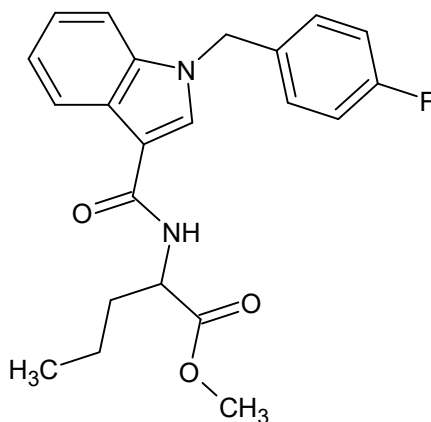




MEP-FUBICA

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



1. GENERAL INFORMATION

- IUPAC Name:** methyl 2-(1-(4-fluorobenzyl)-1H-indole-3-carboxamido)pentanoate
- CAS#:** NA
- Synonyms:** methyl *N*-{1-[(4-fluorophenyl)methyl]-1H-indole-3-carbonyl} norvalinate; MMB-FUBICA isomer 1
- 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 ₂₂ H ₂₃ FN ₂ O ₃	382.43	148.45



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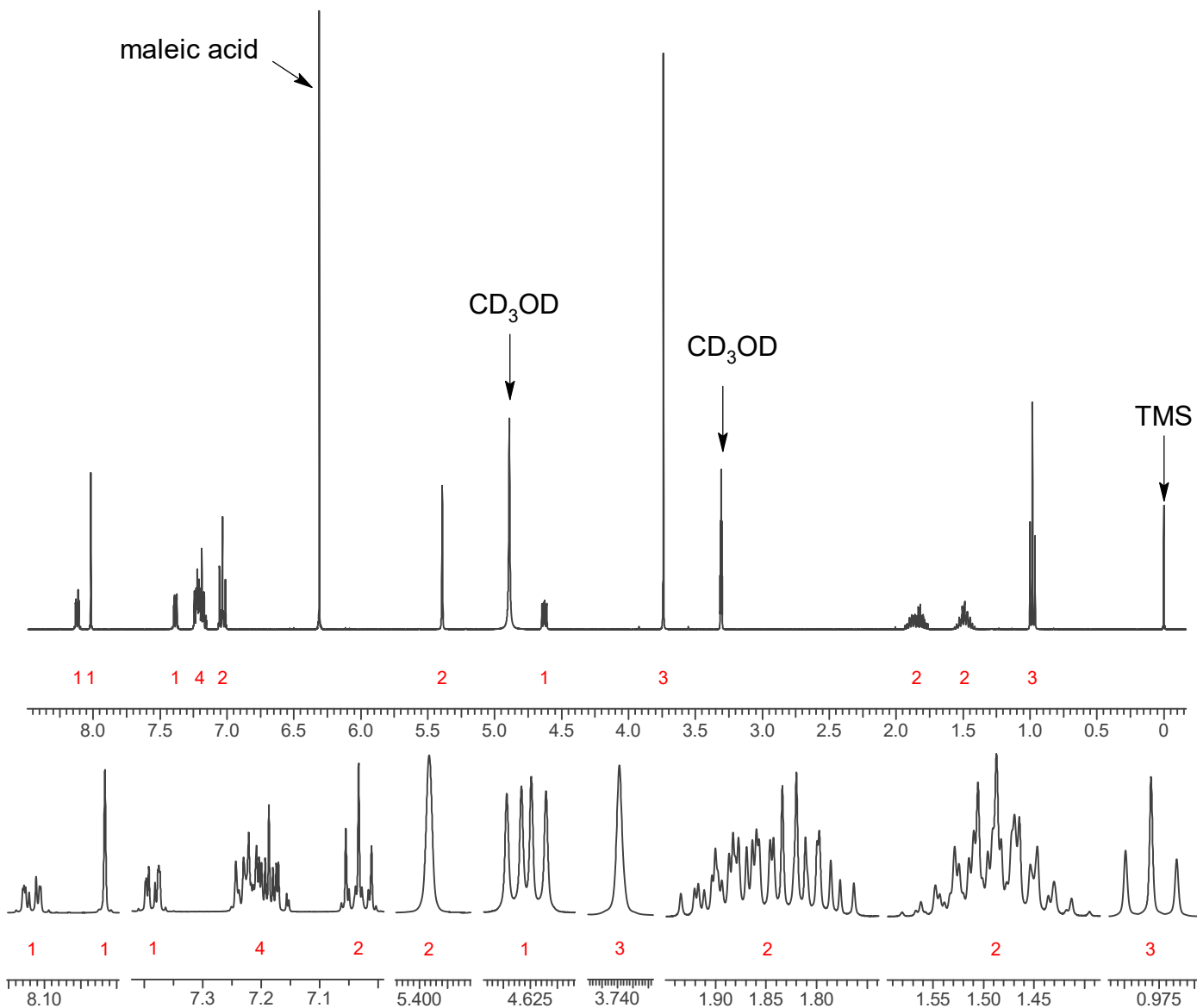
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~13 mg/mL in CD₃OD 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

