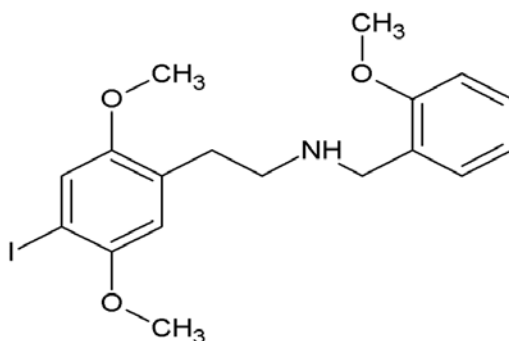




## 25I-NBOMe

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



### 1. GENERAL INFORMATION

**IUPAC Name:** 2-(4-Iodo-2,5-dimethoxyphenyl)-N-(2-methoxybenzyl)ethanamine

**CAS #:** Base: 919797-19-6 HCl: 1043868-97-8

**Synonyms:** 2-C-I-NBOMe, Cimbi-5, 2-(2,5-dimethoxyphenyl-4-iodo)-N-(2-methoxybenzyl)ethanamine; N-Bomb; Smiles

**Source:** DEA Reference Material Collection

**Appearance:** White powder (HCl)

**UV<sub>max</sub>:** 239, 298.5 nm

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>18</sub> H <sub>22</sub> NO <sub>3</sub> I	427	Not Determined
HCl	C <sub>18</sub> H <sub>22</sub> NO <sub>3</sub> I·HCl	463	157.3



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## 3. QUALITATIVE DATA

### 3.1 NUCLEAR MAGNETIC RESONANCE

#### Method NMR CDCl<sub>3</sub>

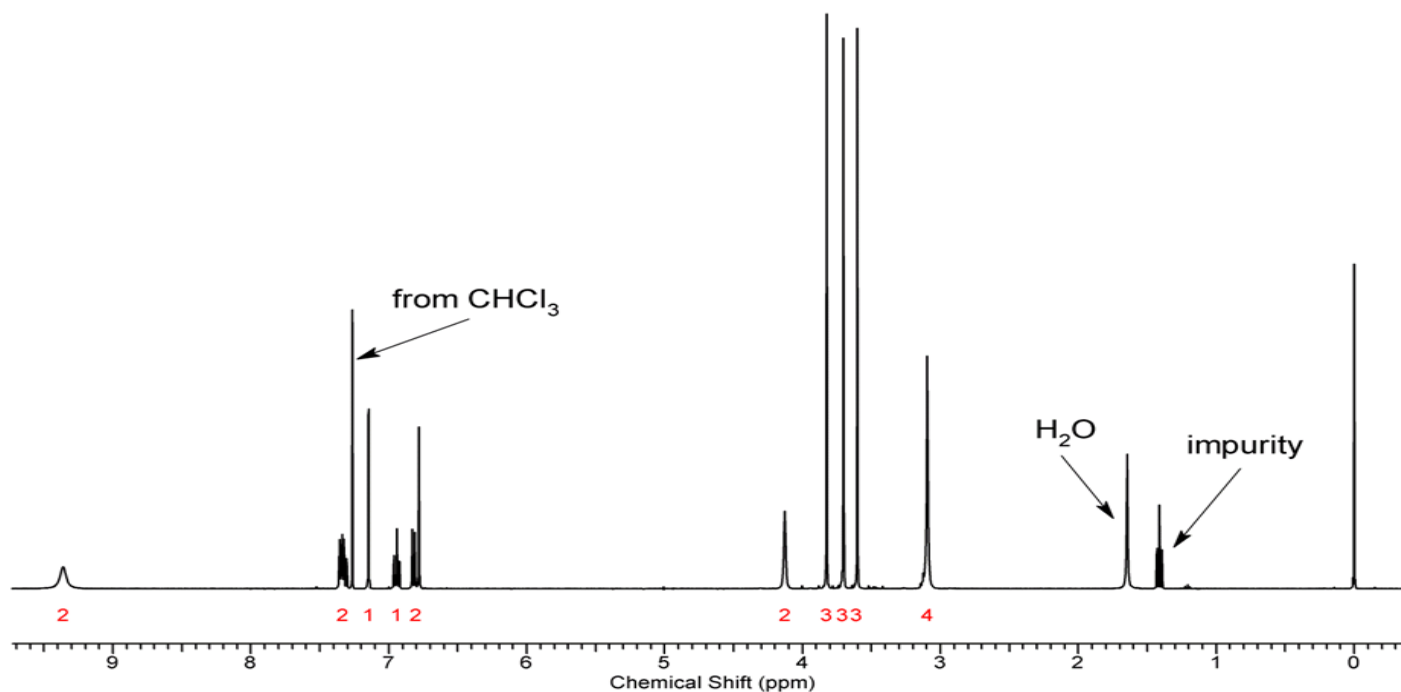
**Sample Preparation:** Sample diluted to ~5 mg/mL in deuteriochloroform (CDCl<sub>3</sub>) containing TMS for 0 ppm reference

