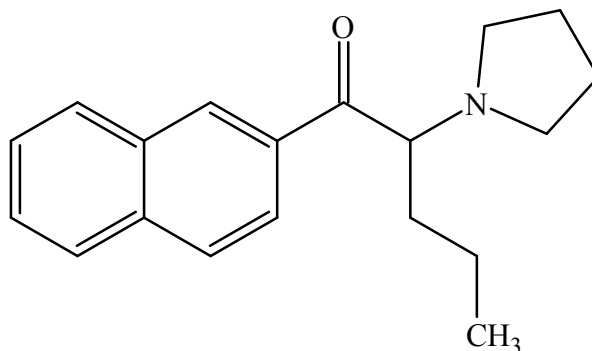




Naphyrone

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



1. GENERAL INFORMATION

IUPAC Name: 1-(naphthalen-2-yl)-2-(pyrrolidin-1-yl)pentan-1-one

CAS#: 850352-53-3 (base), 850352-11-3 (HCl)

Synonyms: β -naphyrone, O-2482, NRG-1, naphthylpyrovalerone, naphpyrovalerone

Source: DEA Reference Material Collection

Appearance: White Powder

UV_{max} (nm): Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{19}H_{23}NO$	281	Not Determined
HCl	$C_{19}H_{23}NO \cdot HCl$	317	248.2



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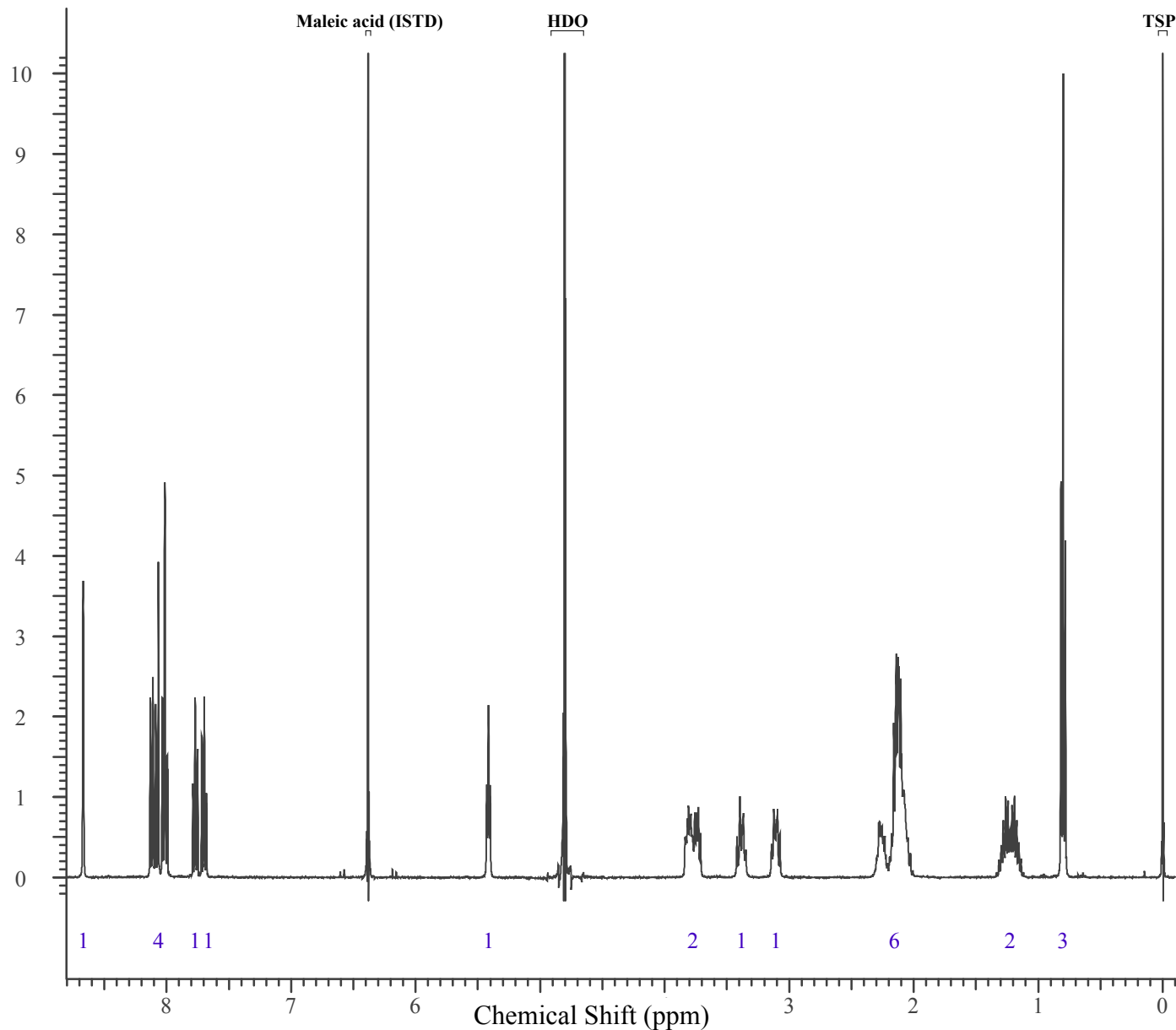
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 mg/mL in deuterium oxide (D₂O) containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