¹HNMR: MEP-FUBICA; LOT # 0502952-7; CD₃OD; 400MHz





MEP-FUBICA



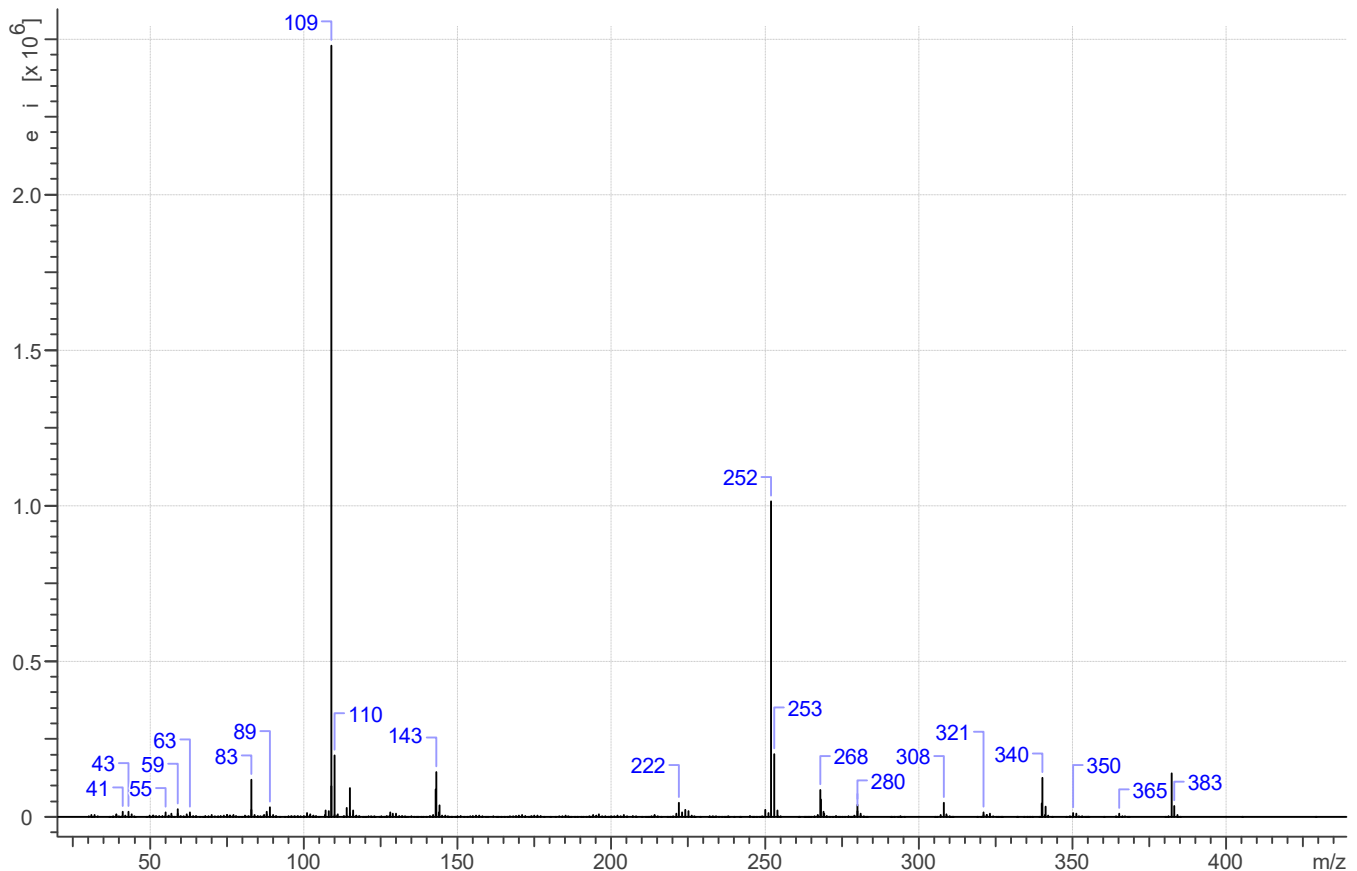
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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: HP-5 MS (or equivalent); 30m x 0.25 mm x 0.25 μ m
Carrier Gas: Helium at 1.5 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 280°C at 12 °C/min
 3) Hold final temperature for 30.0 min
Injection Parameters: Split Ratio = 25:1, 1 μ L injected
MS Parameters: Mass scan range: 30-550 amu Threshold: 150
Tune file: stune.u Acquisition mode: scan
Retention Time: 20.422 min

EI Mass Spectrum: MEP-FUBICA; LOT # 0502952-7





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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): MEP-FUBICA; LOT # 0502952-7

