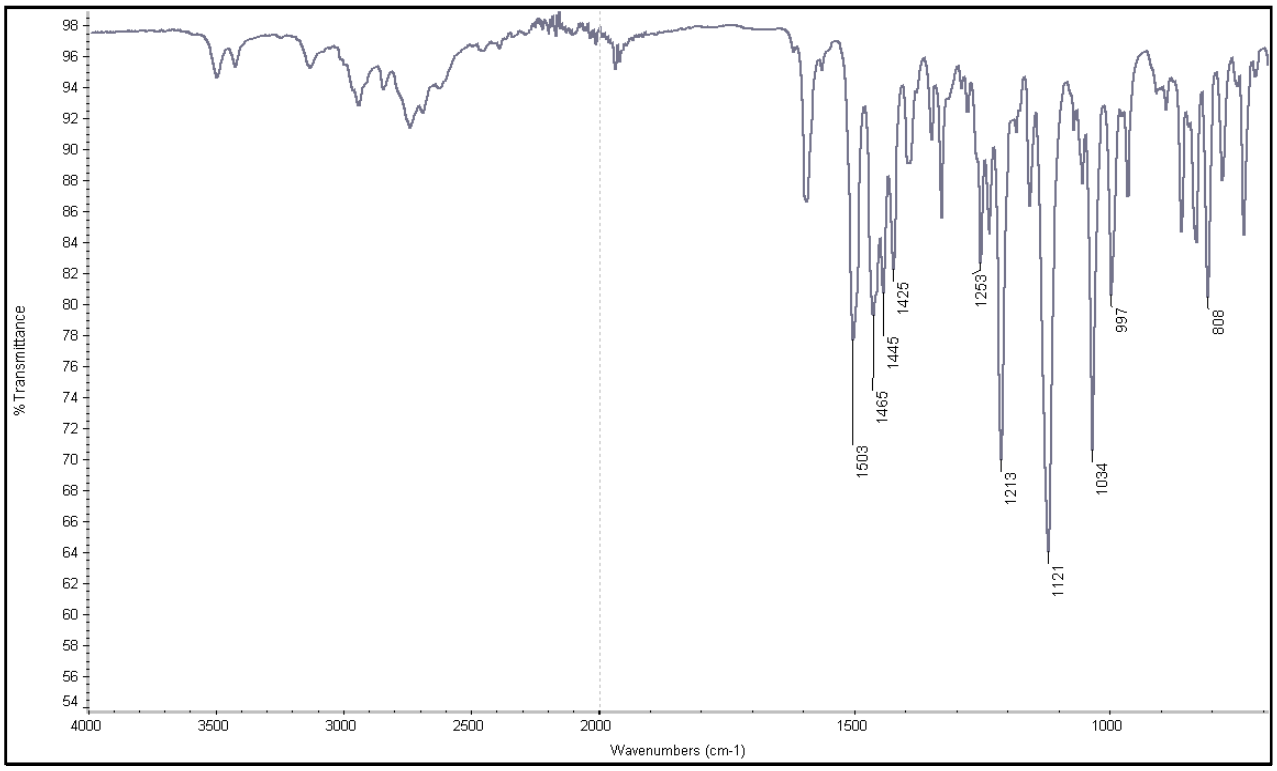
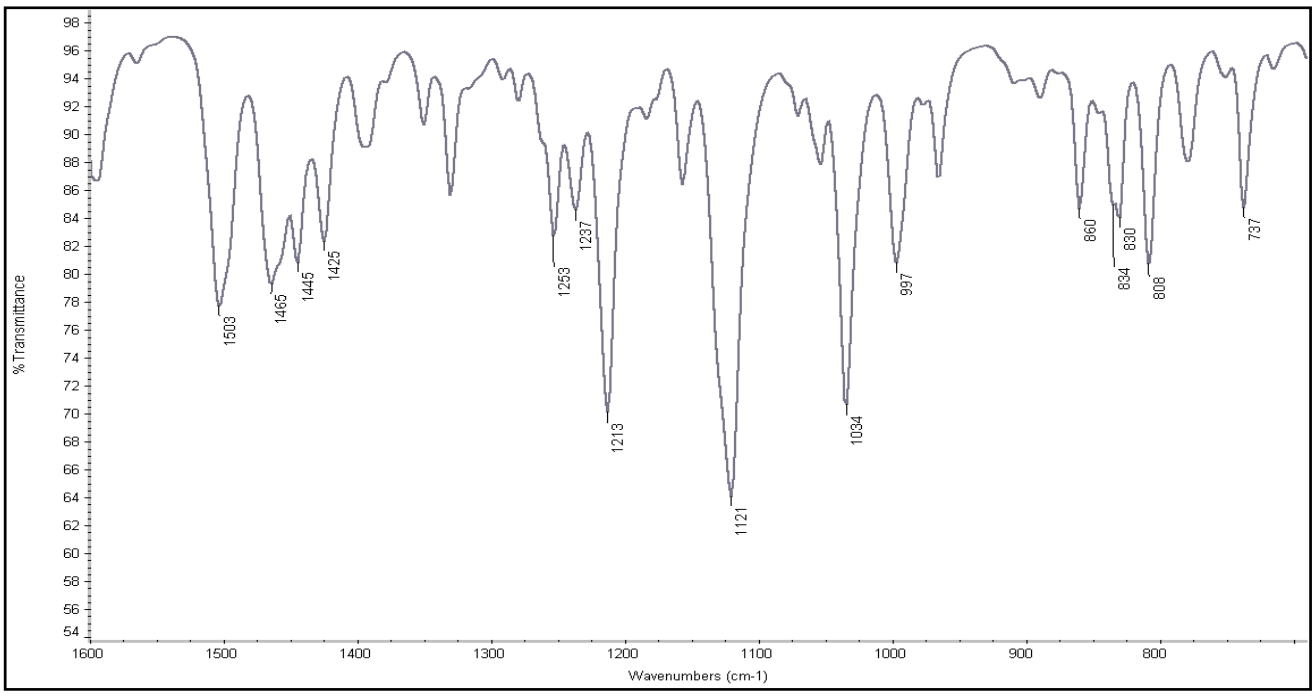


