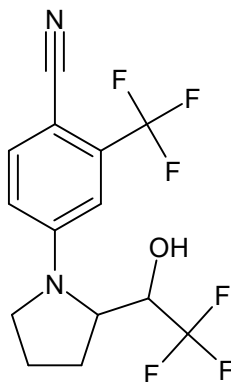




LGD 4033

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



1. GENERAL INFORMATION

IUPAC Name: 4-[2-(2,2,2-trifluoro-1-hydroxyethyl)pyrrolidin-1-yl]-2-(trifluoromethyl)benzonitrile

CAS#: 1165910-22-4

Synonyms: LGD-4033

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 ₁₄ H ₁₂ F ₆ N ₂ O	338.25	106.09



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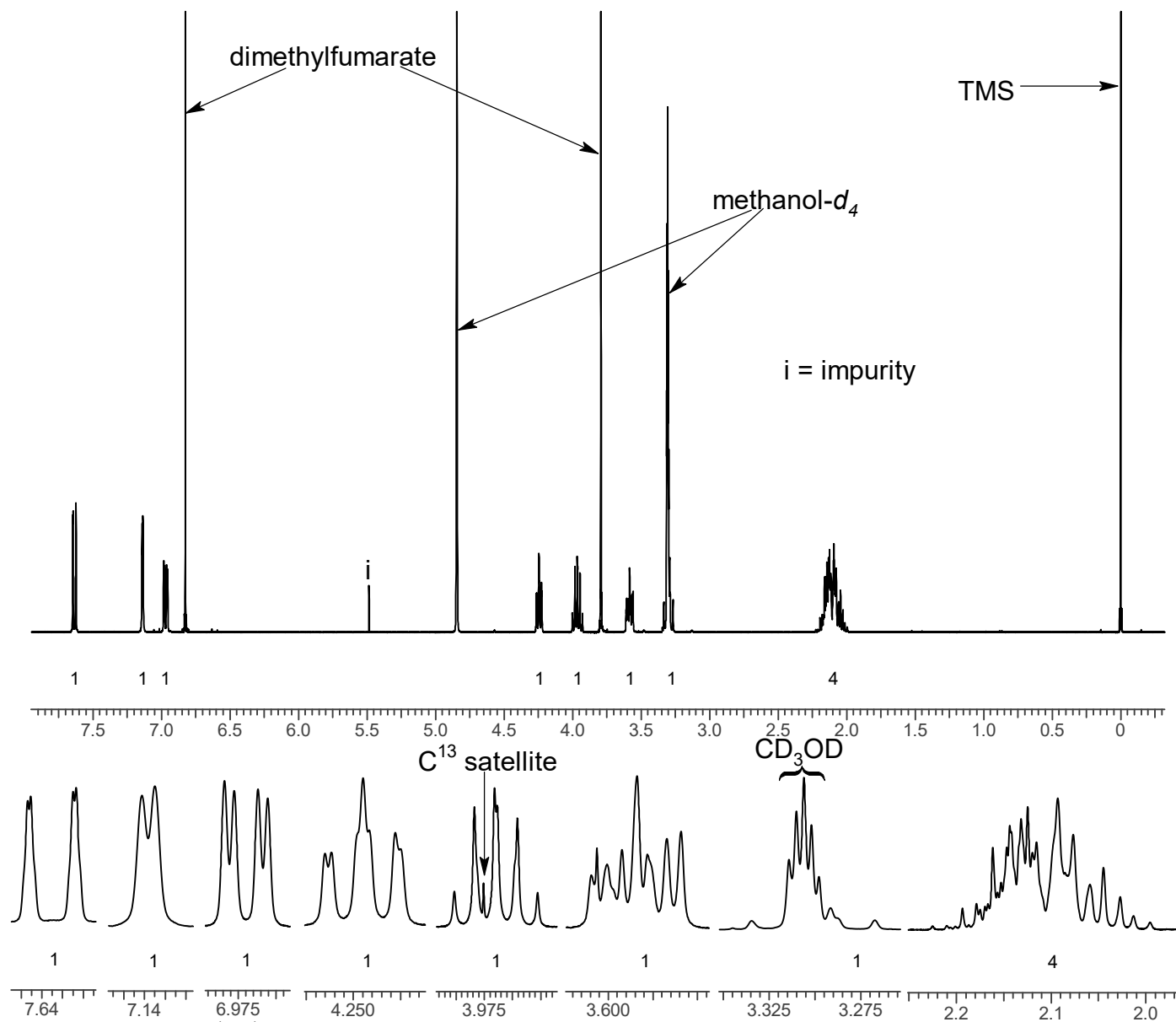
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~14 mg/mL in methanol- d_4 containing TMS for 0 ppm reference and dimethylfumarate 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: LGD 4033; Lot# RM-170505-01; methanol- d_4 ; 400MHz





