Analytical Profile of 5-fluoro MN-18

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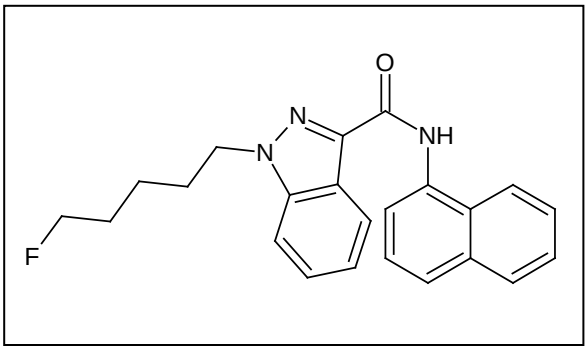
Melissa F. Hehir, Patrick Chepaitis, Georgia Bureau of Investigation, Headquarters Laboratory – Decatur, GA

Table of contents:

Part 1. Cayman Chemical Company Data



Name: 5-fluoro MN-18

Synonyms: 1-(5-fluoropentyl)-N-1-naphthalenyl-1H-indazole-3-carboxamide

CAS#: N/A

Molecular Formula: $C_{23}H_{22}FN_3O$

Molecular Weight: 375.5 g/mol

SMILES: O=C(Nc2cccc1ccccc12)c4nn(CCCCCF)c3ccccc34

InChl Key: XBSWUIWDRFCAGZ-UHFFFAOYAH

InChl: InChI=1/C23H22FN3O/c24-15-6-1-7-16-27-21-14-5-4-12-19(21)22(26-27)23(28)25-20-13-8-10-17-9-2-3-11-18(17)20/h2-5,8-14H,1,6-7,15-16H2,(H,25,28)

Background:

5-fluoro MN-18 is a synthetic cannabinoid modeled after the potent cannabinoid agonist AM2201 (K_i = 1.0nM for CB_1, 2.6nM for CB_2).[1] in that the indole ring of AM2201 has been replaced with an indazole moiety, and the acyl naphthyl group at the 3 position of the indole has been replaced with a 1-aminonaphthylcarboxamide group. 5-fluoro MN-18 began appearing on illicit drug sites during the summer of 2013. Although the physiological and toxicological properties of this compound have not yet been reported, other indazole-based cannabinoid agonists with reported binding affinities such as AKB48 have been detected in herbal smoking mixtures.[2]

[1] Makriyannis, A., and Deng, H. Cannabimimetic indole derivatives. **PCT/US2000/28832** 1-25 (2001 Apr 26).