**Instrument:** Varian Mercury 400 MHz NMR spectrometer with proton detection probe

**Parameters:**

- Spectral width: at least containing -3 ppm through 13 ppm
- Pulse angle: 90°
- Delay between pulses: 45 seconds
- Number of scans (NT): 8
- Number of steady state scans: 0
- Oversampling: 4 or more
- Shimming: automatic gradient shimming of Z1-4 shims
- Phasing, Drift Correction: automatic or manual

<sup>1</sup>H NMR: 2,5I-NBOMe HCl Lot # N17-P11B CDCl<sub>3</sub>, 400MHz

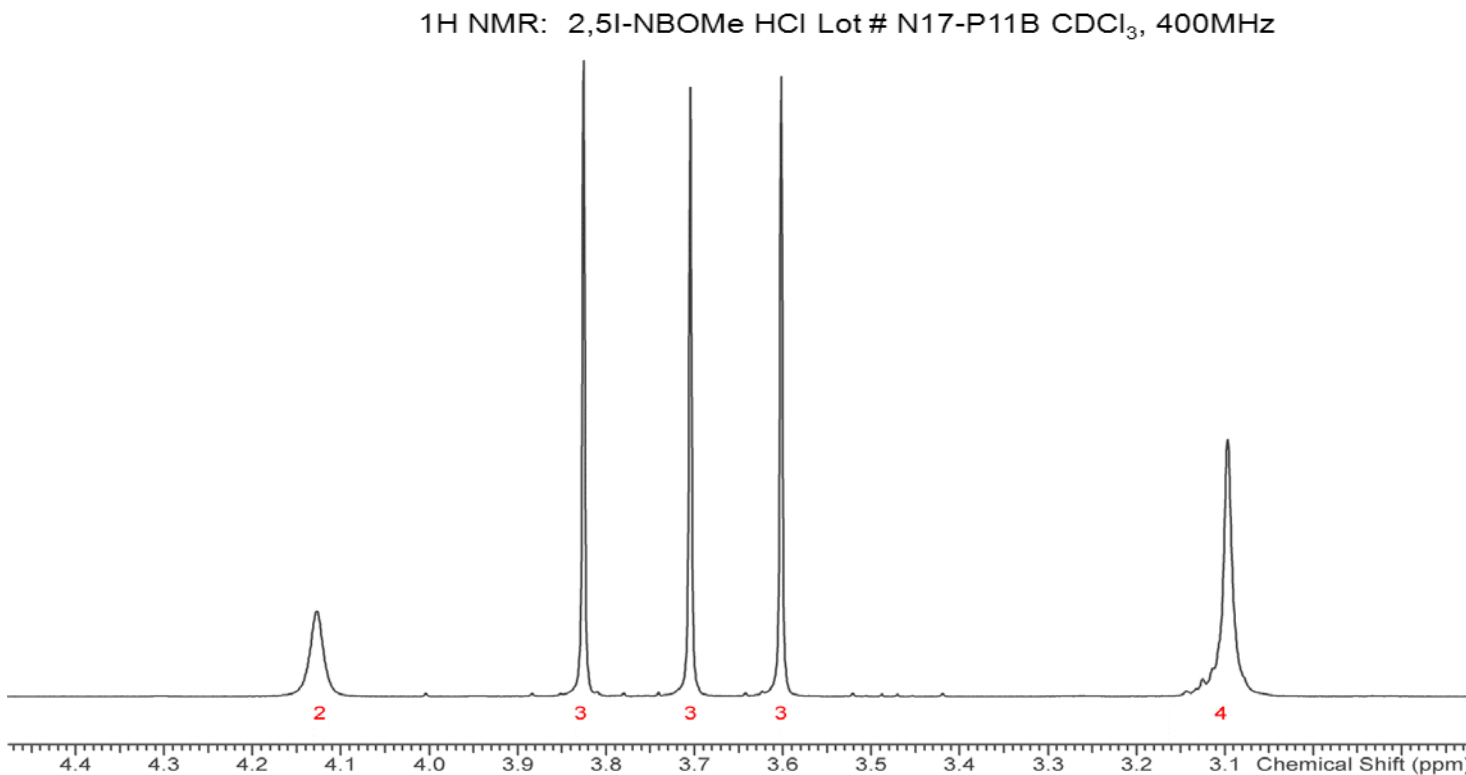
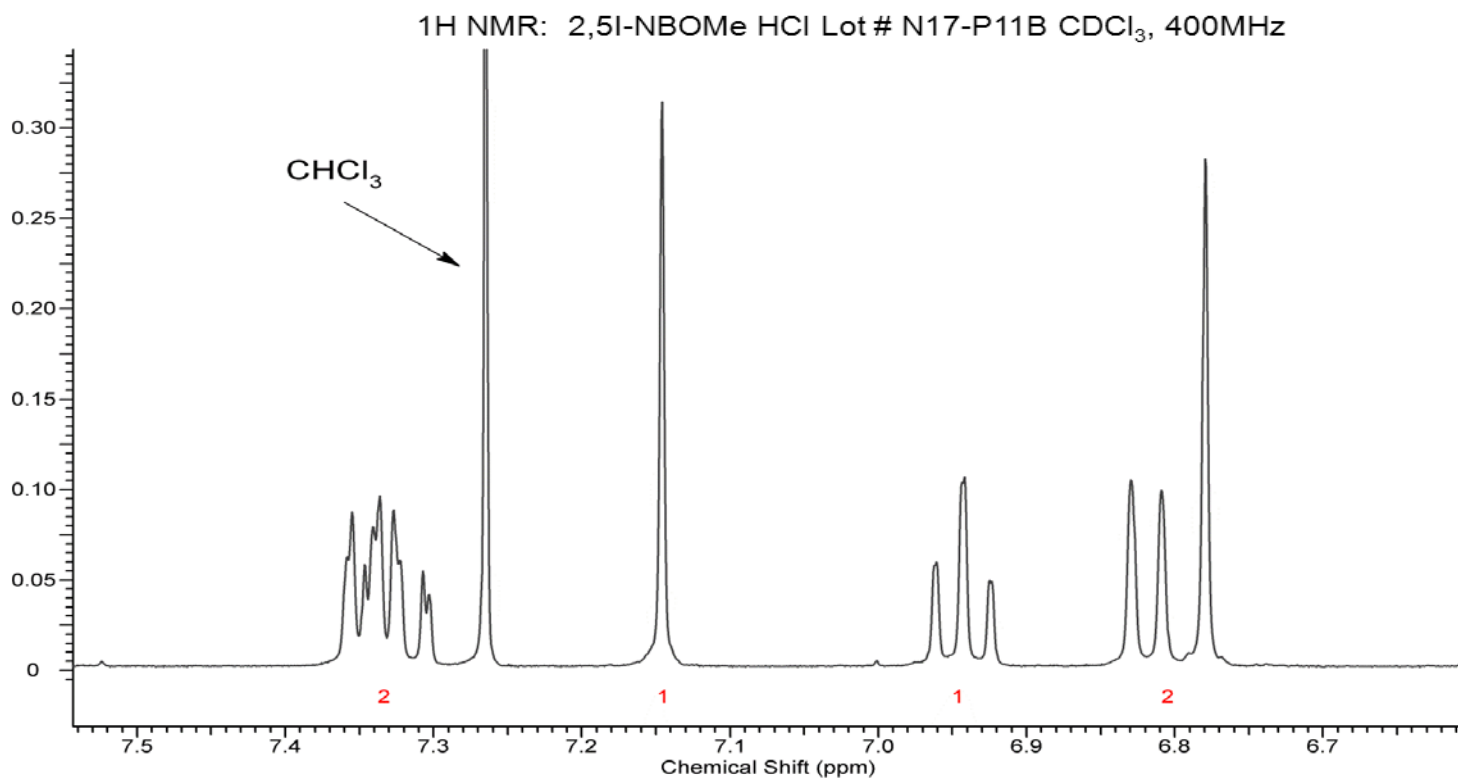




