

1. GENERAL INFORMATION

IUPAC Name:	<i>N</i> -(1-amino-3-methyl-1-oxobutan-2-yl)-1-(5-fluoropentyl)-1 <i>H</i> -indazole-3-carboxamide
CFR:	Not Scheduled (10/2013)
CAS#:	Not Available
Synonyms:	5-Fluoro-AB-PINACA
Source:	DEA Reference Material Collection
Appearance:	White powder (base)
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 ₁₈ H ₂₅ FN ₄ O ₂	348	85.3

3. ADDITIONAL RESOURCES

No resources identified as of 10/2013.

4. QUALITATIVE DATA

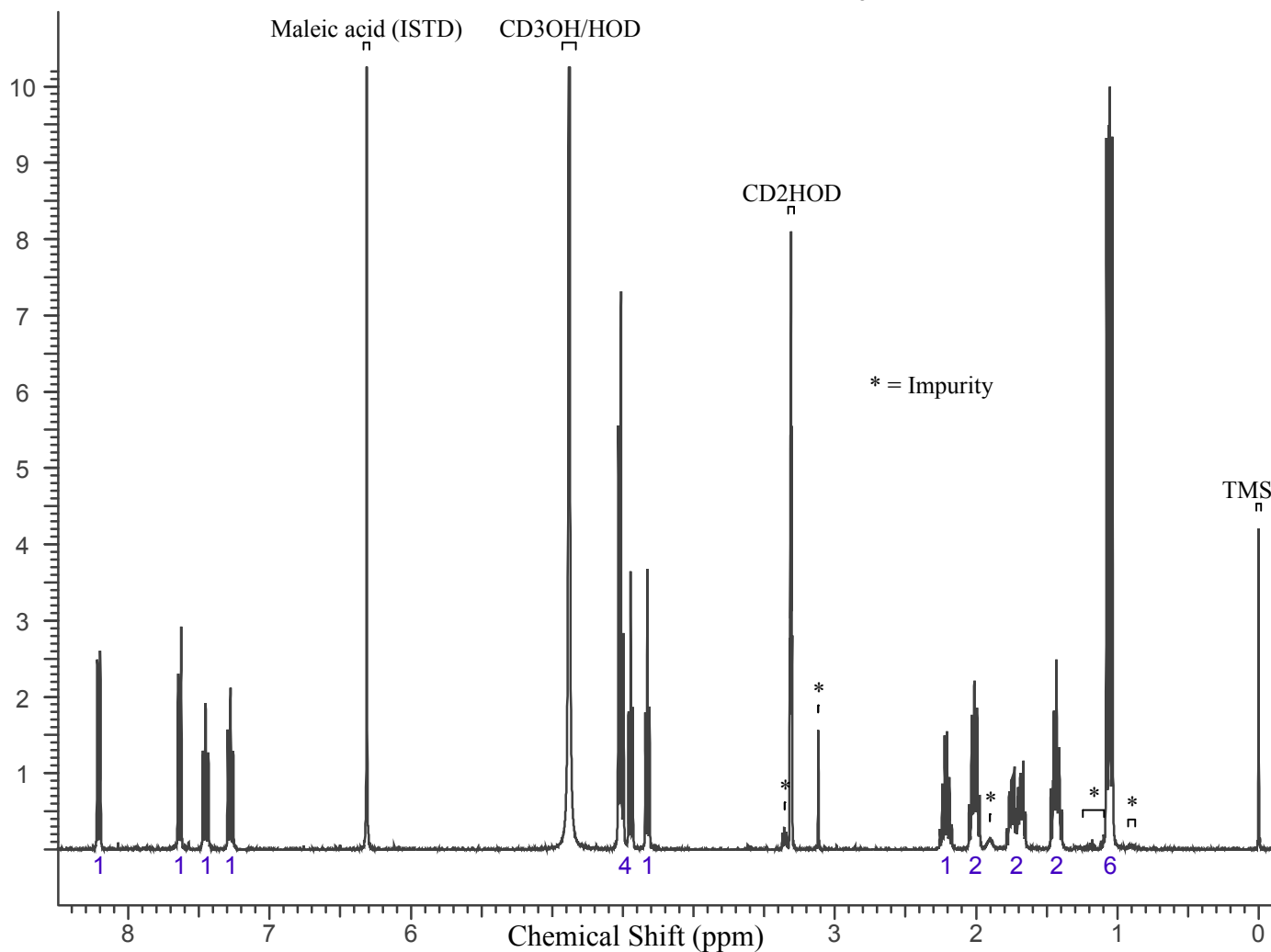
4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CD₃OD