[2] Uchiyama, N., *et al. Forensic Science International* **227** (1–3): 21–32

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 5-fluoro MN-18

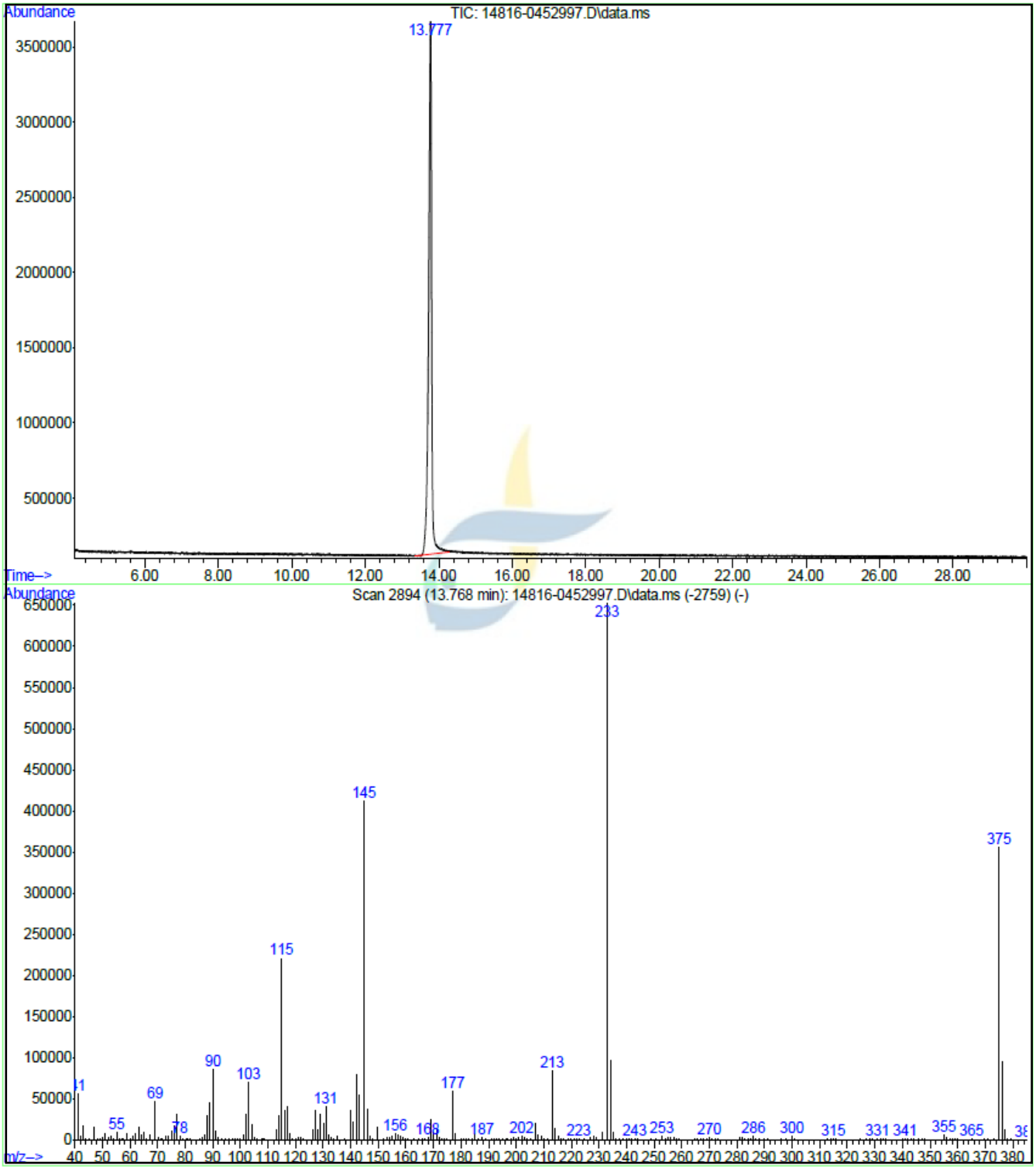


Figure 2. Fourier Transform Infrared Spectroscopy of 5-fluoro MN-18

Experiment Parameters:
PerkinElmer Spectrum 65
Number of scans: 16 (background subtracted)
Resolution: 4 cm^{-1}
Scan Range: 600-4000 cm^{-1}
Sample prepared as KBr pellet

