

1. GENERAL INFORMATION

IUPAC Name:	<i>N</i> -[2-(5-methoxy-1 <i>H</i> -indol-3-yl)ethyl]- <i>N</i> -(prop-2-en-1-yl)prop-2-en-1-amine
CFR:	Unscheduled (as of 1/2013)
CAS #:	92882-98-4
Synonyms:	5-MeO-DALT, 5-methoxy-DALT, <i>N,N</i> -diallyl-5-methoxytryptamine, <i>N</i> -allyl- <i>N</i> -[2-(5-methoxy-1 <i>H</i> -indol-3-yl)ethyl]prop-2-en-1-amine, diallyl-[2-(5-methoxy-1 <i>H</i> -indol-3-yl)ethyl]amine, <i>N</i> -[2-(5-methoxy-1 <i>H</i> -indol-3-yl)ethyl]- <i>N</i> -prop-2-enyl-2-propen-1-amine, <i>N</i> -[2-(5-methoxy-1 <i>H</i> -indol-3-yl)ethyl]- <i>N</i> -prop-2-enylprop-2-en-1-amine, <i>N</i> -[2-(5-methoxy-1 <i>H</i> -indol-3-yl)ethyl]- <i>N</i> -prop-2-enyl-prop-2-en-1-amine
Source:	DEA Reference Material Collection
Appearance:	White powder
Kovat's Index:	Pending
UV_{max} (nm):	220.6, 275.1

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₇ H ₂₂ N ₂ O	270	105.1

3. ADDITIONAL RESOURCES

[Forendex](#)

[Wikipedia](#)

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CDCl₃

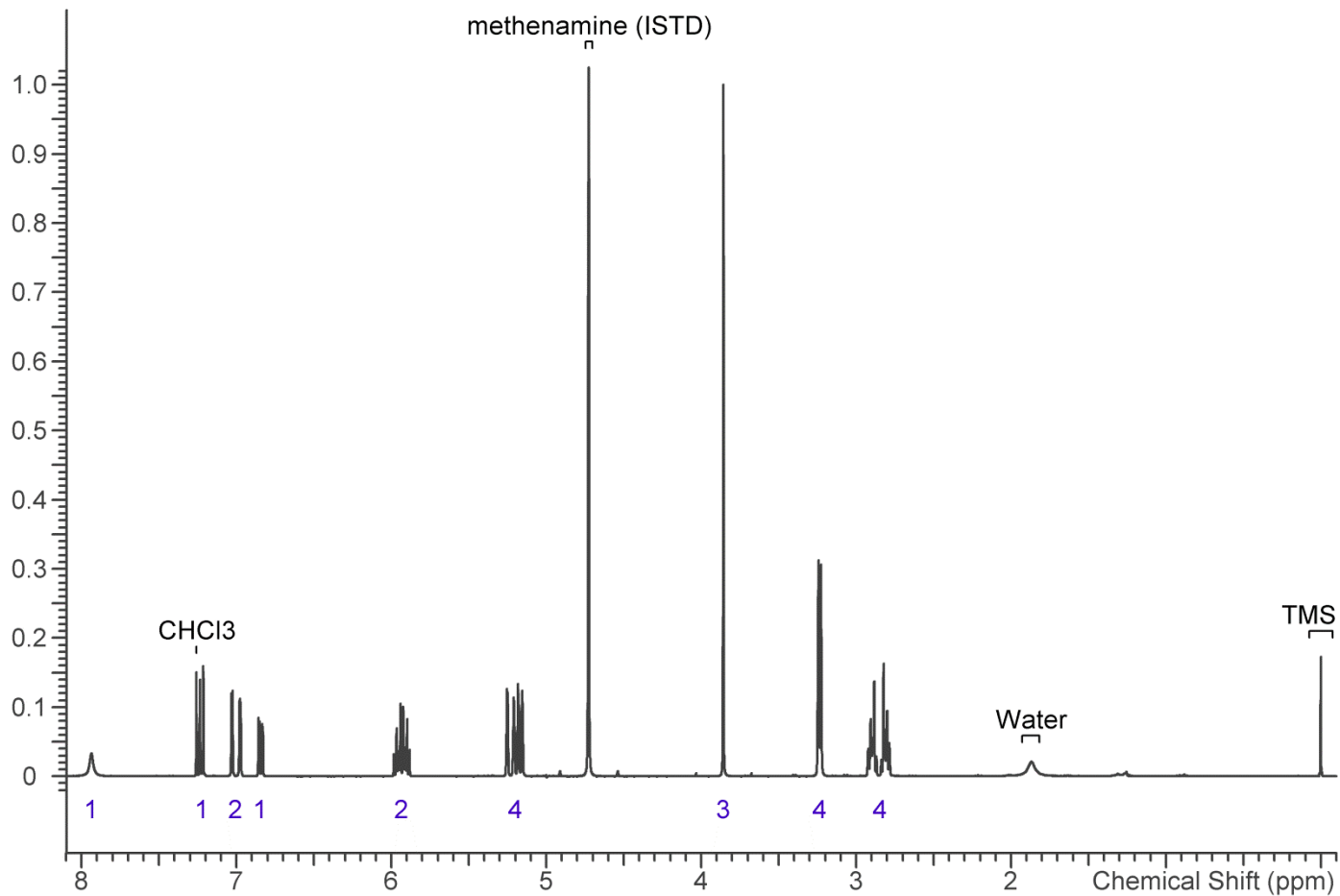
Sample Preparation: Dilute analyte to ~10 mg/mL in deuteriochloroform (CDCl₃) containing TMS for 0 ppm reference and methenamine as quantitative internal standard.

