

1. GENERAL INFORMATION

IUPAC Name:	1-(5-fluoropentyl)-N-(tricyclo[3.3.1.1 ^{3,7}]dec-1-yl)-1H-indazole-3-carboxamide
CFR:	Not Scheduled (2/2013)
CAS #:	Not Available
Synonyms:	5F-APINACA; APINACA 5-Fluoropentyl analog; 5F-AKB-48
Source:	DEA Reference Material Collection
Appearance:	White powder
Kovat's Index:	Pending
UV_{max}:	Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₂₃ H ₃₀ FN ₃ O	383	54.9

3. ADDITIONAL RESOURCES

No resources identified as of 02/08/2013.

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CDCl₃

Sample Preparation: Dilute analyte to ~25 mg/mL in deuteriochloroform (CDCl₃) containing TMS for 0 ppm reference and dimethylsulfone as quantitative internal standard.

Instrument:

Varian Mercury 400 MHz NMR spectrometer with proton detection probe

Parameters:

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

Pulse angle: 90°

Delay between pulses: 45 seconds

Number of scans (NT): 8

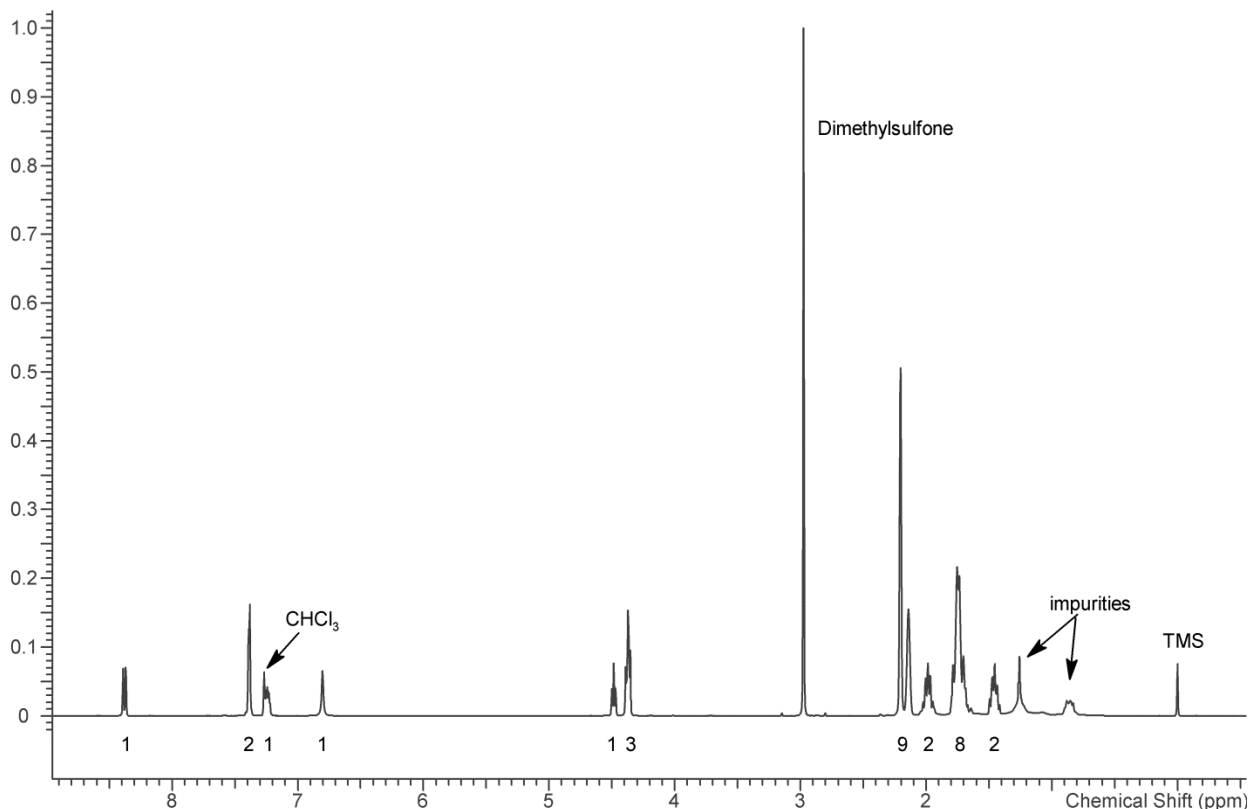
Number of steady state scans: 0

Oversampling: 4 or more

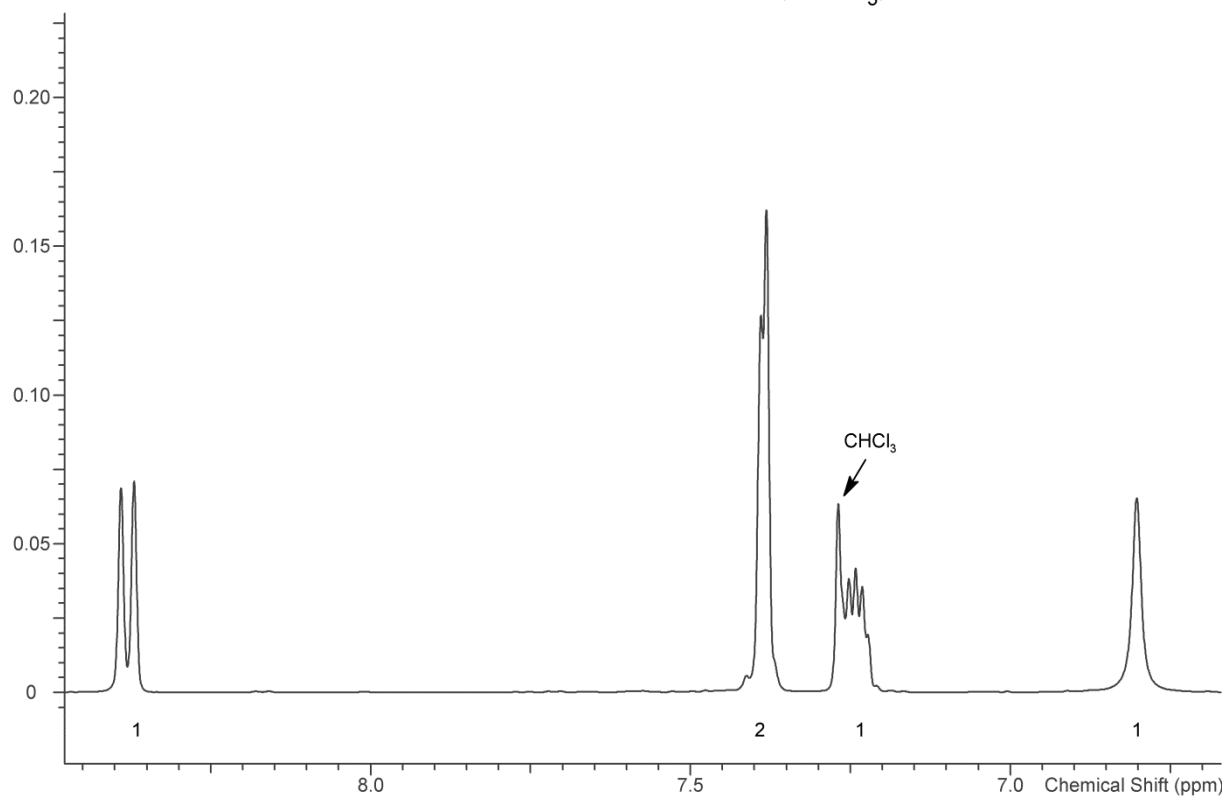
Shimming: automatic gradient shimming of Z1-4 shims