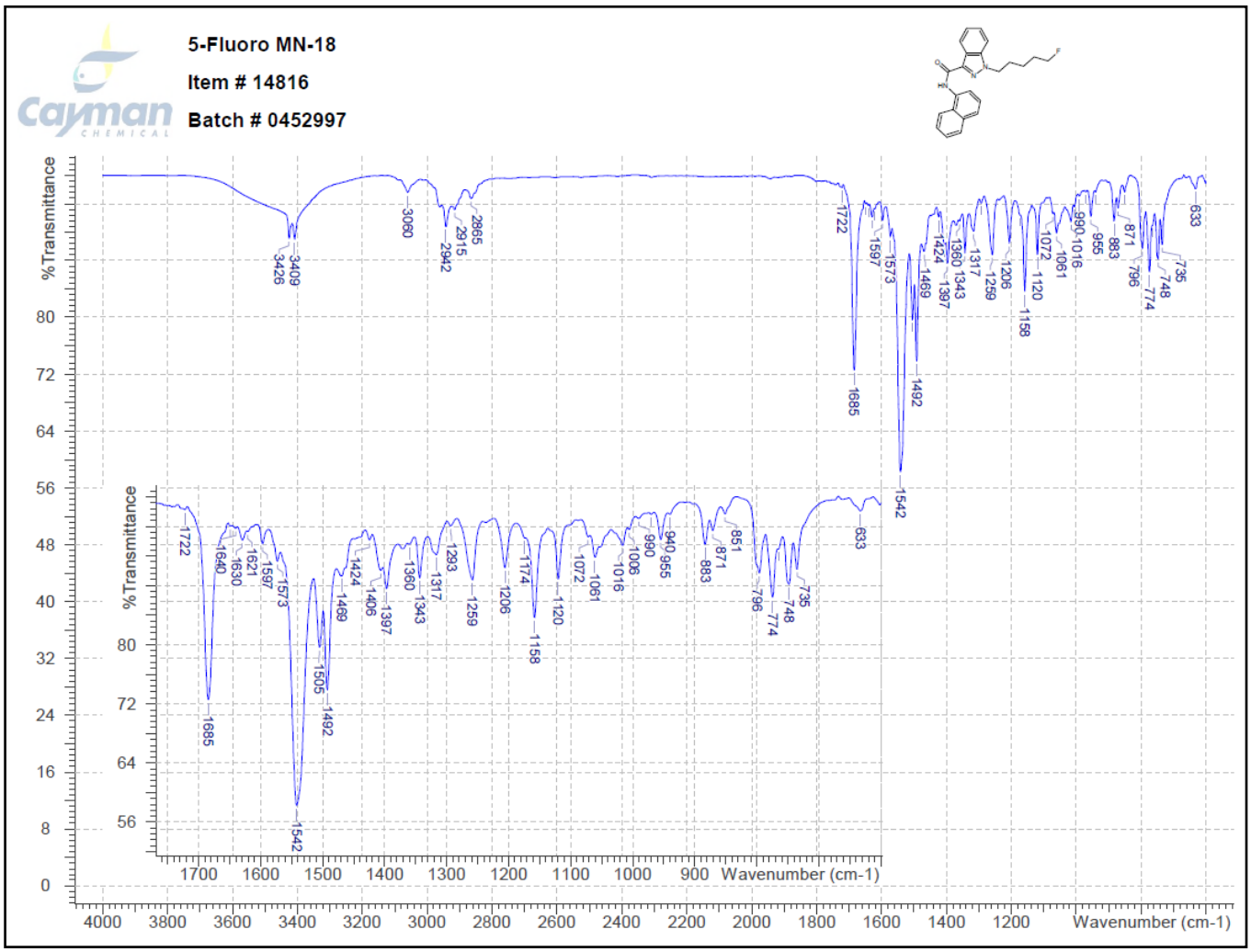


Figure 3. 1H Nuclear Magnetic Resonance Spectroscopy of 5-fluoro MN-18

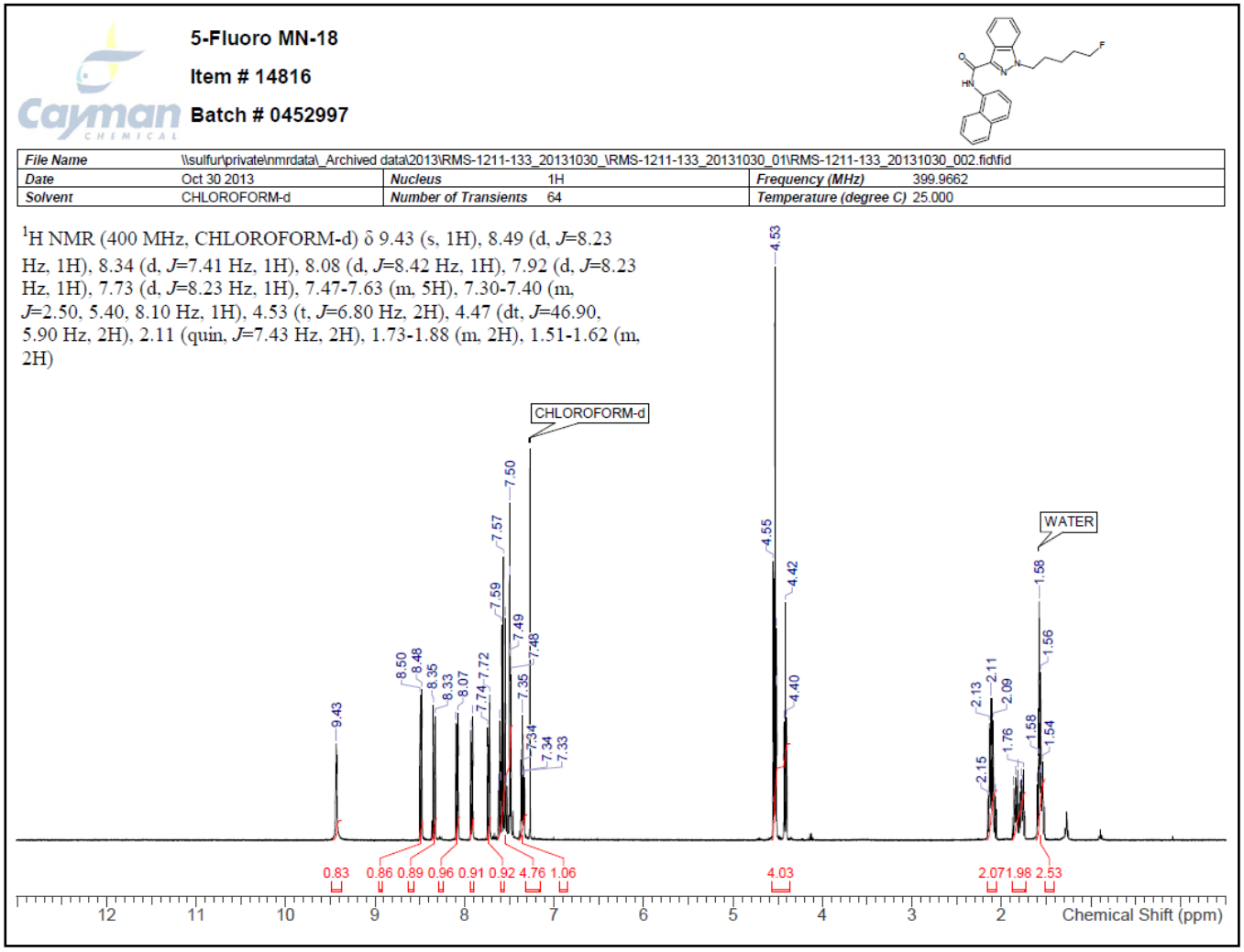


Figure 4. 1H Nuclear Magnetic Resonance Spectroscopy of 5-fluoro MN-18, Enhanced for Detail