Instrument: 400 MHz NMR spectrometer
Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

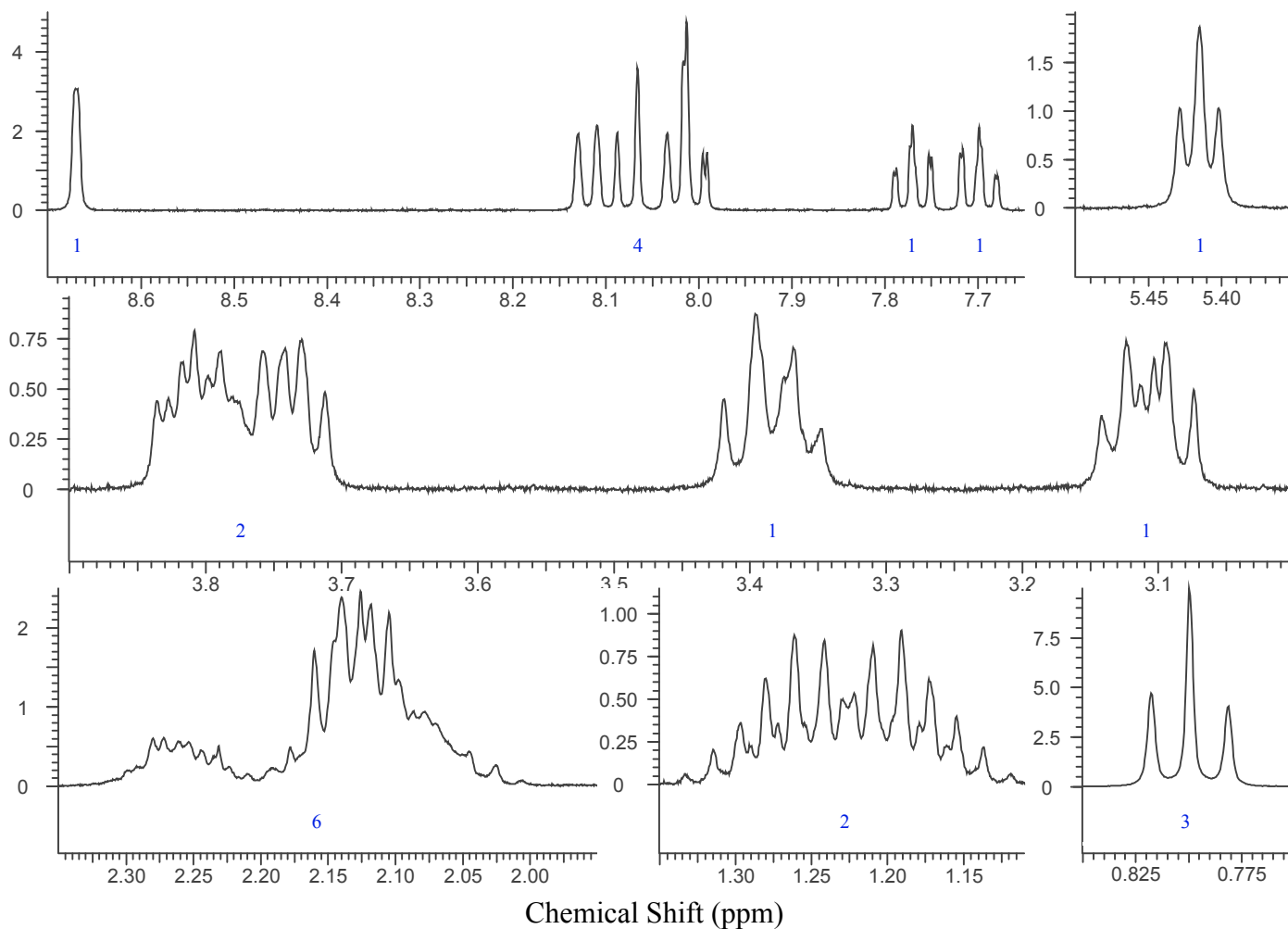
¹H NMR: Naphyrone HCl; Lot 2011DEA003-24A; D₂O, 400 MHz