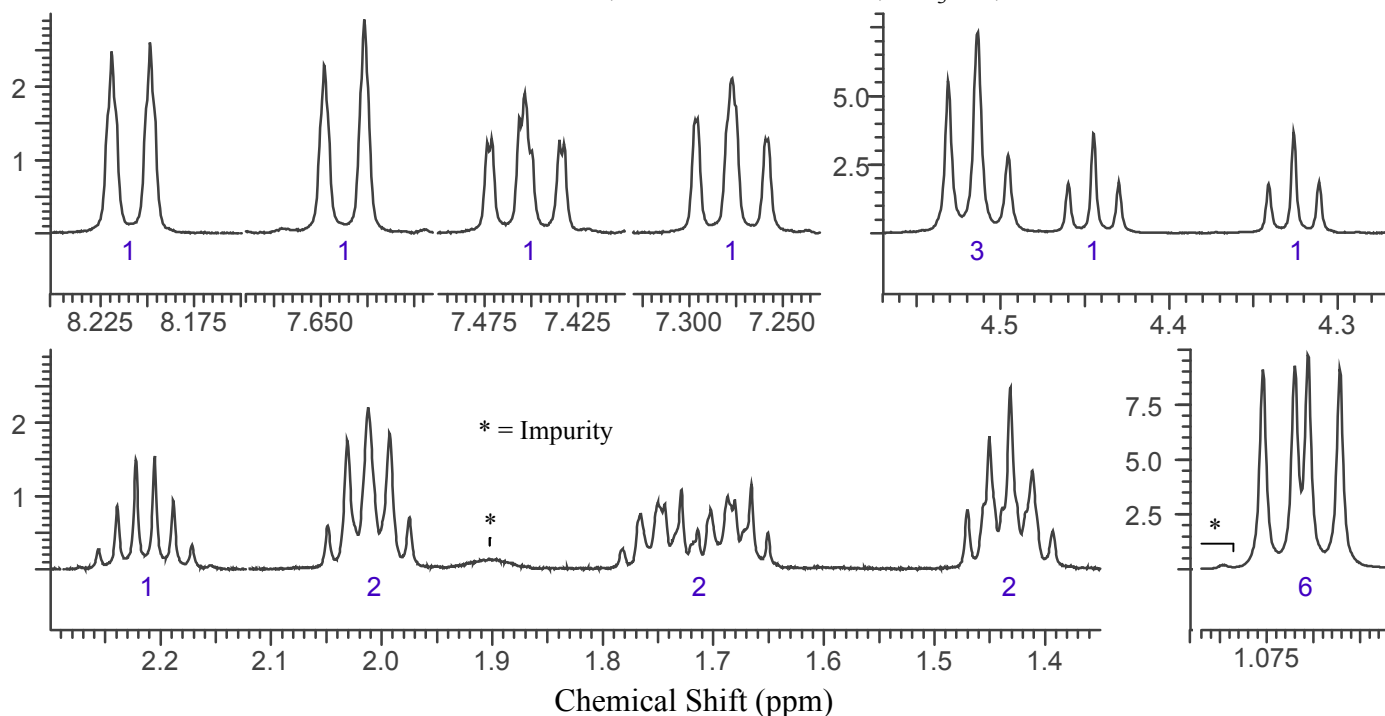
Sample Preparation: Dilute analyte to ~10 mg/mL in methanol-*d*₄ (CD₃OD) containing TMS for 0 ppm reference and maleic acid as quantitative internal standard.

