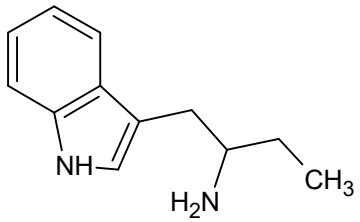
a-Ethyltryptamine

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



1. GENERAL INFORMATION

IUPAC Name: 1-(1*H*-indol-3-yl)butan-2-amine

CAS#: 2235-90-7

Synonyms: *alpha*-Ethyltryptamine, α-ET, 3-Indolybutylamine, NSC 88061, Ro 3-1932

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	$C_{12}H_{16}N_2$	188	100.5
HCl	$C_{12}H_{16}N_2$ HCl	225	Not Determined

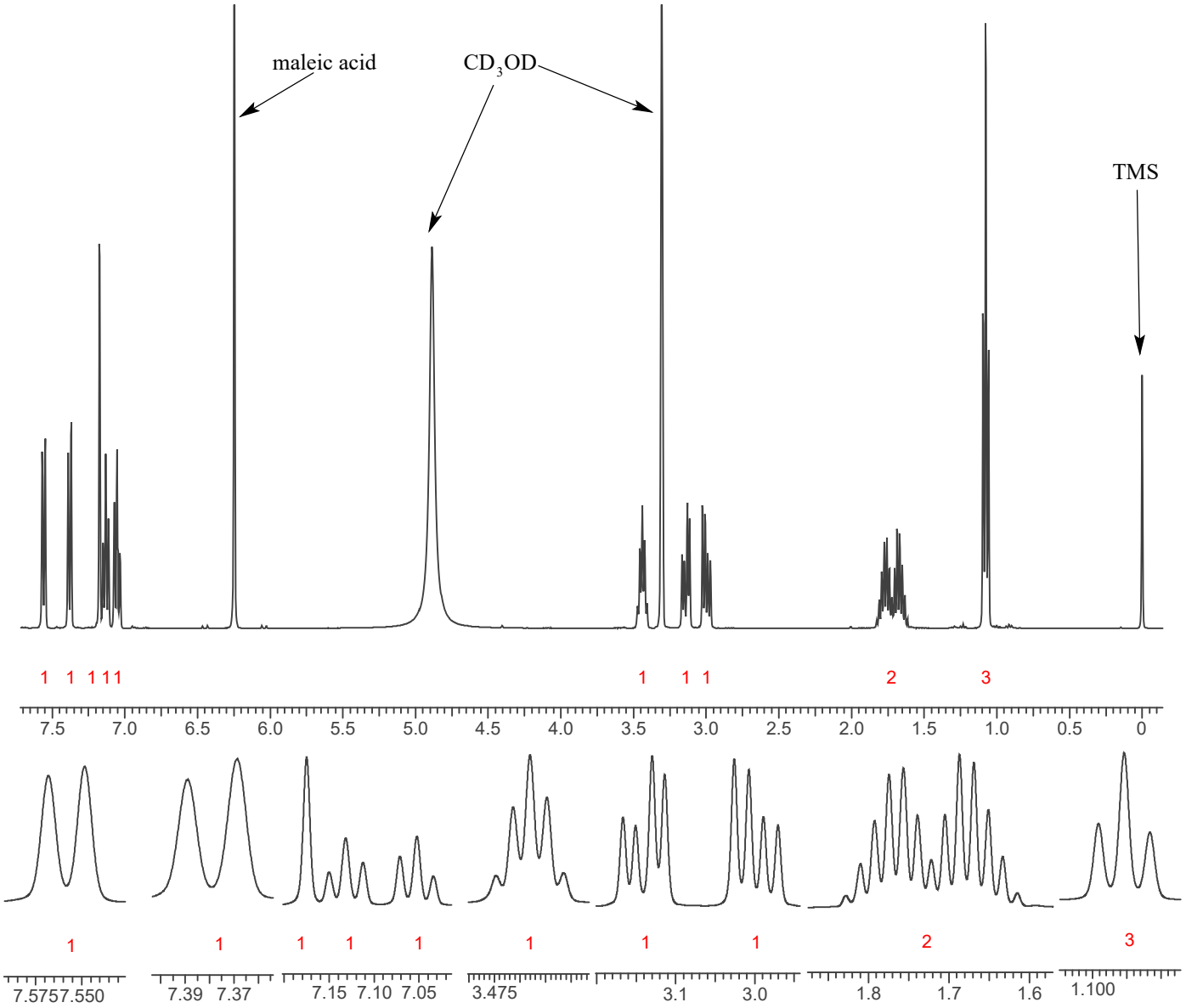
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 mg/mL in CD_3OD containing TMS 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

