

1. GENERAL INFORMATION

IUPAC Name:	2-(2,5-dimethoxy-4-propylphenyl)-N-(2-methoxybenzyl)ethanamine
CFR:	Not Scheduled (8/2013)
CAS#:	Not Available
Synonyms:	25P-NB2OMe
Source:	DEA Reference Material Collection
Appearance:	White powder (HCl)
Kovat's Index:	Pending
UV_{max} (nm):	Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₂₁ H ₂₉ NO ₃	343	Not Determined
HCl	C ₂₁ H ₂₉ NO ₃ · HCl	379	123.3

3. ADDITIONAL RESOURCES

Casale, J. F.; Hays, P. A. Characterization of Eleven 2,5-Dimethoxy-N-(2-methoxybenzyl)phenethylamine (NBOMe) Derivatives and Differentiation from their 3- and 4-Methoxybenzyl Analogues - Part I. *Microgram J.* **2012**, 9 (2), 84-109.

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CDCl₃

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

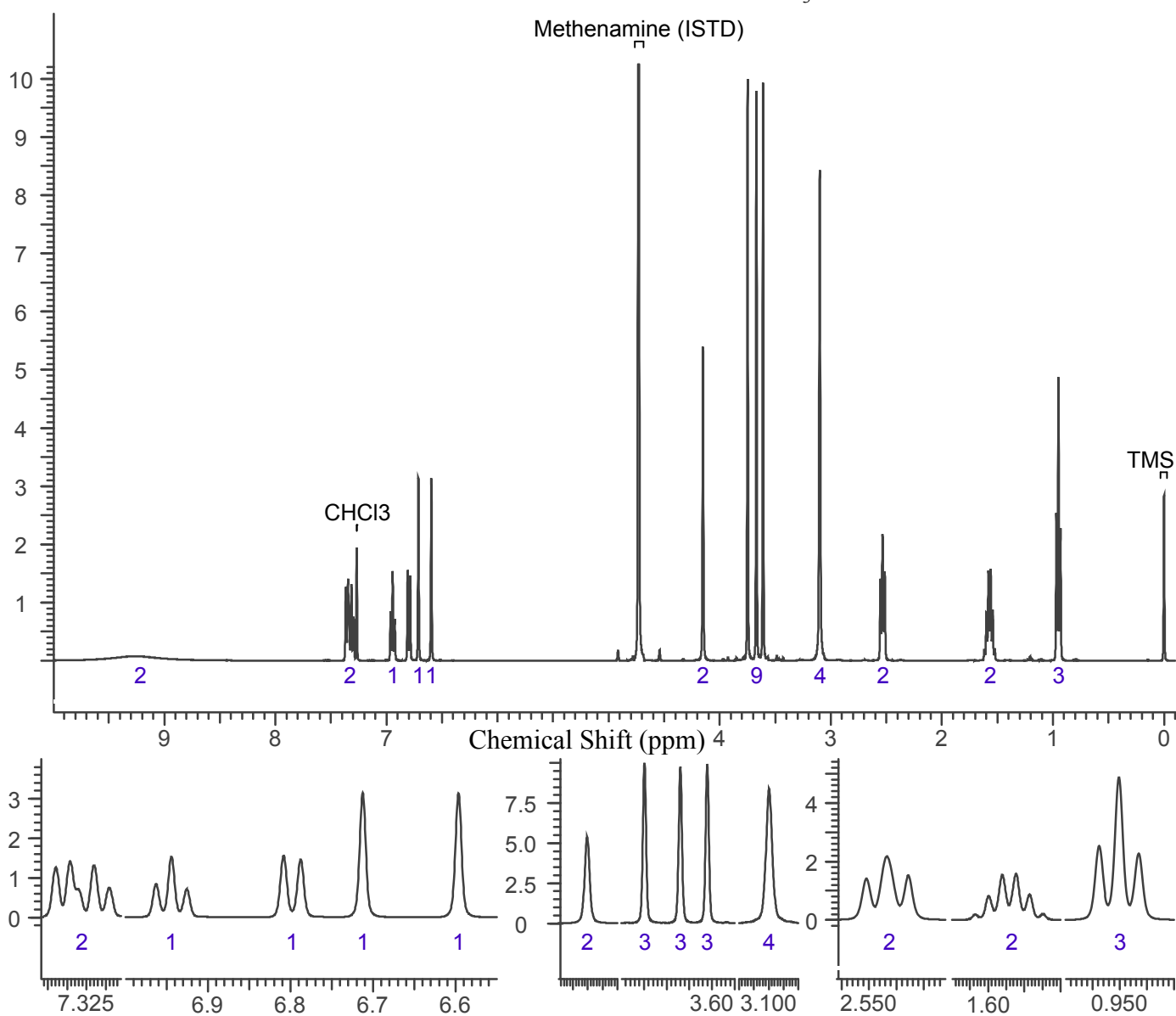
Instrument: 400 MHz NMR spectrometer

Parameters: Spectral width: at least containing -3 ppm through 13 ppm

Pulse angle: 90°

Delay between pulses: 45 seconds

¹H NMR: 25P-NBOMe HCl; Lot N18-P13B; CDCl₃; 400 MHz



4.2 Gas Chromatography/Mass Spectrometry

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

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

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

MS Parameters: Mass scan range: 30-550 amu

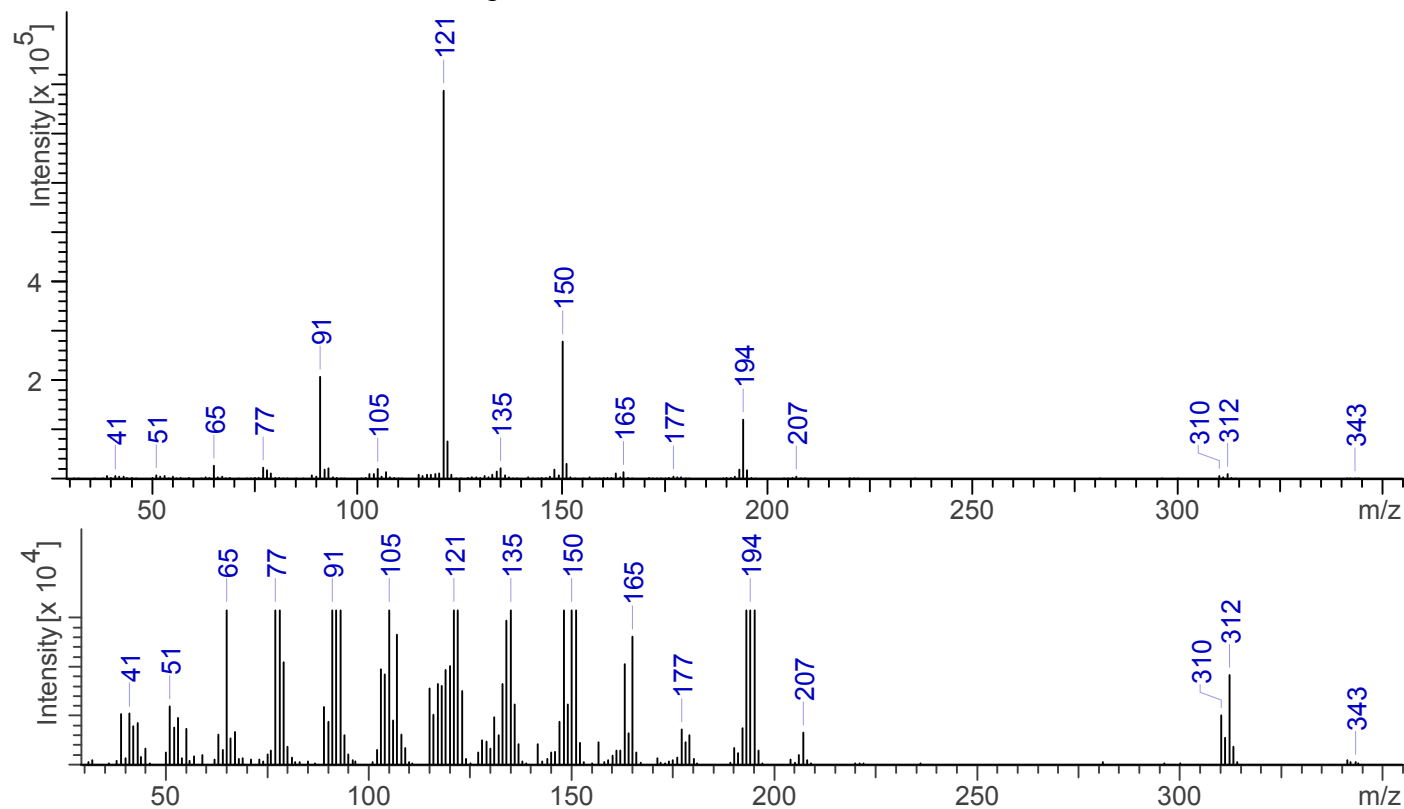
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 16.175 min

EI Mass Spectrum: 25P-NBOMe HCl; Lot N18-P13B



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: 4 cm⁻¹
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): 25P-NBOMe HCl; Lot N18-P13B