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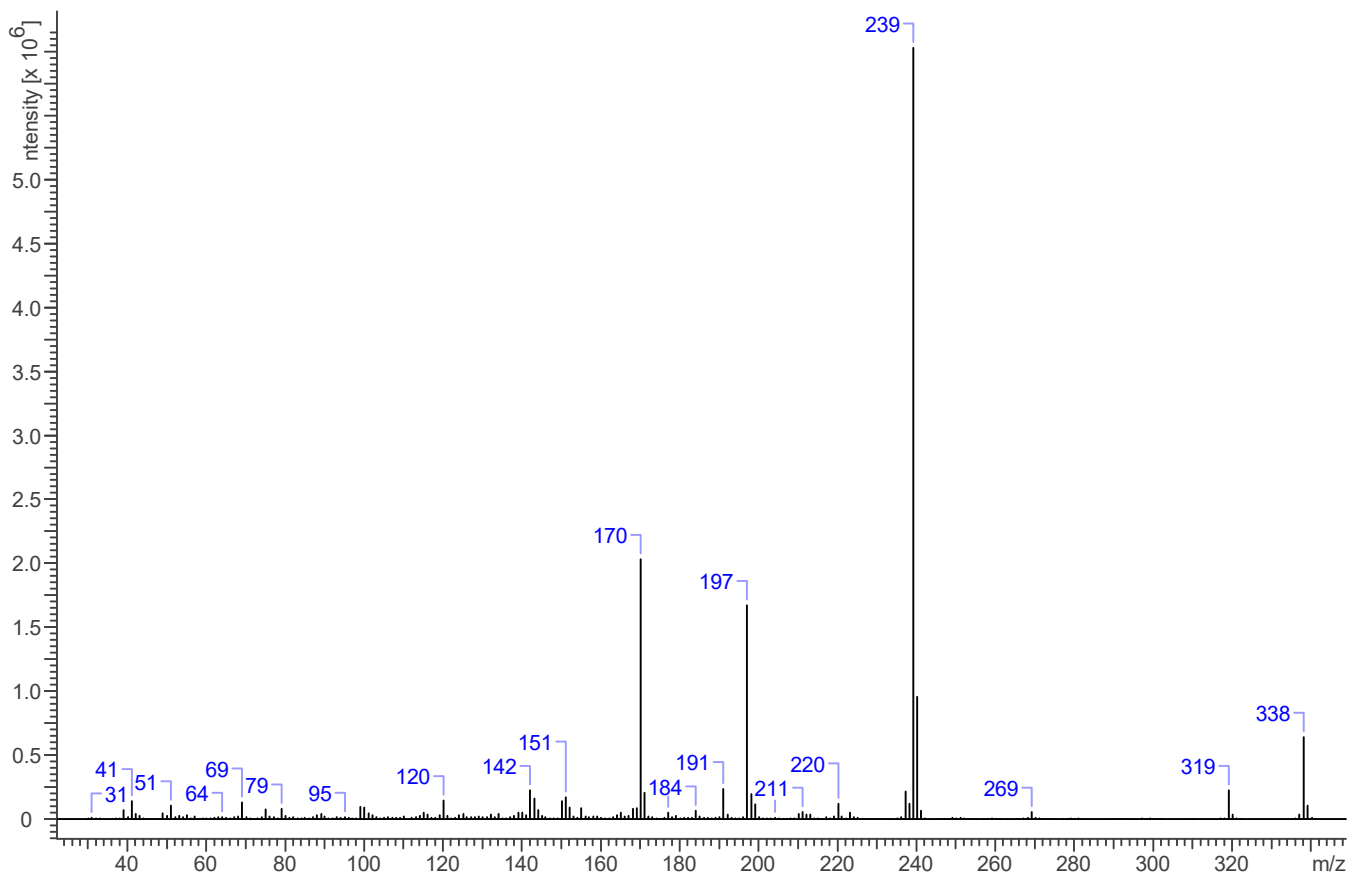


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in 9:1 CHCl₃: 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 μm
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 9.0 min
Injection Parameters: Split Ratio = 25:1, 1 μL injected
MS Parameters: Mass scan range: 30-550 amu Threshold: 250
Tune file: stune.u Acquisition mode: scan
Retention Time: 12.29 min