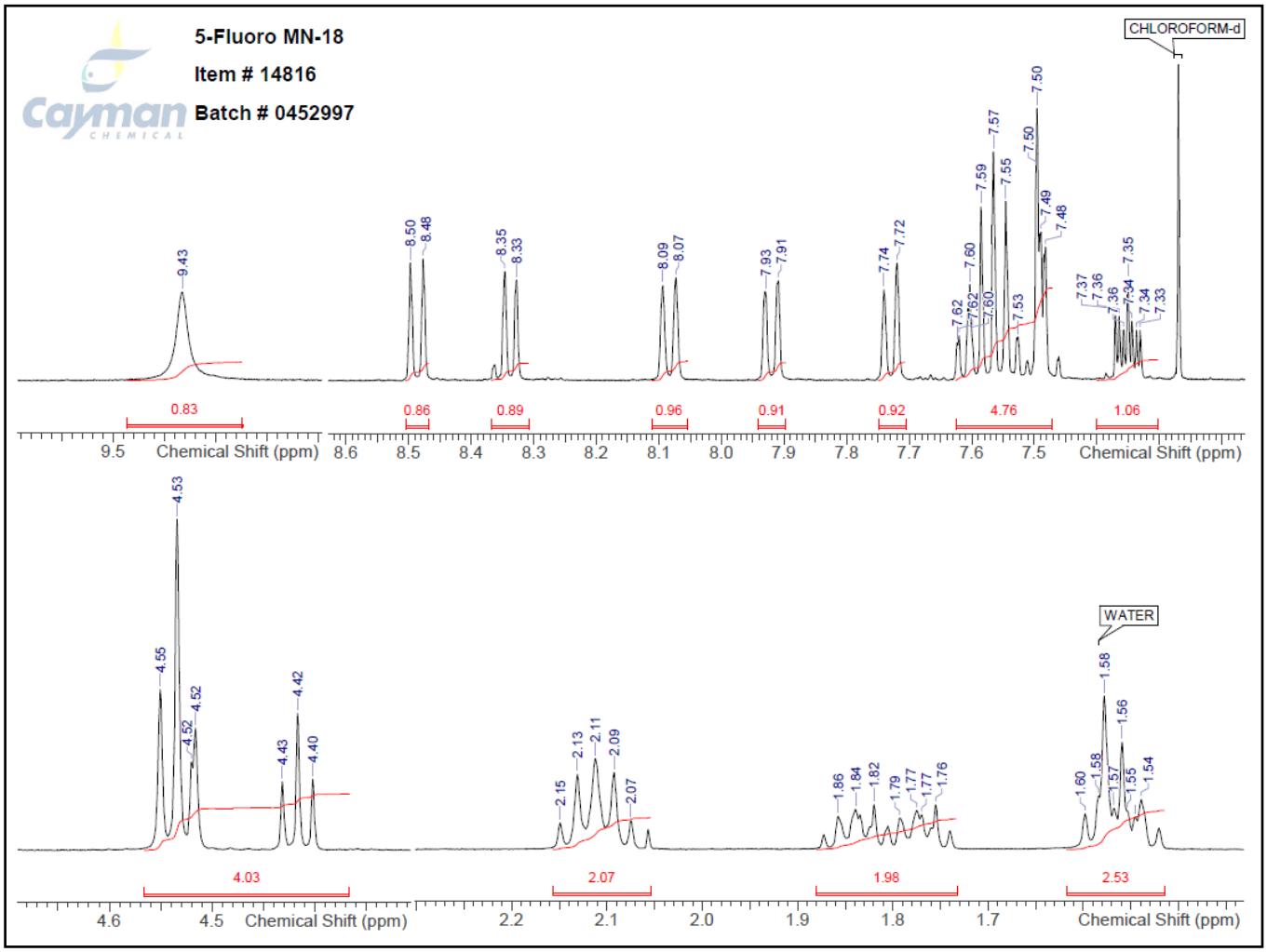
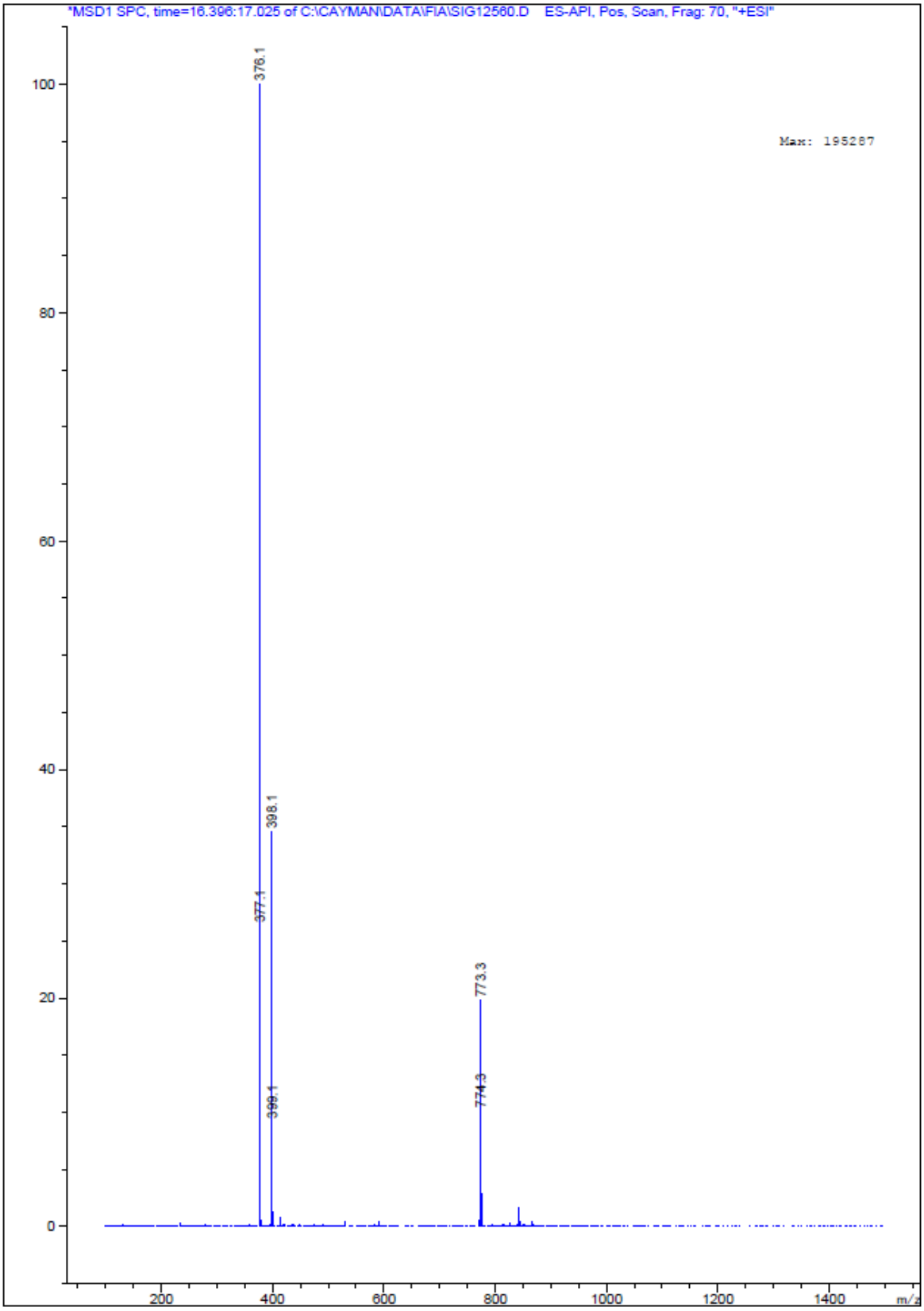
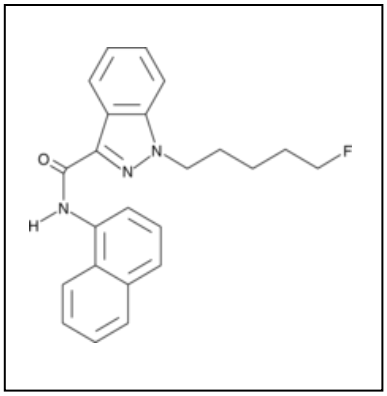