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

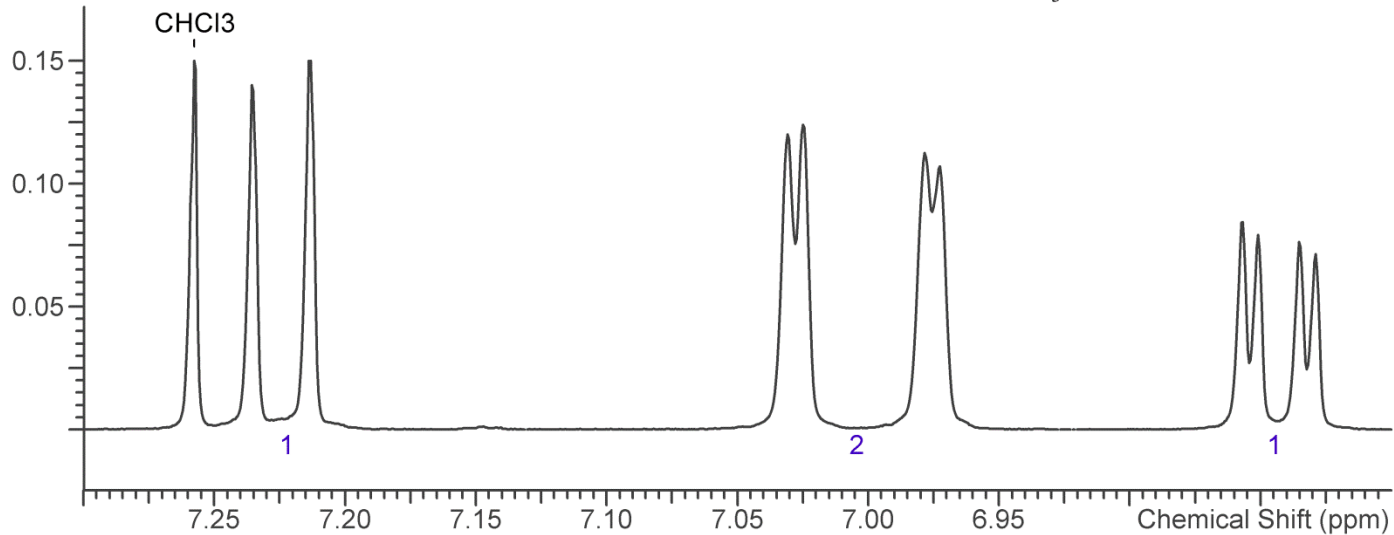
Parameters:

- 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

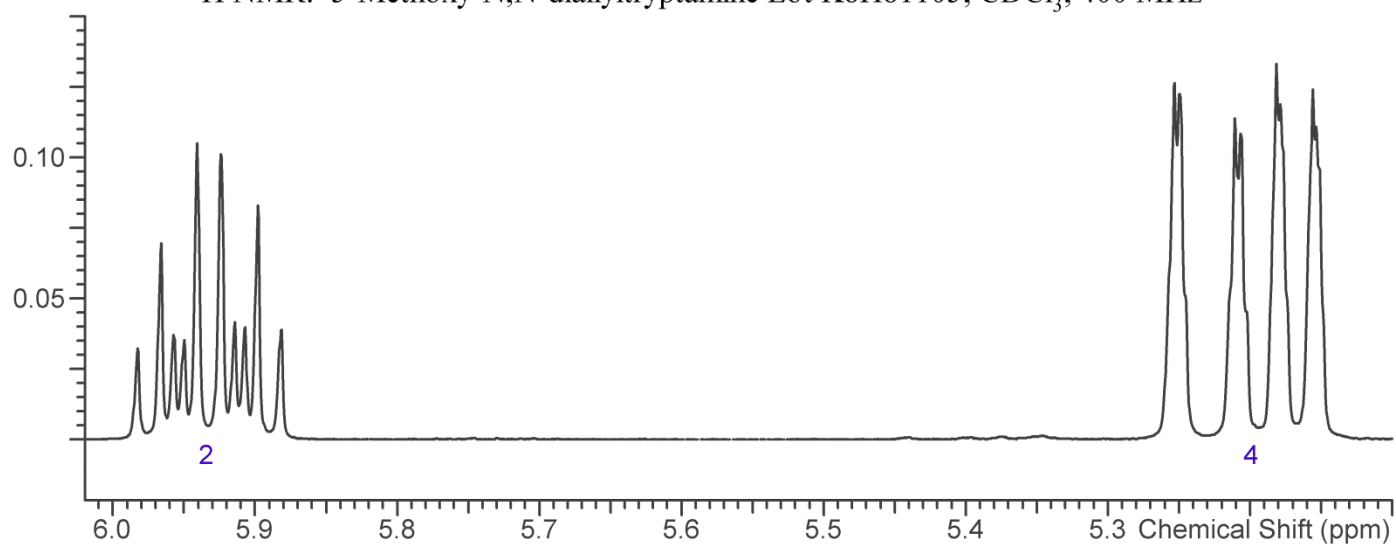
¹H NMR: 5-Methoxy-N,N-diallyltryptamine Lot K8H81105; CDCl₃; 400 MHz



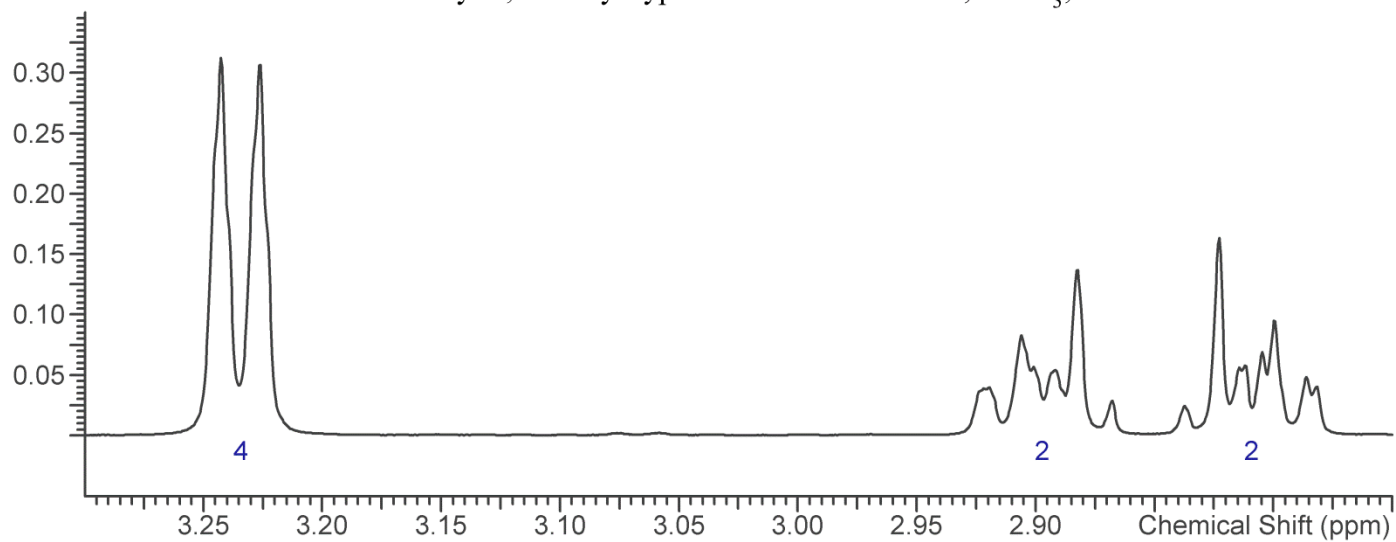
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4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