Instrument: 400 MHz NMR spectrometer
Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

¹H NMR: 5F-AB-PINACA; Lot RM-130816-02; CD₃OD; 400 MHz



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4.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~ 1 mg/mL in methanol

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 mL/min

Temperatures:

Injector: 280°C

MSD transfer line: 280°C

MS Source: 230°C

MS Quad: 150°C

Oven program:

1) 90°C initial temperature for 2.0 min

2) Ramp to 300°C at 14 °C/min

3) Hold final temperature for 17.0 min

Injection Parameters:

Split Ratio = 25:1, 1 μL injected

MS Parameters:

Mass scan range: 29-750 amu

Threshold: 50

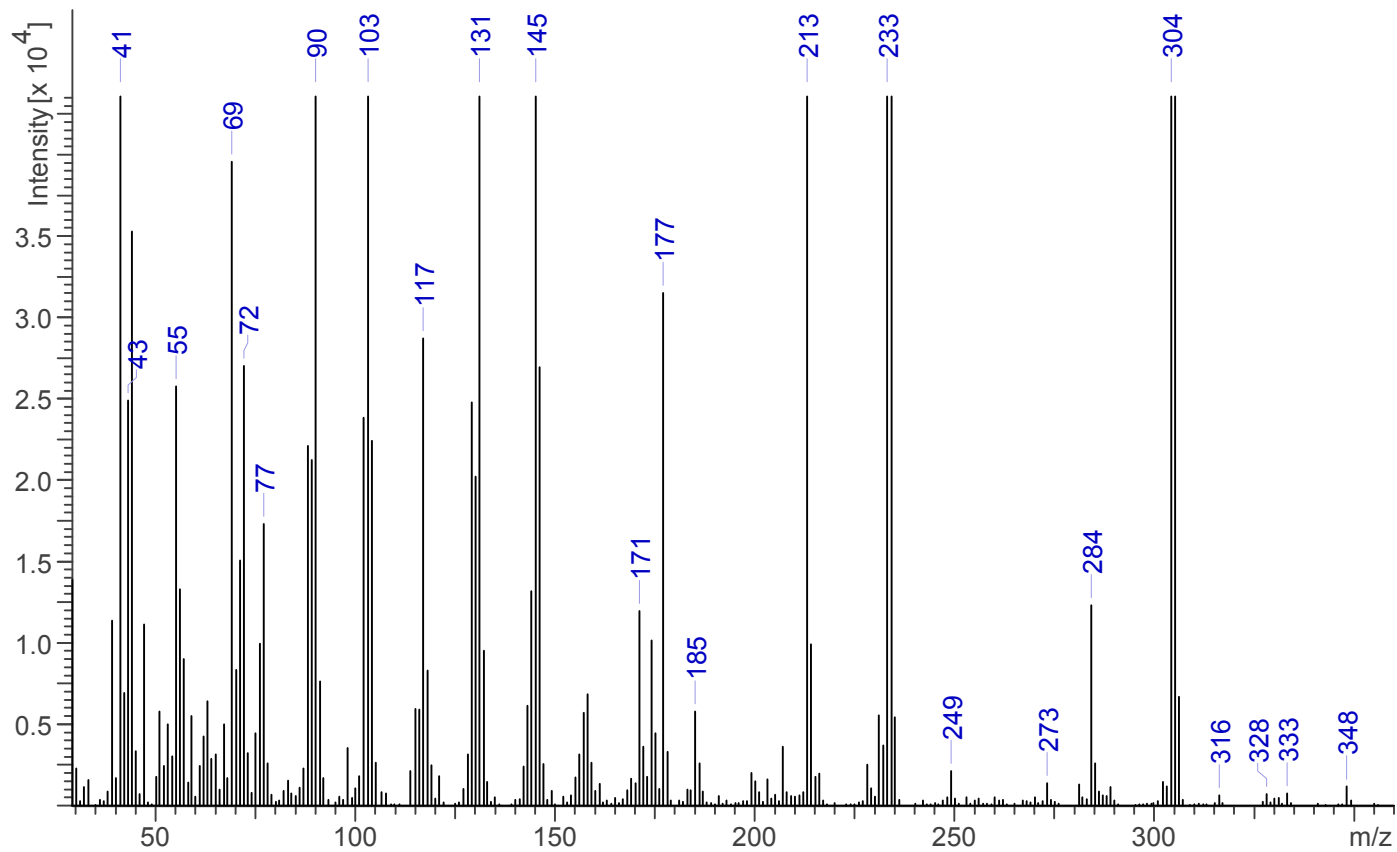
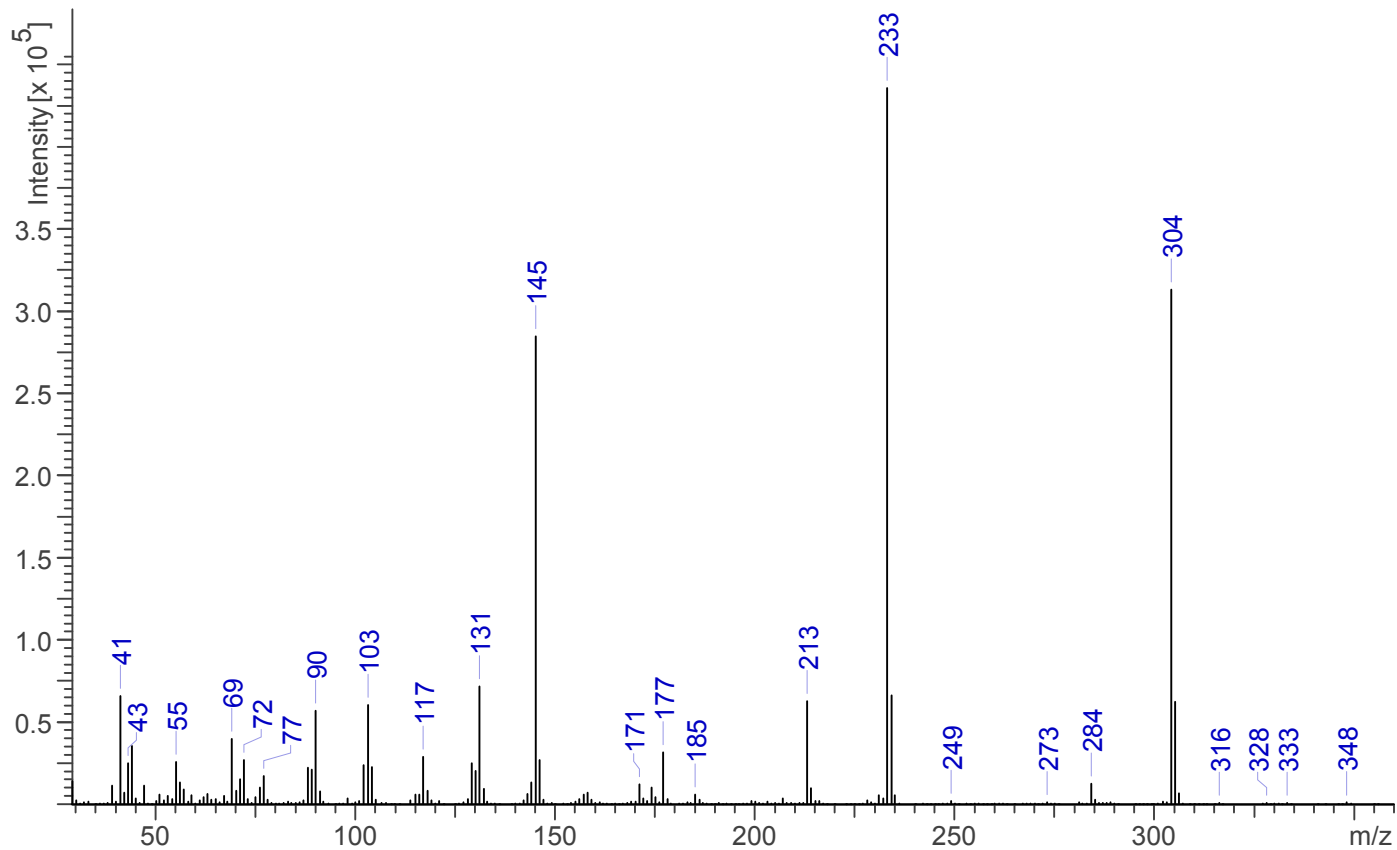
Tune file: stune.u

Acquisition mode: scan

Retention Time:

18.218 min

EI Mass Spectrum: 5F-AB-PINACA; Lot RM-130816-02



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): 5F-AB-PINACA; Lot RM-130816-02