Figure 8: Expanded Infrared Spectroscopy of 30C-NBOMe (hydrochloride)



High Performance Liquid Chromatography (HPLC):

Instrument: Agilent 1260 Infinity

LC Parameters: **Column:** Zorbax Eclipse Plus C18 3.0 x 100mm 35-micron

Column compartment: 40ºC

Mobile phase: A: Ammonium Phosphate buffer

B: Acetonitrile

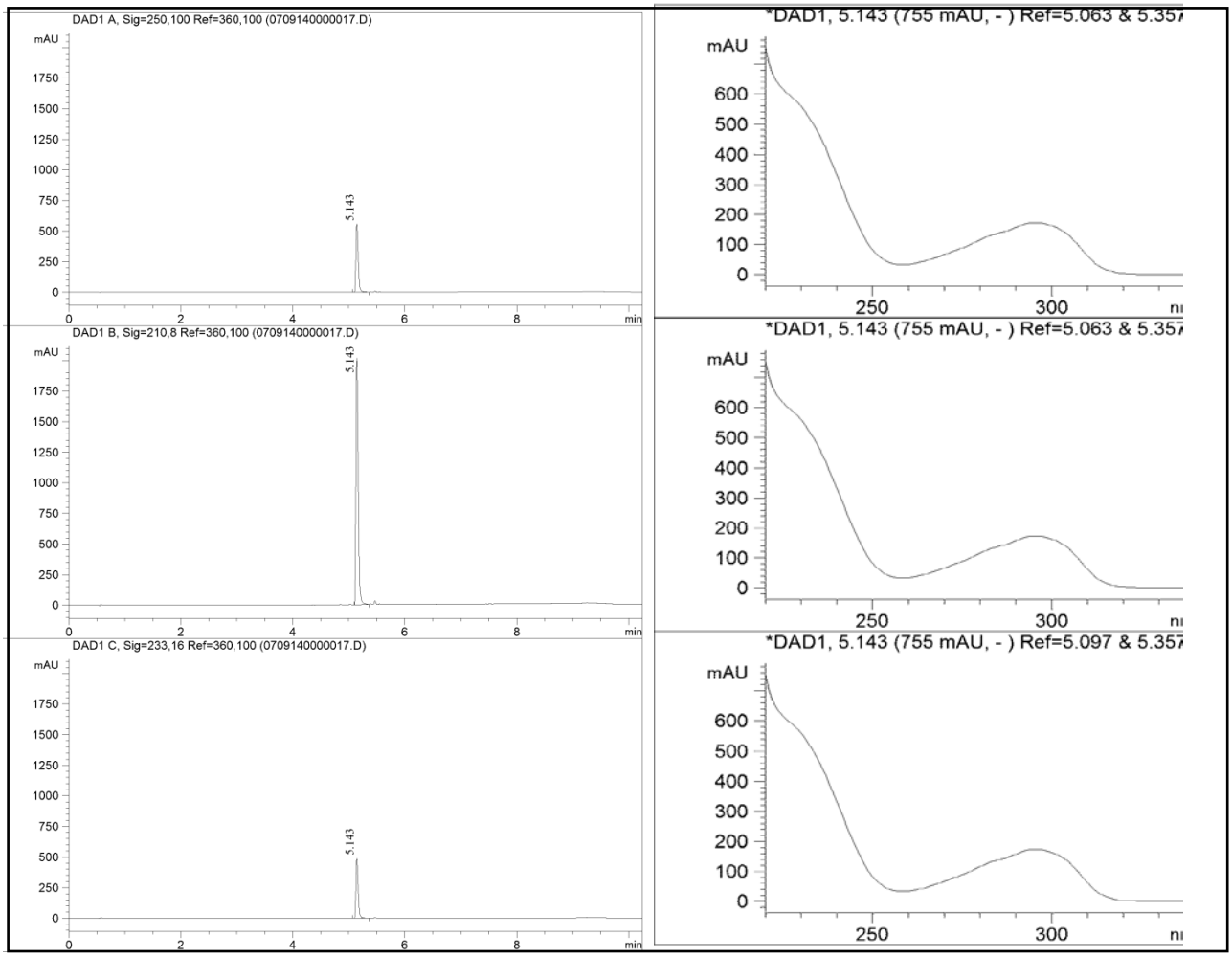
Time	%A	%B	Flow
0	95	5	1.000 mL/min
0.67	95	5	1.000 mL/min
0.68	85	15	1.000 mL/min
2.00	85	15	1.000 mL/min
6.70	15	85	1.000 mL/min
6.70	15	85	1.000 mL/min
7.50	15	85	1.000 mL/min
8.00	5	95	1.000 mL/min
8.00	5	95	2.700 mL/min
8.50	5	95	2.700 mL/min
9.75	95	5	1.000 mL/min
10.25	95	5	1.000 mL/min