Phasing, Drift Correction: automatic or manual

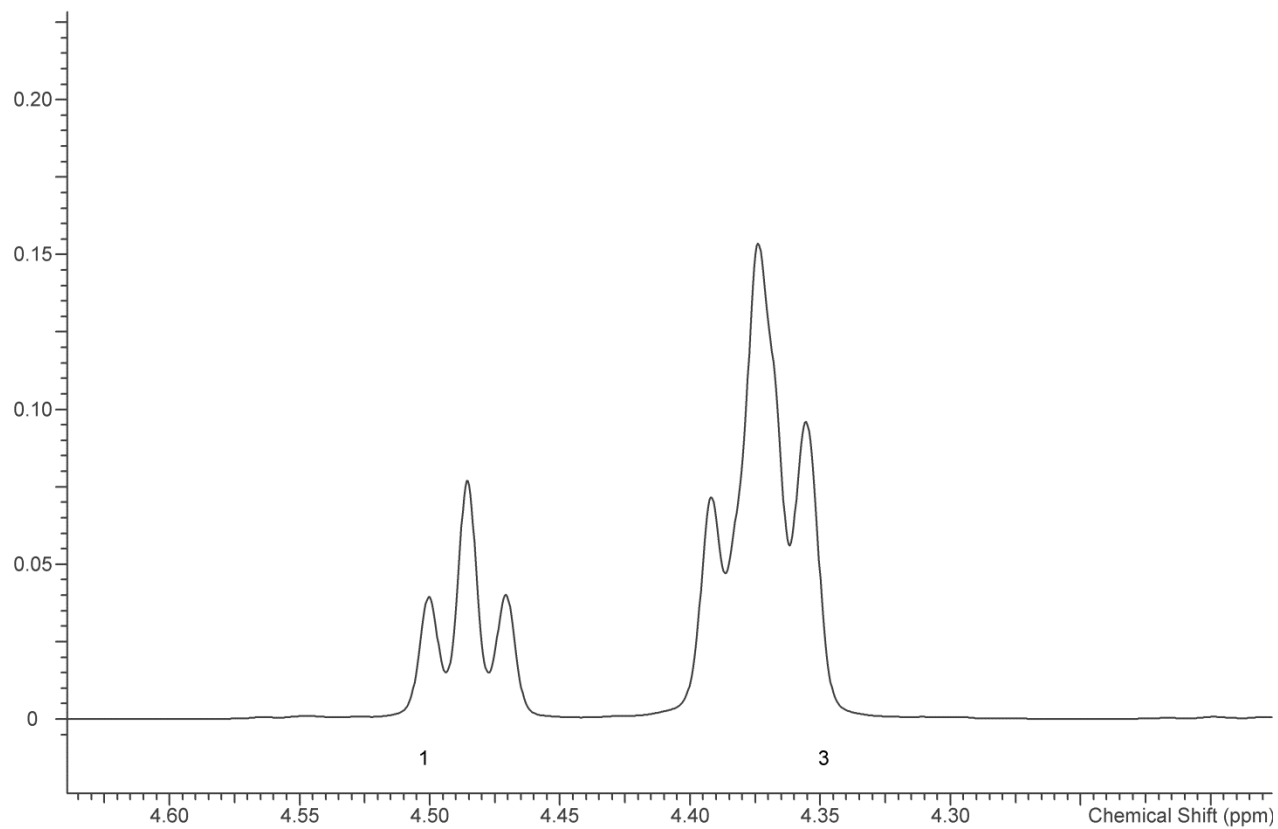
¹H NMR: 5-Fluoro-AKB-48 Lot # N1-P53EMG; CDCl₃; 400 MHz