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### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

**Sample Preparation:** Dilute analyte to ~1 mg/mL in MeOH.

**Instrument:** Gas chromatograph operated in split mode with MS detector

**Column:** DB-1 MS or equivalent; 30m x 0.25mm x 0.25 $\mu$ 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:

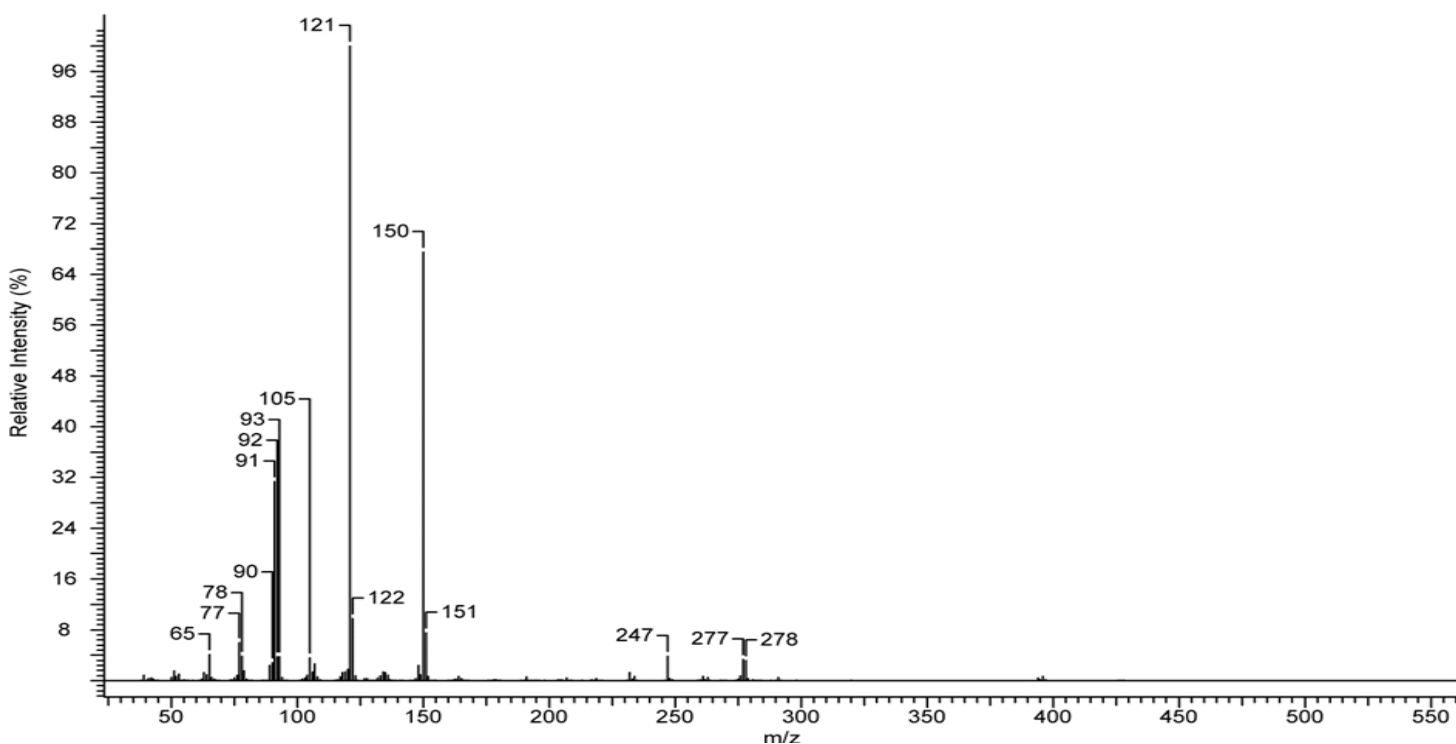
- 1) 100°C initial temperature for 1.0 min
- 2) Ramp to 300°C at 12°C/min
- 3) Hold final temperature for 9.0 min