Instrument: Agilent gas chromatograph operated in split mode with MS detector

Column: DB-1 MS; 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

Injection Parameters: Split Ratio = 20:1, 1 μ L injected

MS Parameters: Mass scan range: 30-550 amu

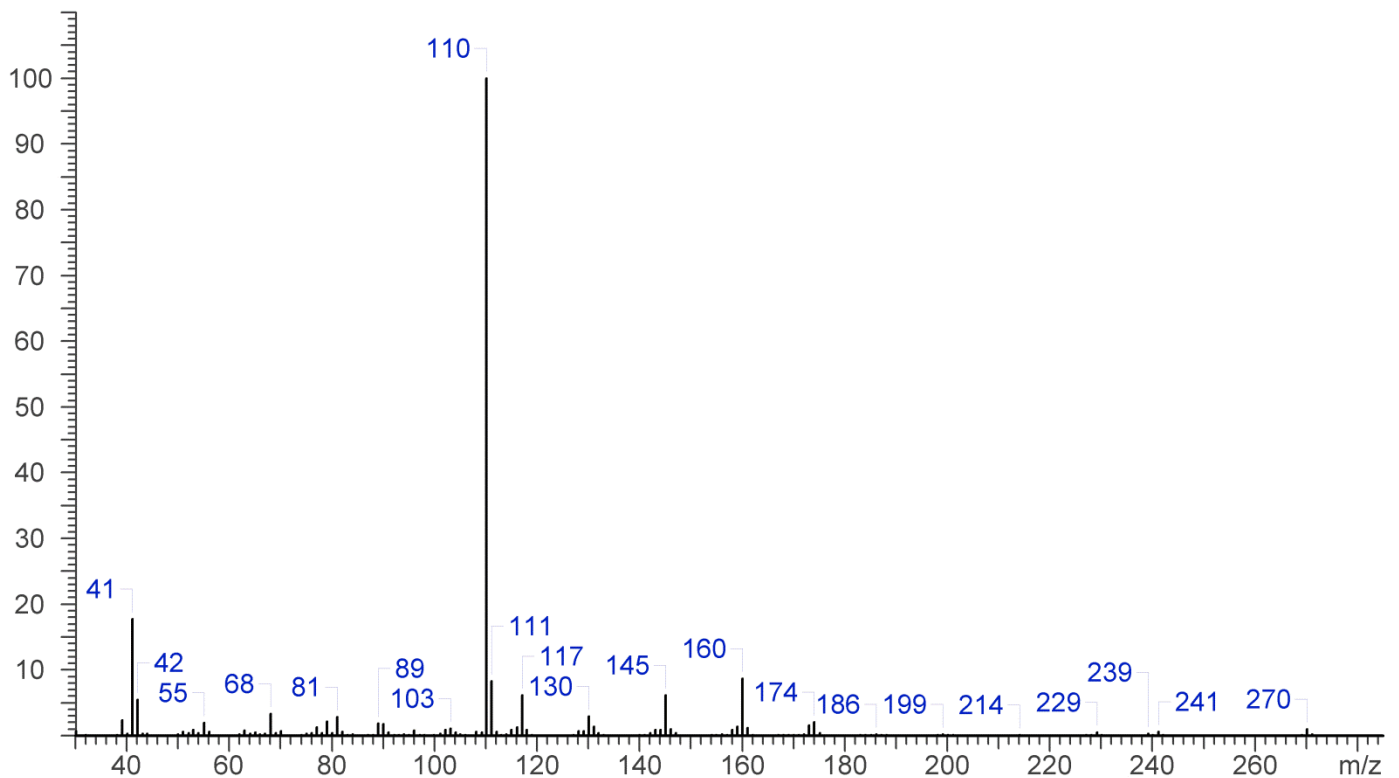
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 14.339 min