^{1}HNMR: α-Ethyltryptamine; Lot# 0448839-14; CD_3OD; 400MHz

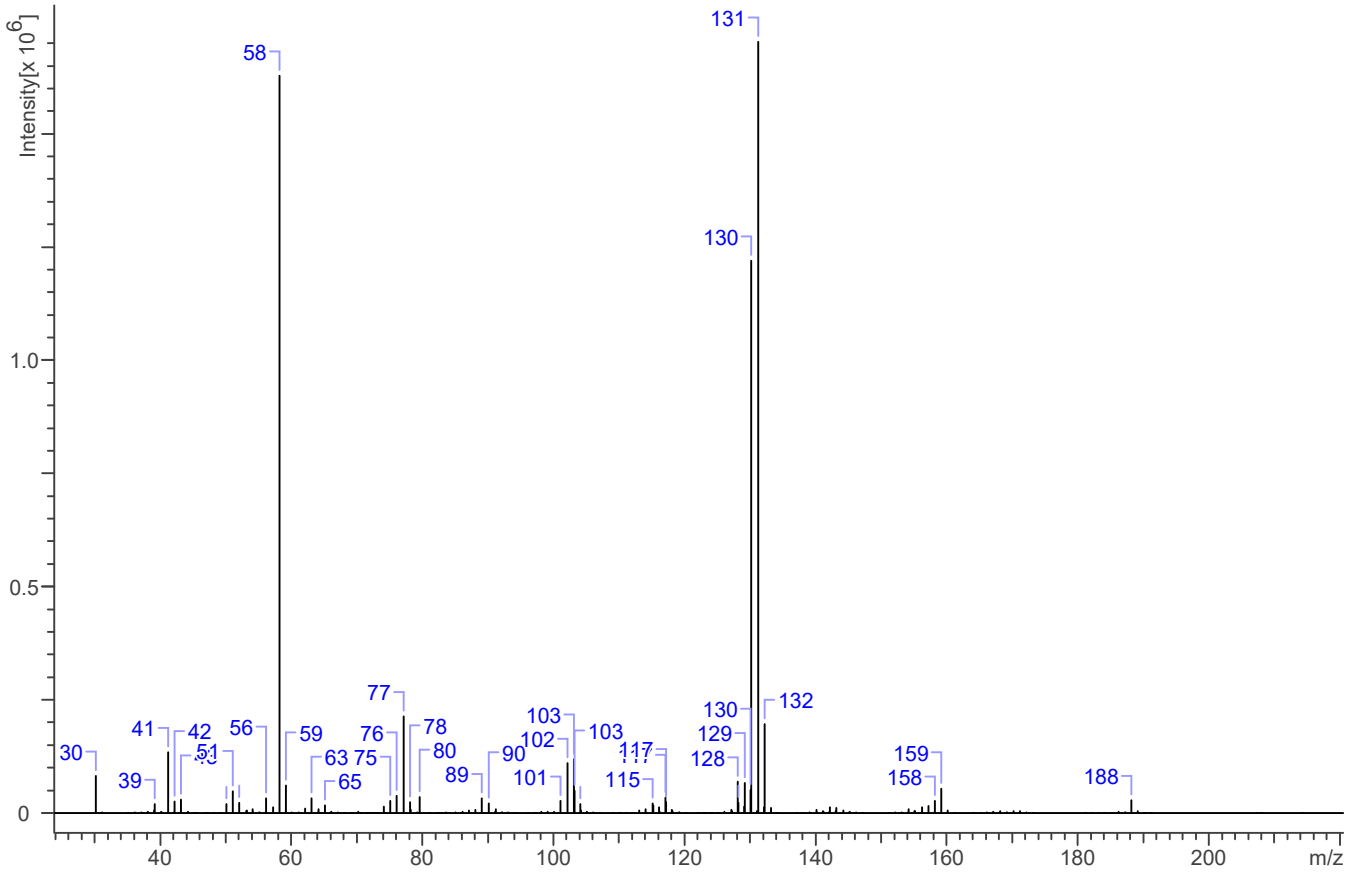


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~ 3 mg/mL in $CHCl_3$

Instrument:	Agilent gas chromatograph operated in split mode with MS detector	
Column:	DB-5 MS (or equivalent); 15m x 0.25 mm x 0.25 µm	
Carrier Gas:	Helium at 1.5 mL/min	
Temperatures:	Injector: 280°C	MSD transfer line: 280°C
	MS Source: 250°C	MS Quad: 150°C
	Oven program:	
	1) 90°C initial temperature for 1.0 min	
	2) Ramp to 315°C at 30 °C/min	
	3) Hold final temperature for 6.0 min	
Injection Parameters:	Split Ratio = 25:1, 1 µL injected	
MS Parameters:	Mass scan range: 30-550 amu	Threshold: 150
	Tune file: stune.u	Acquisition mode: scan
Retention Time:	5.18 min	