Figure 5. ESI-MS of 5-fluoro MN-18



Part 2. Georgia Bureau of Investigation Data



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Synonyms: 1-(5-fluoropentyl)-N-1-naphthalenyl-1H-indazole-3-carboxamide

CAS#: N/A

Molecular Formula: $C_{23}H_{22}FN_3O$

Molecular Weight: 375.5 g/mol

Source: Cayman Chemicals lot # 0452997-17

Appearance: crystalline solid

SMILES: O=C(Nc2cccc1ccccc12)c4nn(CCCCCF)c3ccccc34

InChl Key: XBSWUIWDRFCAGZ-UHFFFAOYAH

InChl: InChI=1/C23H22FN3O/c24-15-6-1-7-16-27-21-14-5-4-12-19(21)22(26-27)23(28)25-20-13-8-10-17-9-2-3-11-18(17)20/h2-5,8-14H,1,6-7,15-16H2,(H,25,28)

Gas Chromatography/Mass Spectrometry (GCMS):

Sample Preparation: EtOH

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

GC Parameters

Column: HP Ultra-112m × 200µm × 0.33µm

Carrier gas: Helium

Oven program:
1) initial temperature 70ºC for 2 min.
2) ramp to 275ºC at 30ºC/min.
3) hold at 275ºC for 18 min.

Injection parameters: 1µL injection; split ratio: 100:1

Inlet temperature: 275ºC

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 6: Gas Chromatography/Mass Spectrometry of 5-fluoro MN-18

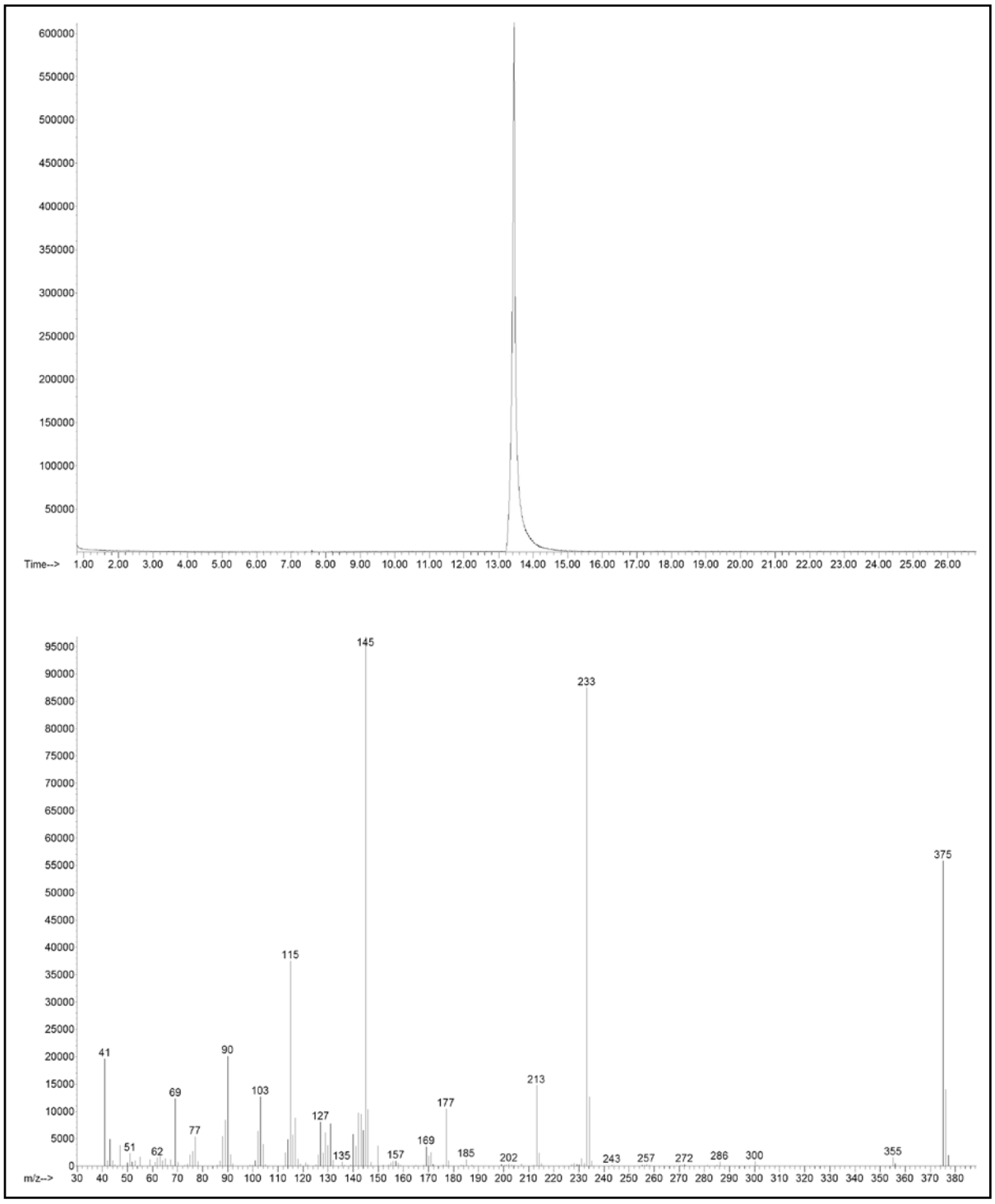
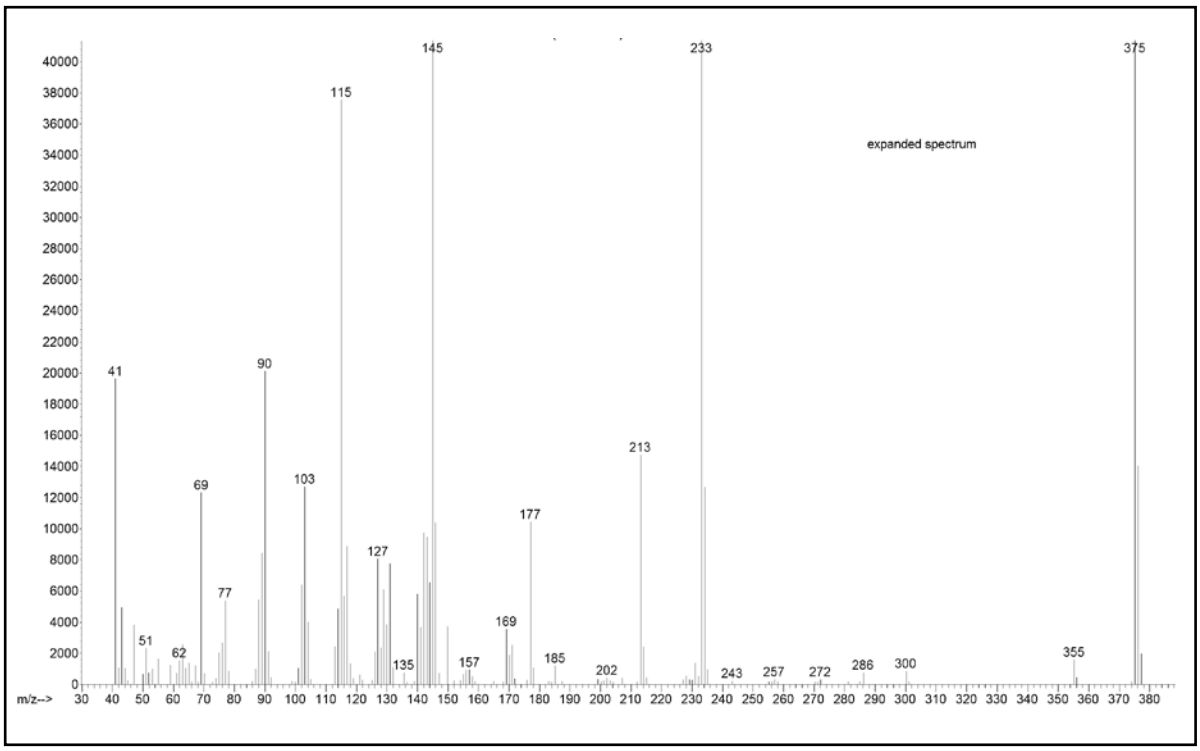