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3.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~ 4 mg/mL in methanol

Instrument:

Agilent gas chromatograph operated in split mode with MS detector

Column:

DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 μ m

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



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**Injection Parameters:**

Split Ratio = 25:1, 1 μ L injected

MS Parameters:

Mass scan range: 34-550 amu

Threshold: 100

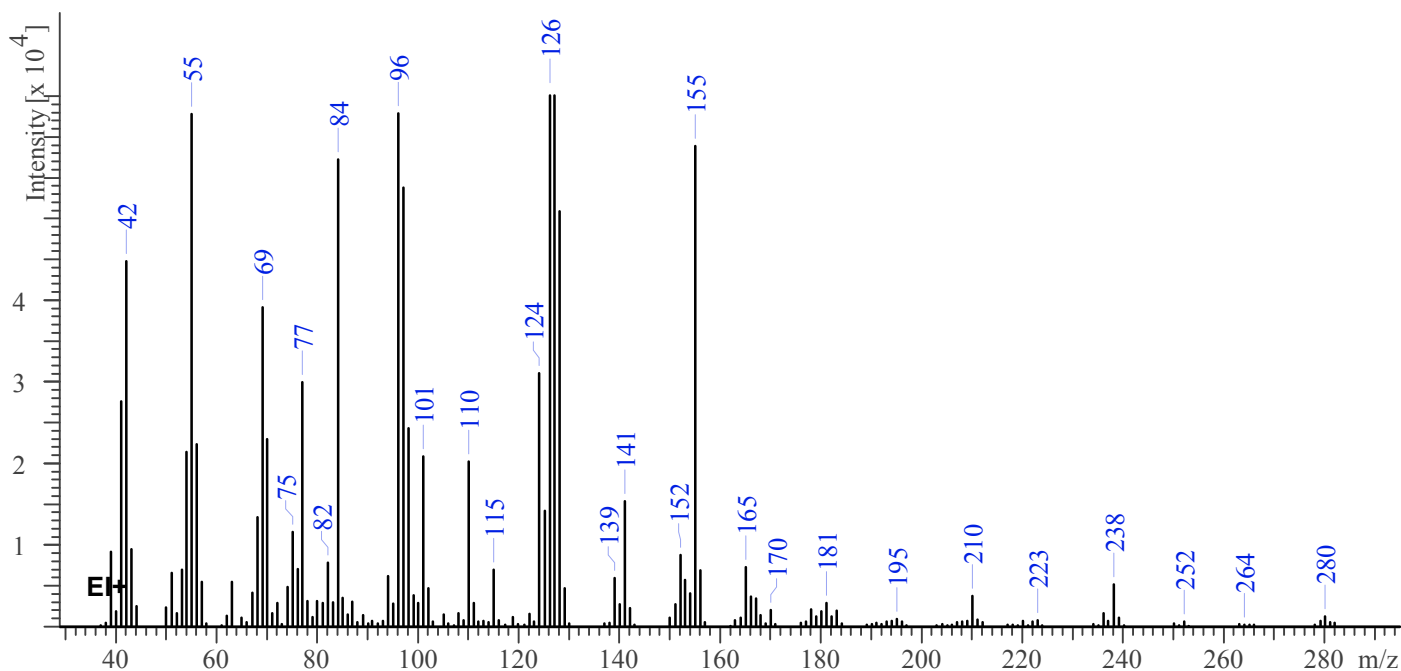
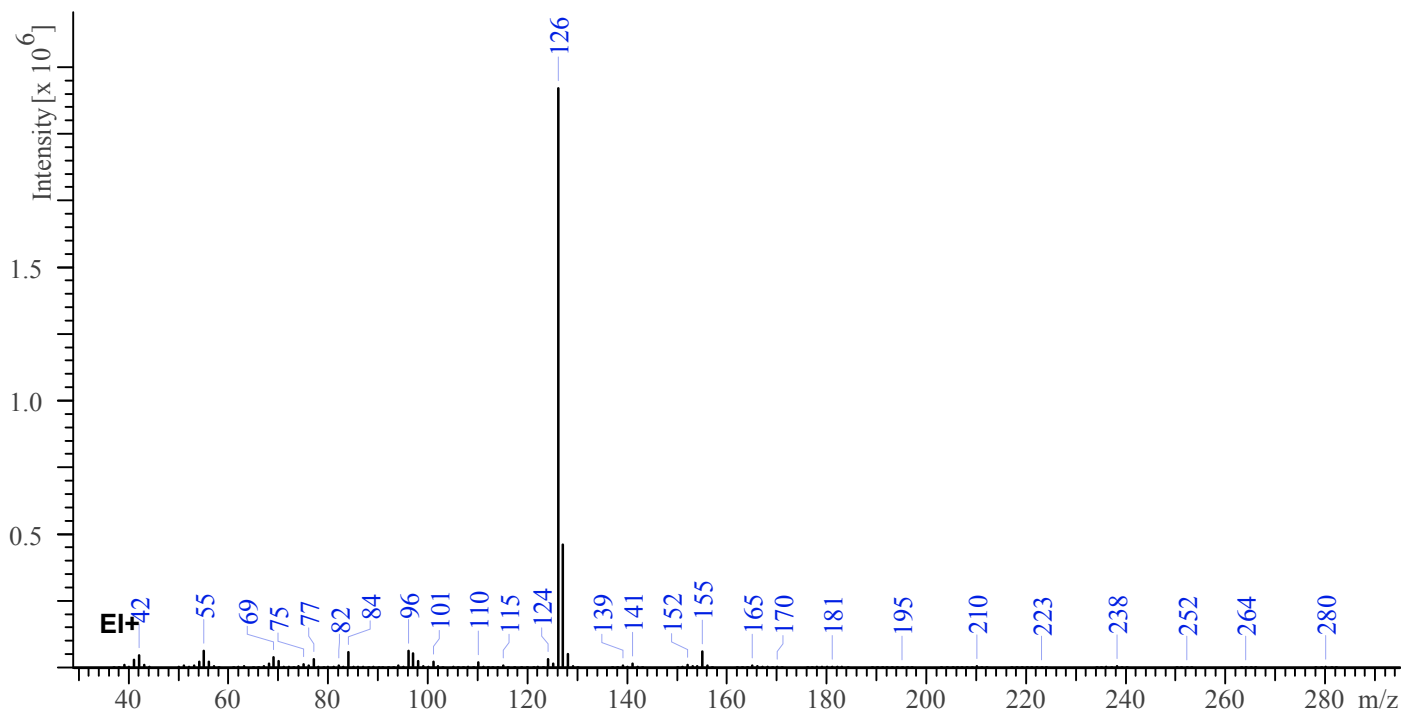
Tune file: stune.u

Acquisition mode: scan

Retention Time:

14.834 min

EI Mass Spectrum: Naphyrone HCl; Lot 2011DEA003-24A





Naphyrone

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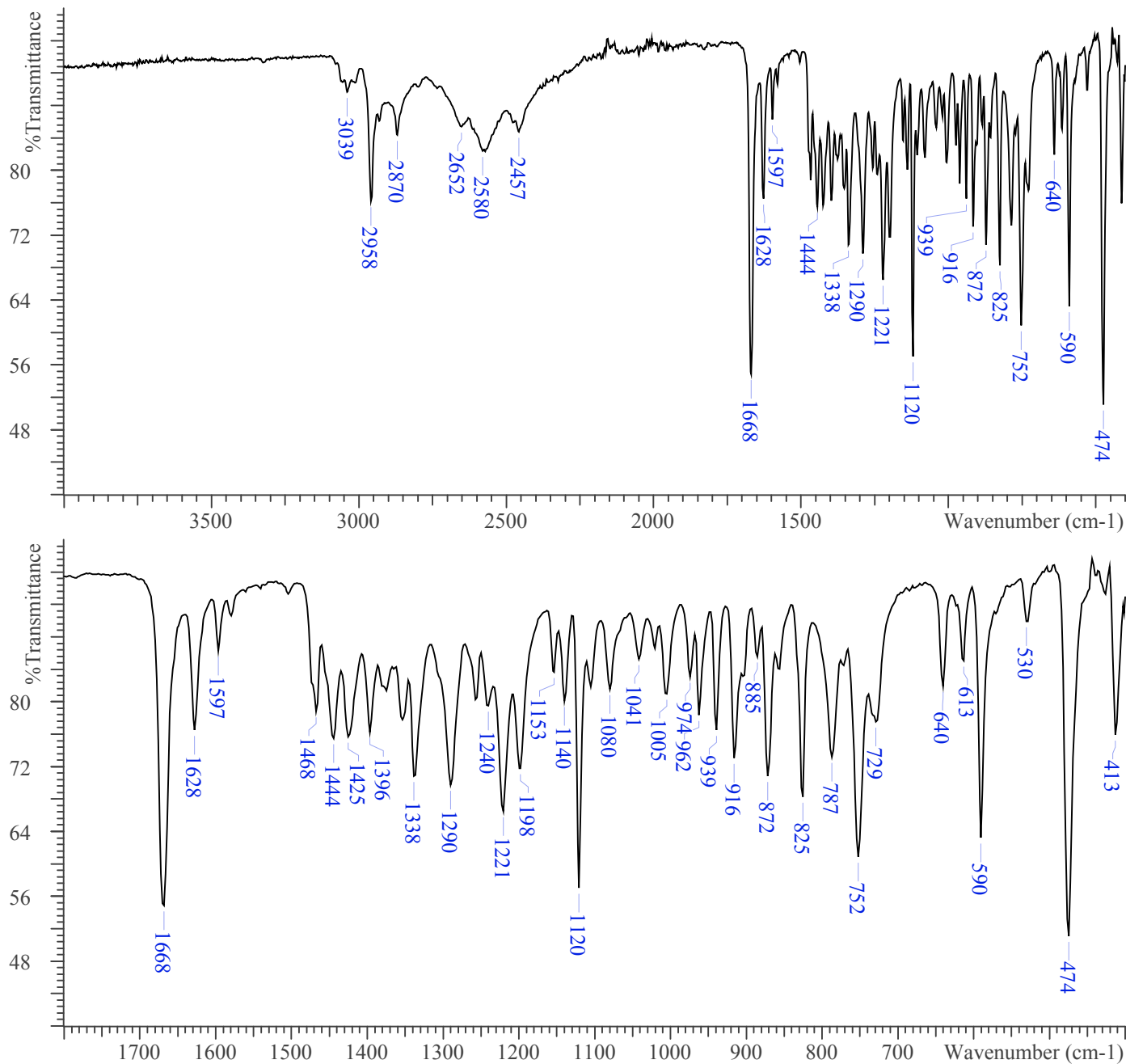


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (3 bounce)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4 cm⁻¹
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): Naphyrone HCl; Lot 2011DEA003-24A





Naphyrone

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4. ADDITIONAL RESOURCES

De Paoli, G.; Maskell, P.D.; Pounder, D.J. Naphyrone: analytical profile of the new "legal high" substitute for mephedrone. *J. Forensic Leg. Med.* **2011**, 18 (2), 93.

Brandt, S.D.; Wootton, R.C.; De Paoli G.; Freeman S. The Naphyrone Story: The Alpha or Beta-naphthyl Isomer? *Drug Test. Analysis* **2010**, 2, 496-502.

Brandt, S.D.; Sumnall, H.R.; Measham, F.; Cole, J. Analysis of second-generation 'legal highs' in the UK: Initial findings. *Drug Test. Analysis* **2010**, 2, 377-382.

[Forendex](#)

[Wikipedia](#)