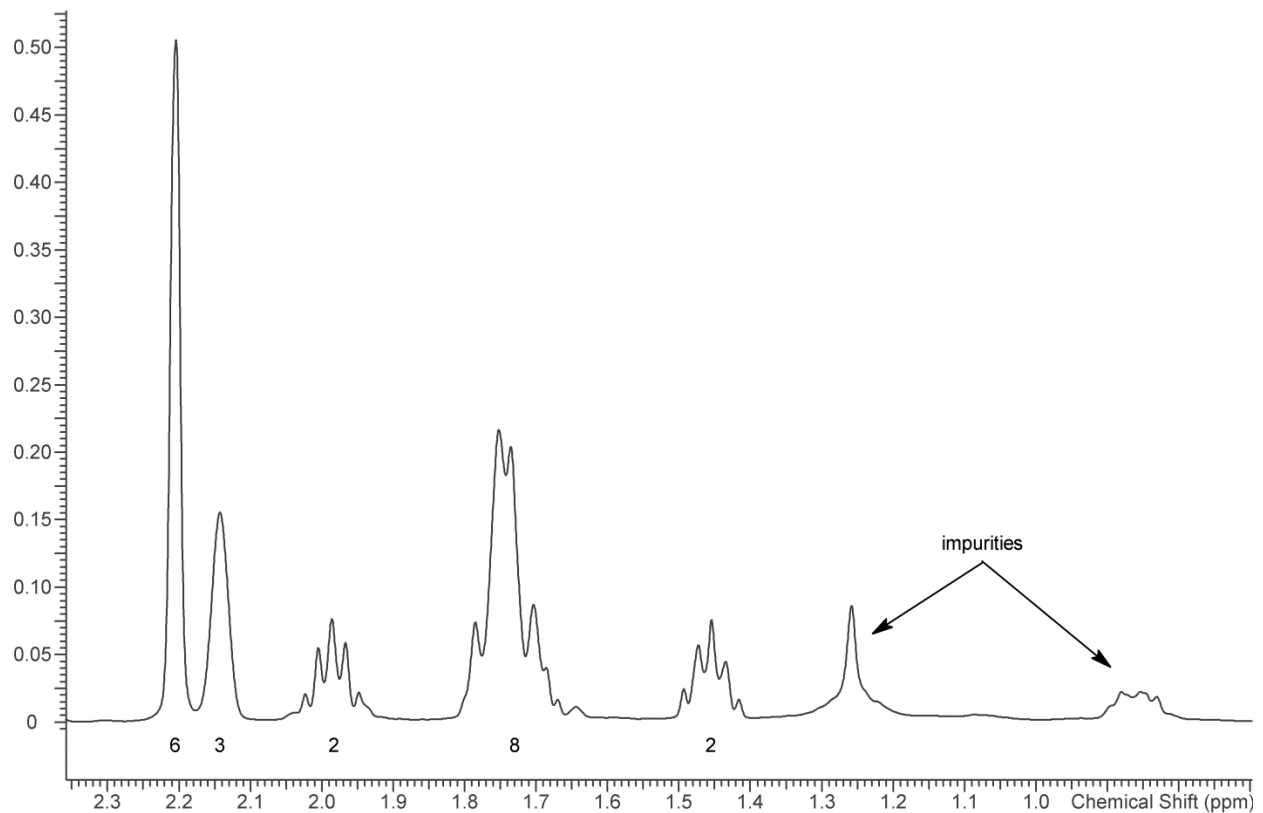
1H NMR: 5-Fluoro-AKB-48 Lot # N1-P53EMG; CDCl₃; 400 MHz