EI Mass Spectrum: α-Ethyltryptamine; Lot# 0448839-14

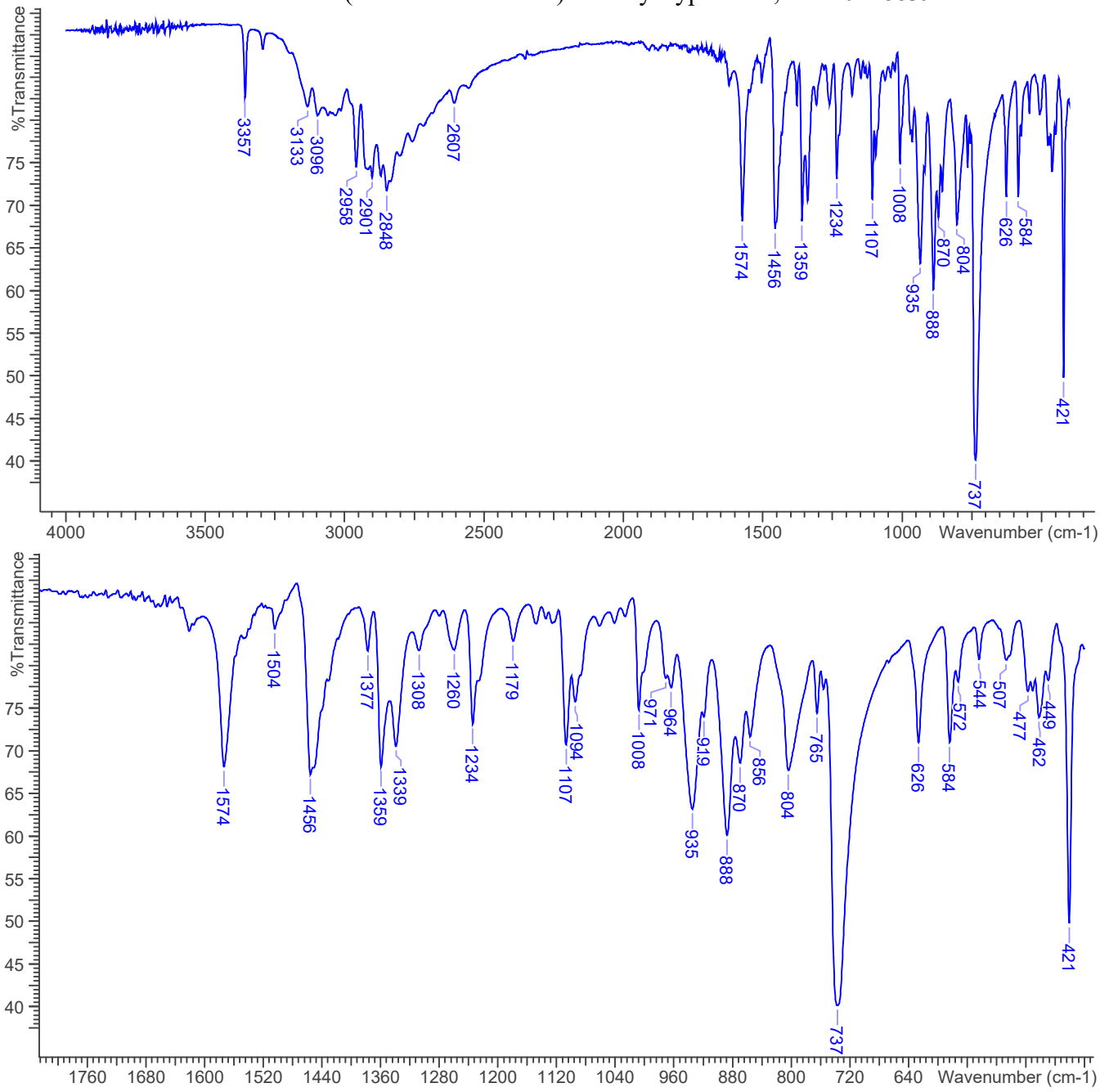


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (1 bounce)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4 cm^{-1}
Sample gain: 1
Aperture: 150

FTIR ATR (Diamond 1 Bounce): α-Ethyltryptamine; Lot# 0448839-14



4. ADDITIONAL RESOURCES

Wikipedia

Forendex