DAD Parameters: **Scan:** 220 – 340nm

Step: 1.0nm

Slitwidth: 4nm

Figure 9: High Performance Liquid Chromatography of 30C-NBOMe (hydrochloride)



Ultraviolet Spectrophotometry (UV):

Instrument: HP 8453

Parameters: **Source:** deuterium lamp

Path length: 1cm

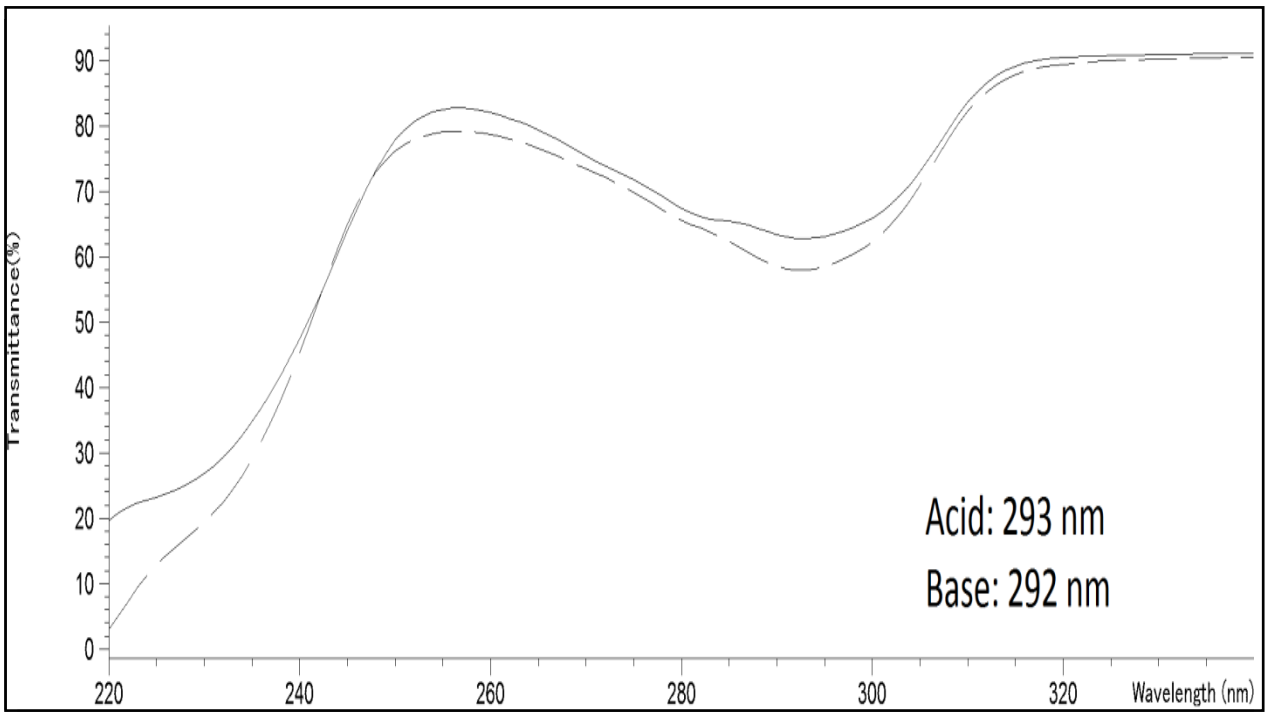
Transmittance

Wavelength range: 220 – 340nm

Integration time: 0.5 sec

Interval: 1nm

Figure 10: Ultraviolet Spectrophotometry of 30C-NBOMe (hydrochloride)



Part 3. External Links:

Forendex