Figure 7: Expanded Gas Chromatography/Mass Spectrometry of 5-fluoro MN-18



Gas Chromatography/Infrared Spectroscopy (GC-FTIR):

Instrument: Agilent 7890A gas chromatograph / Spectra Analysis DiscovIR

GC Parameters:

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

Carrier gas: Helium

Oven program:
1) initial temperature 70ºC for 3 min.
2) ramp to 300ºC at 13ºC/min.
3) hold at 300ºC for 4 min.

Injection parameters: 2µL injection; split ratio: 2:1

Inlet temperature: 275ºC

Flow program: 2mL/min for 17 min, then 1mL/min for 5 min

IR Parameters:

Disk Temperature: -40ºC

Restrictor Temperature: 300ºC

Oven Temperature: 300ºC

Transfer Line Temperature: 300ºC

Dewar Cap Temperature: 20ºC

Disk Speed: 3 mm/min

Spectral Range (cm^{-1}): 4000-650

Chamber Pressure: 0.00001 torr

Resolution: $4cm^{-1}$

Figure 8: Gas Chromatography/Infrared Spectroscopy of 5-fluoro MN-18

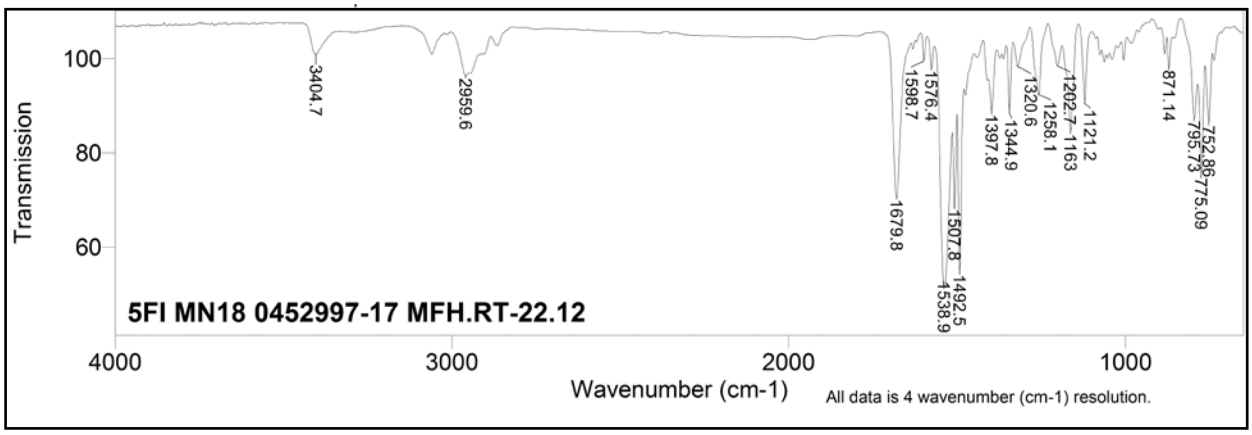
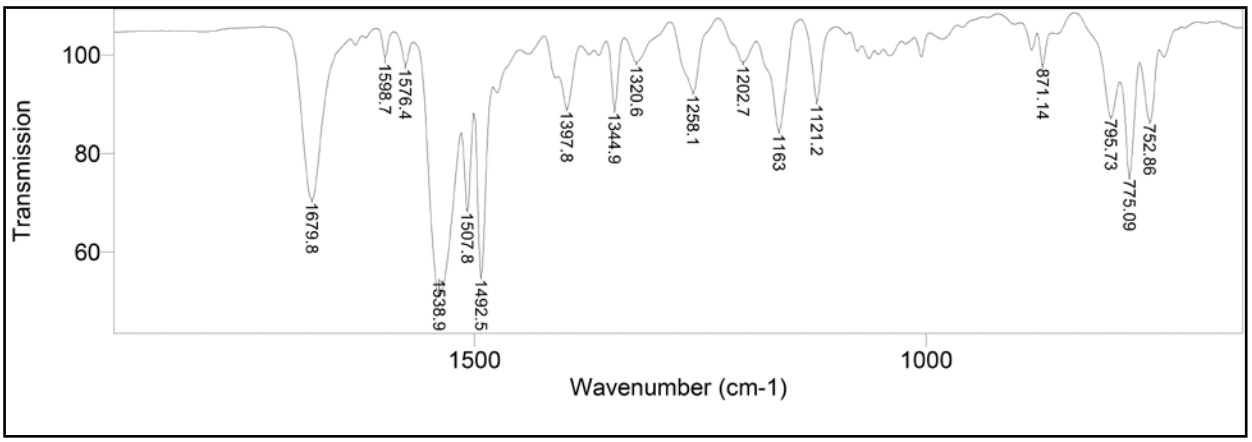


Figure 9: Expanded Gas Chromatography/Infrared Spectroscopy of 5-fluoro MN-18



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

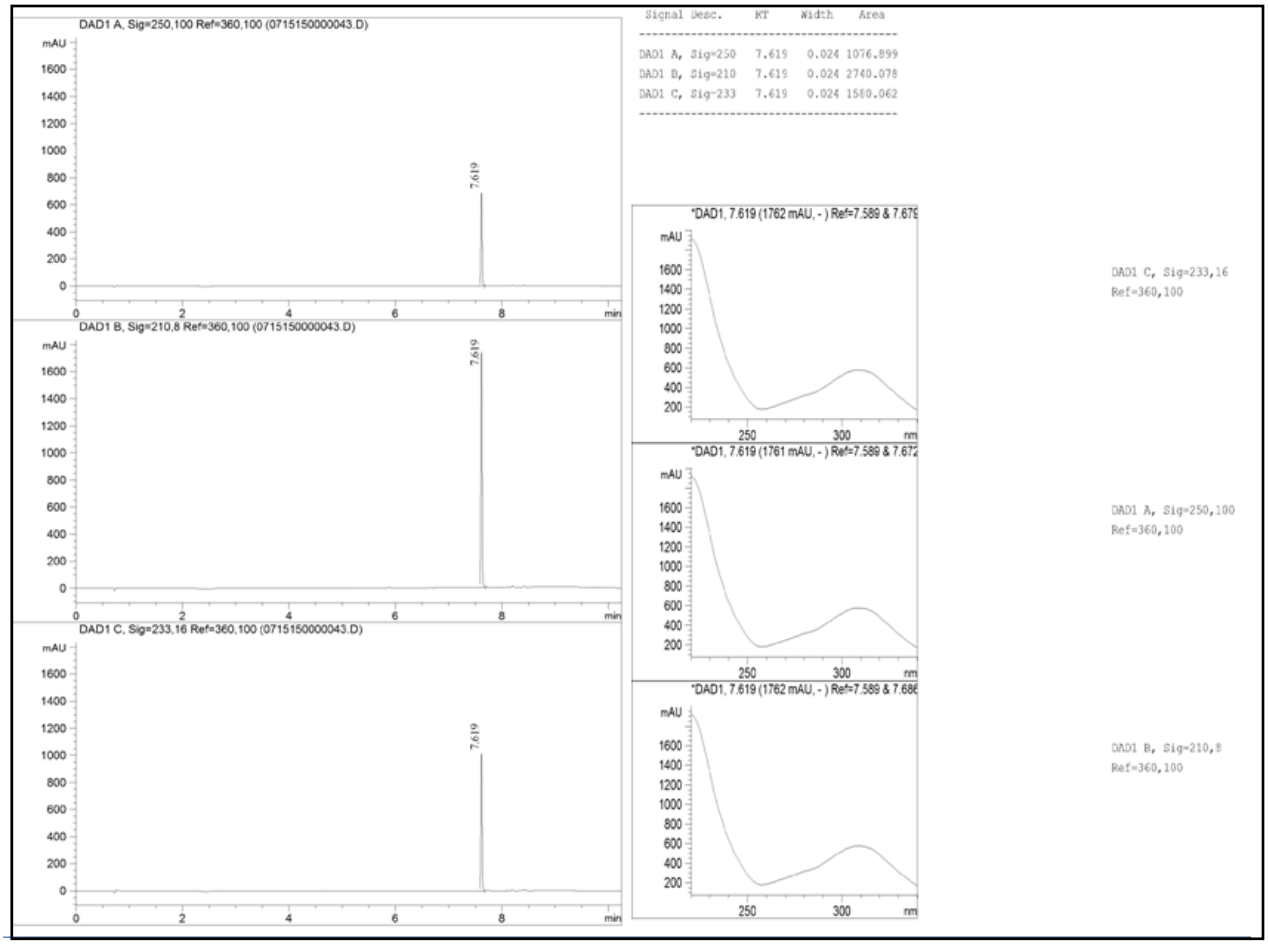
Time	%A	%B	Flow
0	95	5	1.0 mL/min
0.67	95	5	1.0 mL/min
0.68	85	15	1.0 mL/min
2.00	85	15	1.0 mL/min
6.70	15	85	1.0 mL/min
8.00	5	95	2.7 mL/min
9.75	95	5	1.0 mL/min
10.25	95	5	1.0 mL/min