1H NMR: 5-Fluoro-AKB-48 Lot # N1-P53EMG; CDCl₃; 400 MHz



¹H NMR: 5-Fluoro-AKB-48 Lot # N1-P53EMG; CDCl₃; 400 MHz



4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

Instrument: Agilent gas chromatograph operated in split mode with MS detector

Column: DB-1; 30m x .25mm x .25 μ m

Carrier Gas: Helium at 1 mL/min

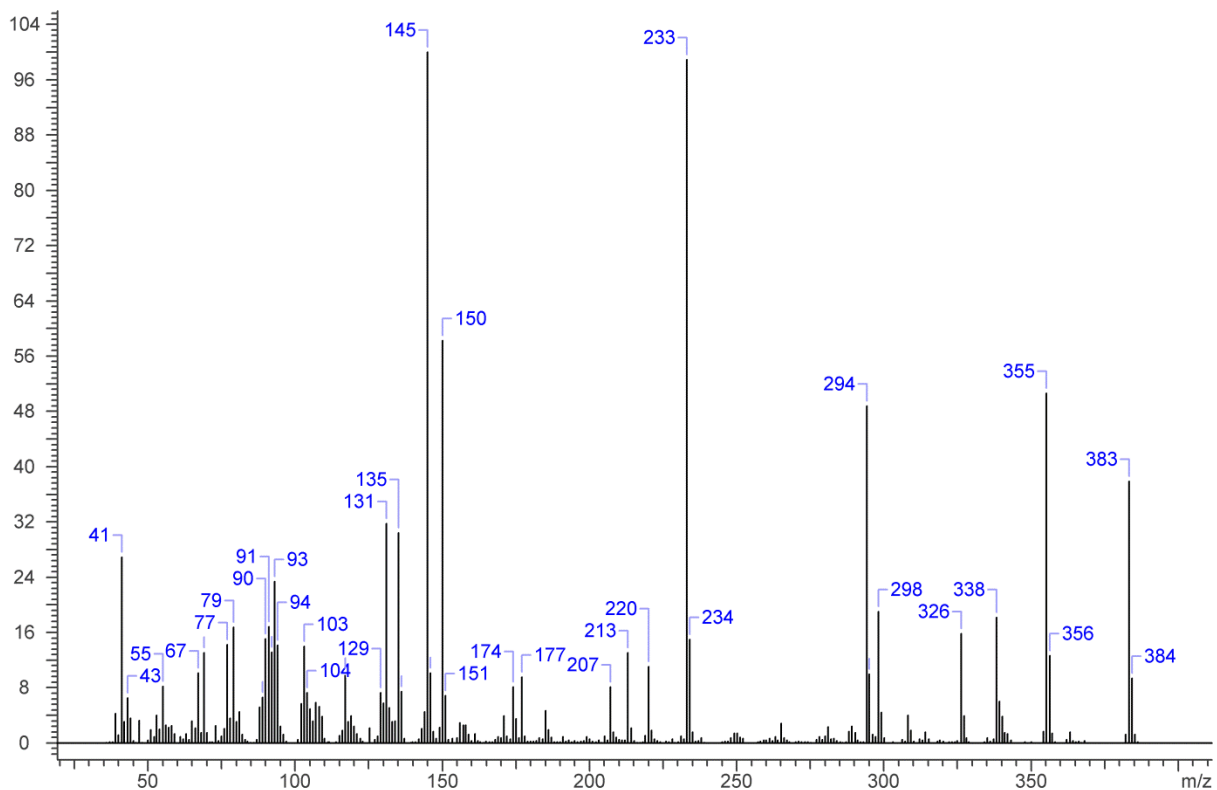
Temperatures: Injector: 280°C
MSD transfer line: 280°C
MS Source: 230°C
MS Quad: 150°C
Oven program:
1) 100°C initial temperature for 1.0 min
2) Ramp to 300°C at 12°C/min
3) Hold final temperature for 9.0 min

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: 20.913 minutes

EI Mass Spectrum: 5-Fluoro-AKB-48 Lot # N1-P53EMG



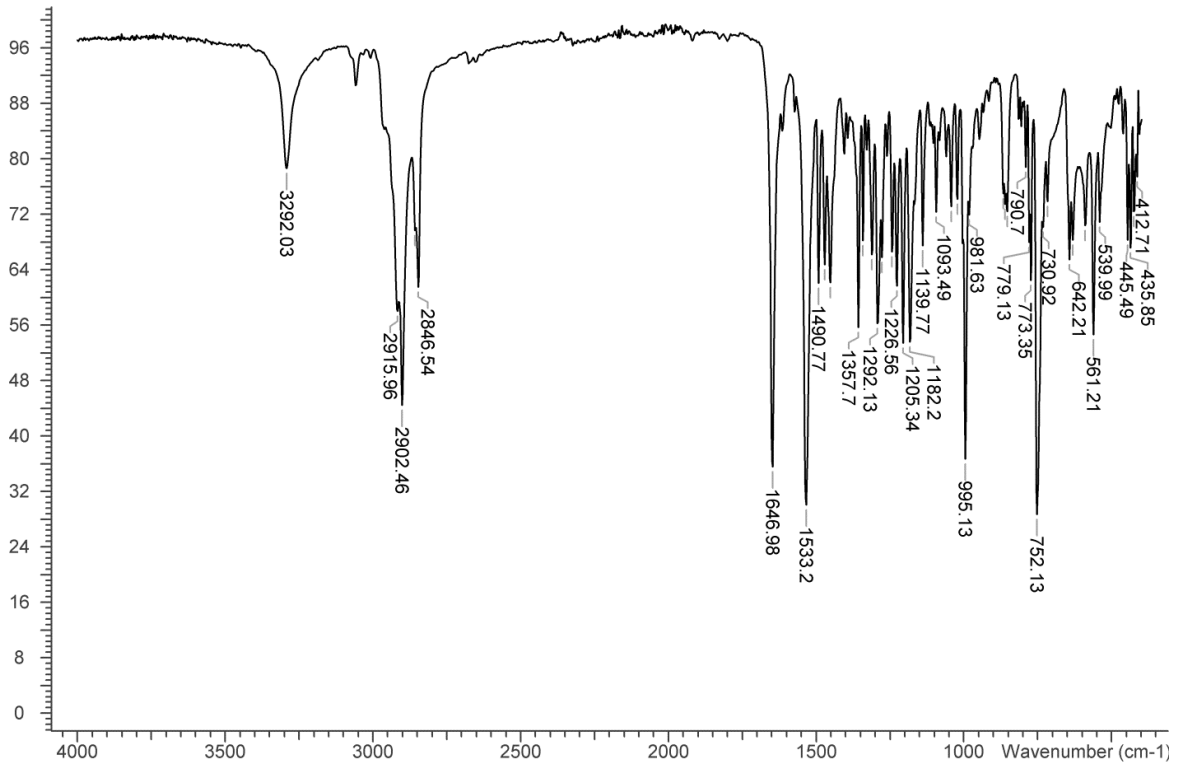
GC/MS Analytical Observation:

Other laboratories have reported observing differences in the abundances of various fragment ions, similar to the variations seen in XLR11, and the cause has not yet been determined. No spectra are available.

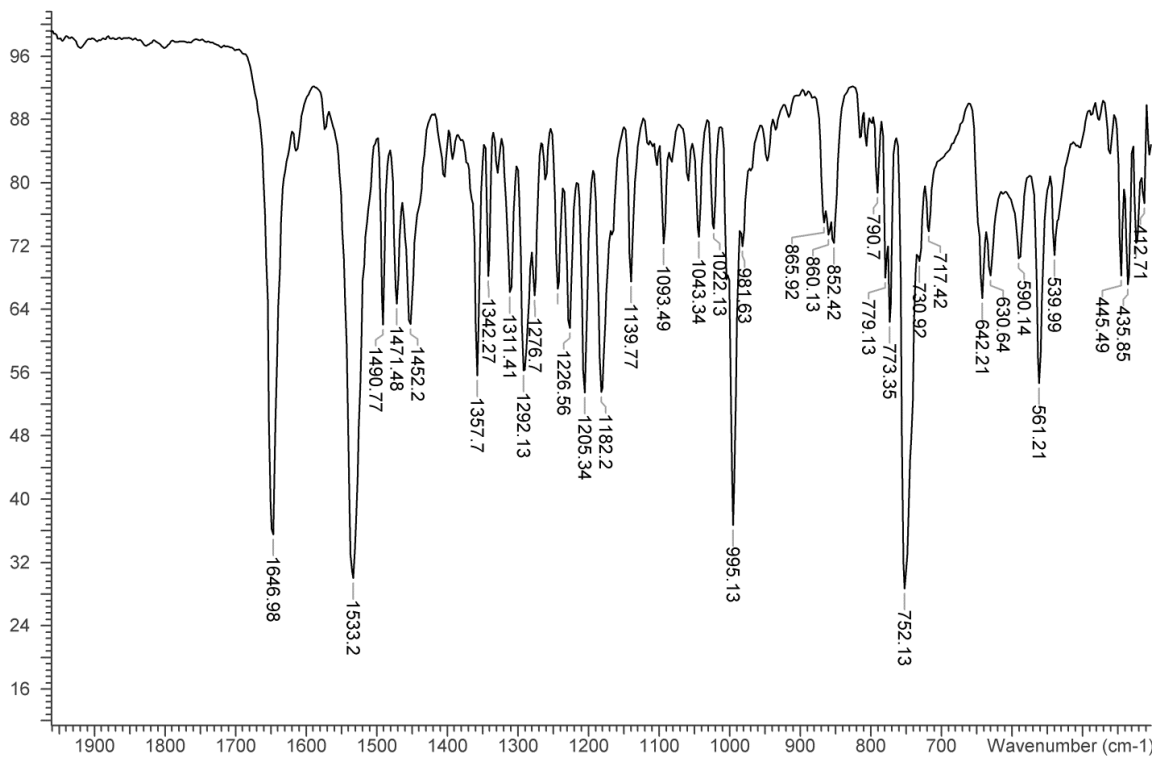
4.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (3 bounce)
Scan Parameters: Number of scans: 32
Number of background scans: 32
Resolution: 4cm⁻¹
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): 5-Fluoro-AKB-48 Lot # N1-P53EMG



FTIR ATR (Diamond, 3 Bounce): 5-Fluoro-AKB-48 Lot # N1-P53EMG



FTIR Analytical Observation:

Due to structural similarities with XLR11, polymorphic characteristics are expected in this compound.