EI Mass Spectrum: LGD 4033; Lot# RM-170505-01





LGD 4033

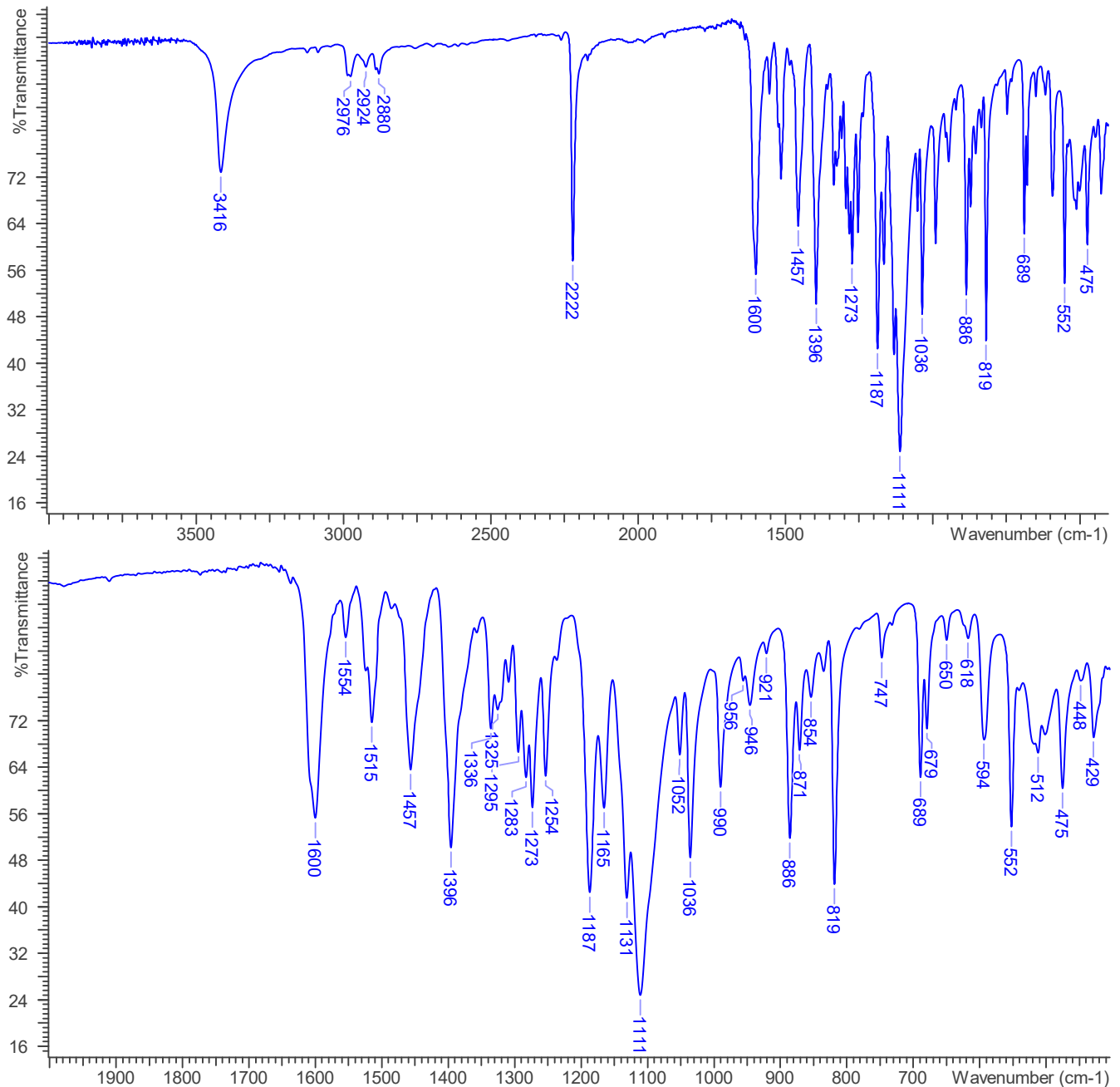
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3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR: Thermo-Scientific iS-10, Smart iTX
Scan Parameters: Number of scans: 32
Number of background scans: 16
Resolution: 4 cm⁻¹
Sample gain: 1
Aperture: 150

FTIR: Thermo-Scientific iS-10, Smart iTX: LGD 4033; Lot# RM-170505-01





LGD 4033

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4. ADDITIONAL RESOURCES

Thevis, M.; Lagojda, A.; Kuehne, D.; *et al.* Characterization of a non-approved elective androgen receptor modulator drug candidate sold via the Internet and identification of in vitro generated phase-I metabolites for human sports drug testing. *Rapid Commun. Mass Spectrom.* 2015. 29. 991-999.