UV Parameters: **Scan:** 220 – 340nm

Step: 1.0nm

Slitwidth: 4nm

Figure 10: High Performance Liquid Chromatography of 5-fluoro MN-18



Ultraviolet Spectrophotometry (UV):

Instrument: HP 8453

Parameters: **Source:** deuterium lamp

Path length: 1cm

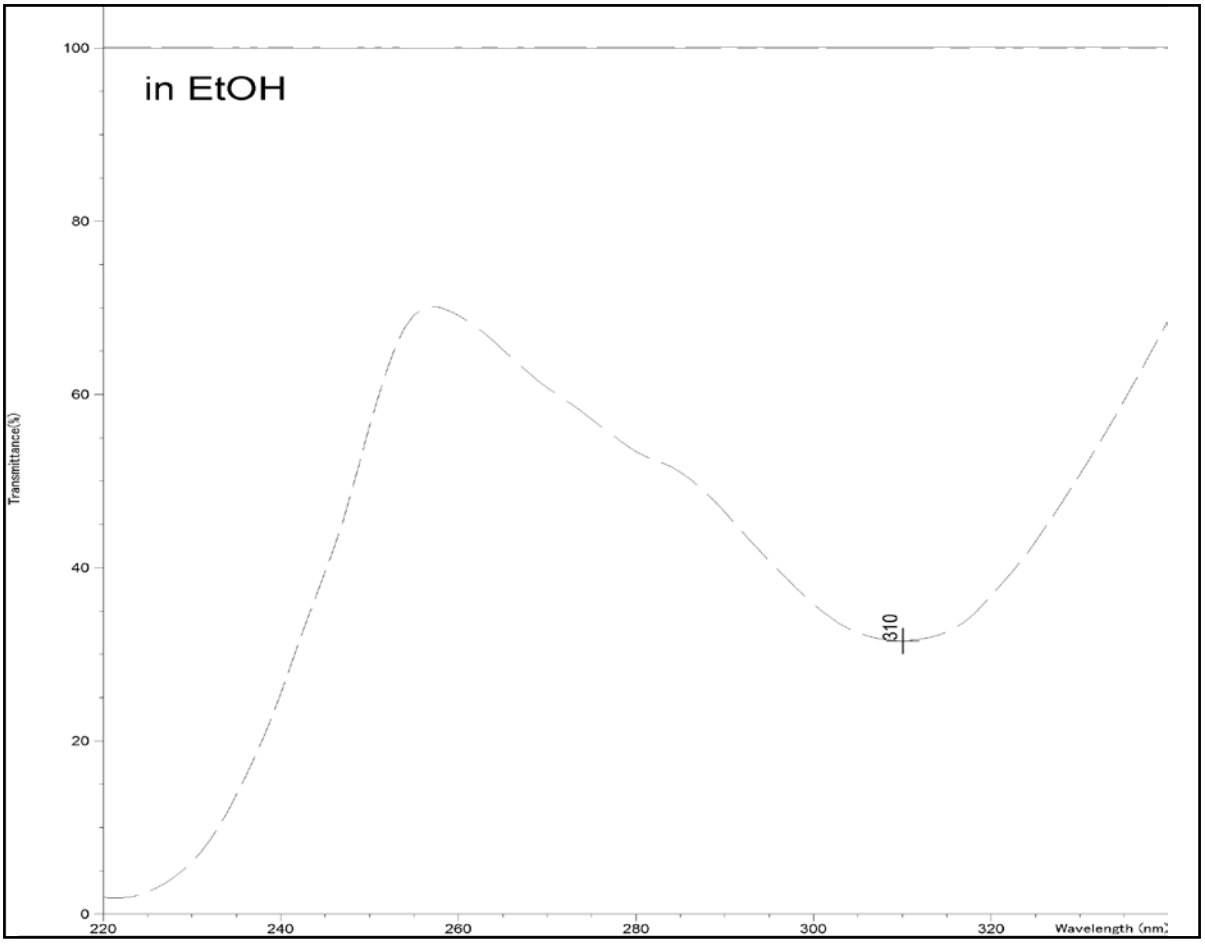
Transmittance

Wavelength range: 220 – 340nm

Integration time: 0.5 sec

Interval: 1nm

Figure 11: Ultraviolet Spectrophotometry of 5-fluoro MN-18



Part 3. External Links:

SAFS Forendex