**Injection Parameters:** Split Ratio = 25:1, 1  $\mu$ L injected

**MS Parameters:**  
Mass scan range: 34-550 amu  
Threshold: 100  
Tune file: stune.u  
Acquisition mode: scan

**Retention Time:** 17.647 minutes

EI Mass Spectrum: 2,5I-NBOMe HCl, Lot # N17-P11B





# 25I-NBOMe

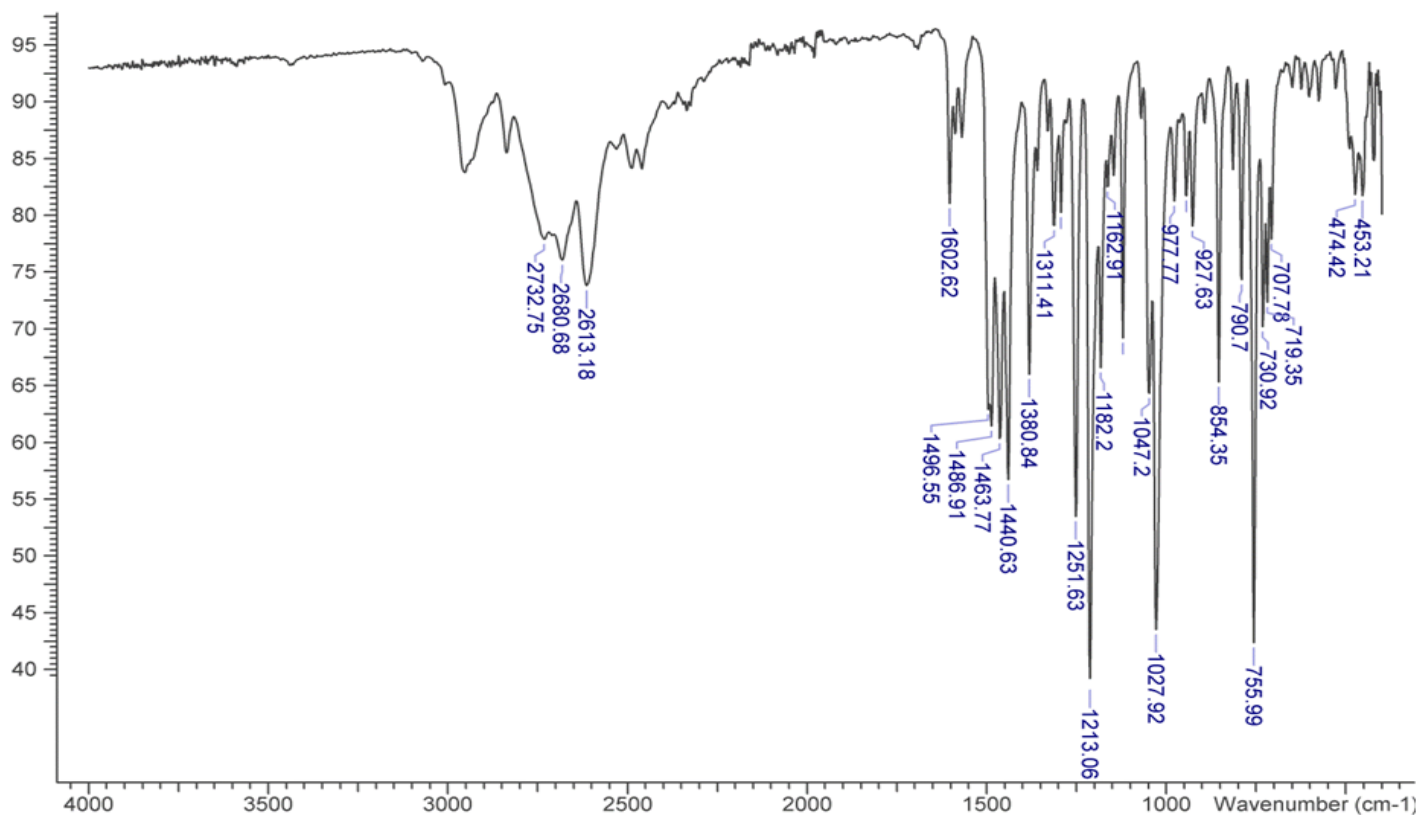


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## 3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (3 bounce)  
**Scan Parameters:** Number of scans: 32  
Number of background scans: 32  
Resolution:  $4\text{cm}^{-1}$   
Sample gain: 8  
Aperture: 150