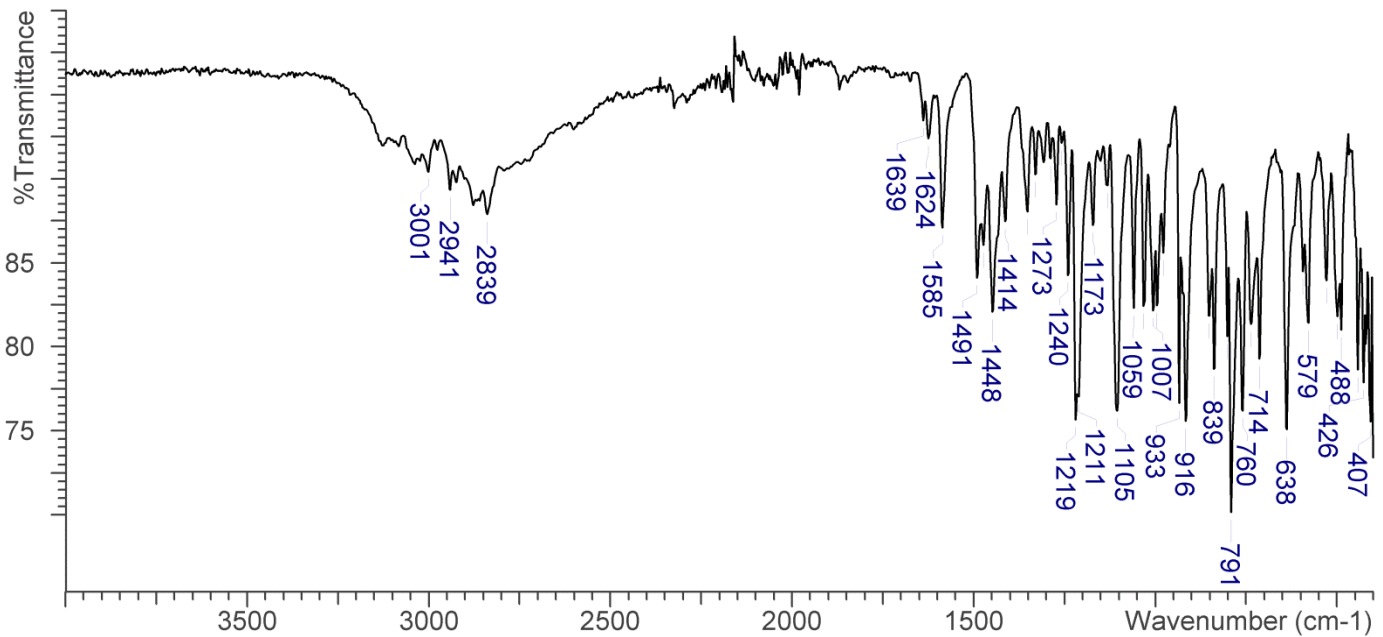
EI Mass Spectrum: 5-Methoxy-N,N-diallyltryptamine Lot K8H81105



4.3 INFRARED SPECTROSCOPY (FTIR)

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

FTIR ATR (Diamond, 3 bounce): 5-Methoxy-N,N-diallyltryptamine Lot K8H81105



FTIR ATR (Diamond, 3 bounce): 5-Methoxy-N,N-diallyltryptamine Lot K8H81105