FTIR (Diamond ATR, 3 Bounce): 2,5I-NBOMe HCl Lot # N17-P11B 32 scans,  $4\text{cm}^{-1}$  resolution



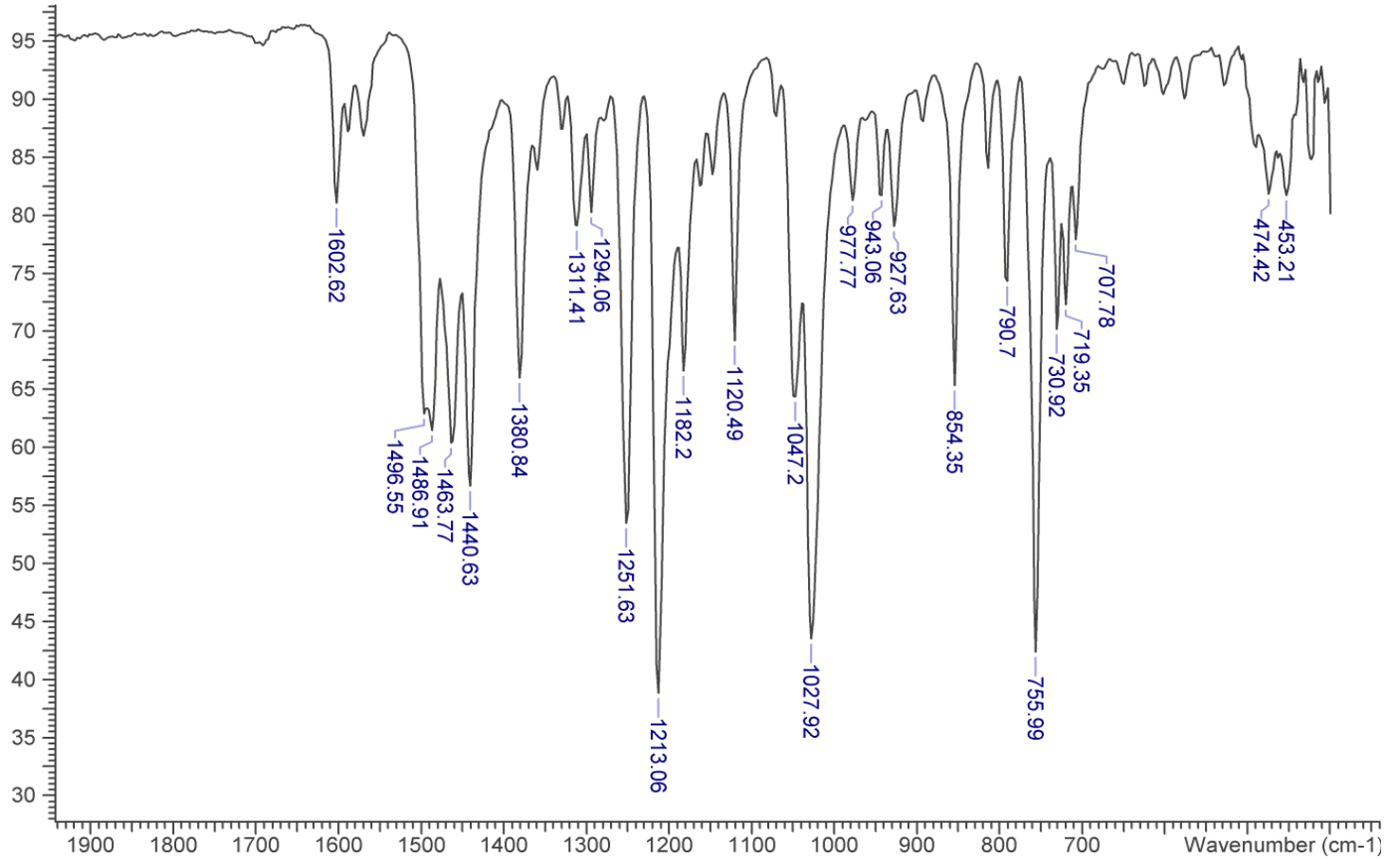


# 25I-NBOMe



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FTIR (Diamond ATR, 3 Bounce): 2,5I-NBOMe HCl Lot # N17-P11B 32 scans, 4cm<sup>-1</sup> resolution



## 4. ADDITIONAL RESOURCES

[Forendex](#)

[Wikipedia](#)