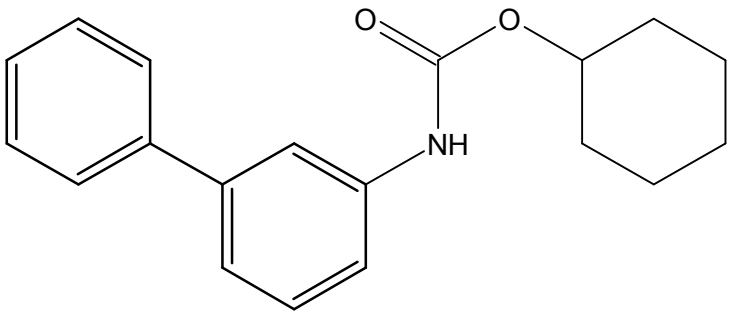
URB-602

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



1. GENERAL INFORMATION

IUPAC Name: cyclohexyl biphenyl-3-yl carbamate

CAS#: 565460-15-3

Synonyms: [1,1'-biphenyl]-3-yl-carbamic acid, cyclohexyl ester

Source: DEA Reference Material Collection

Appearance: White powder

UV_{max}(nm): 235.8

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (^{o}C)
Base	$C_{19}H_{21}NO_2$	295	124.9

3. QUALITATIVE DATA

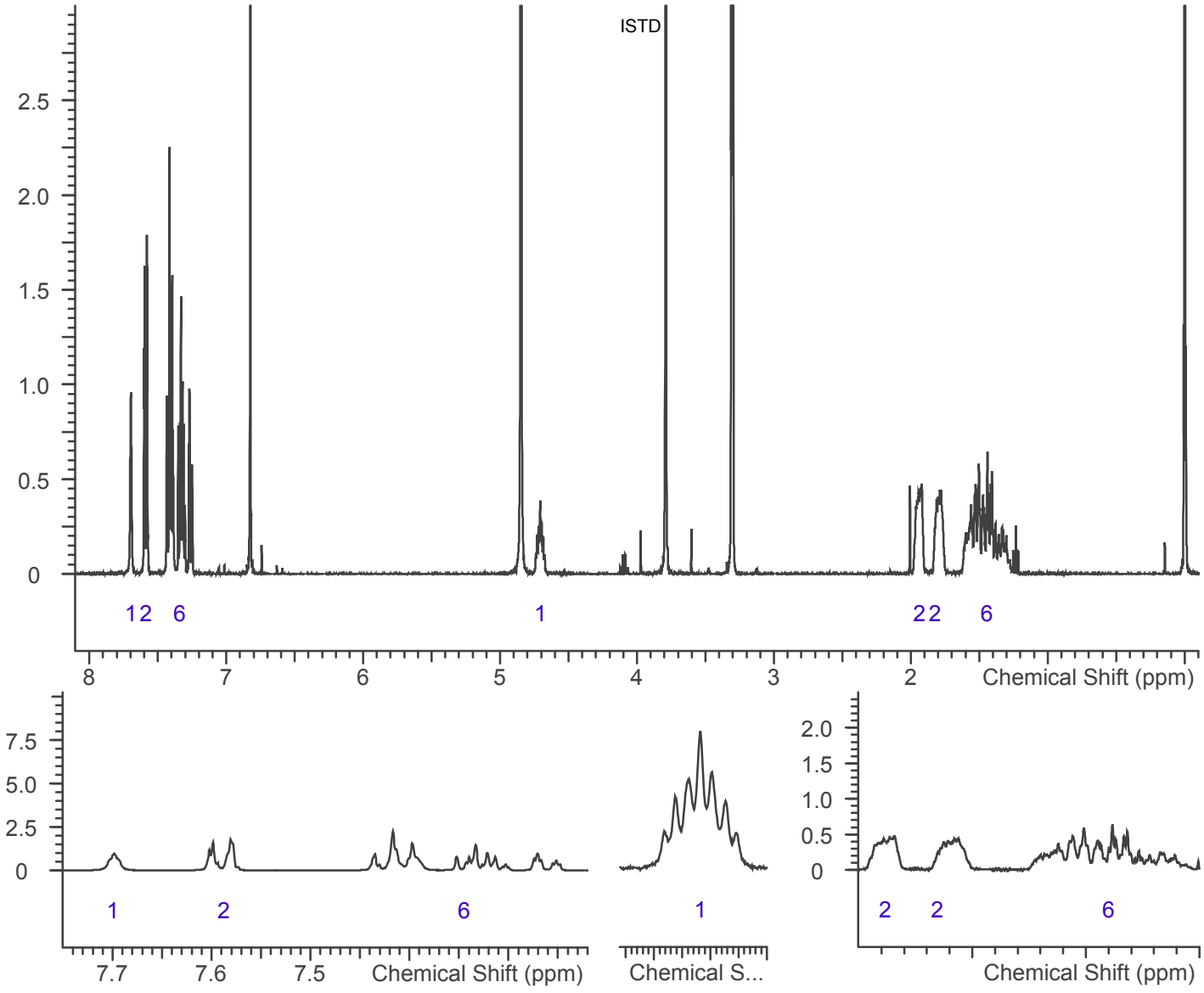
*3.*1 NUCLEAR MAGNETIC RESONANCE

Method NMR CD_3OD

Sample Preparation: Dilute analyte to ~5 mg/mL inCD_3OD 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

^{1}H NMR: URB-602; Lot 0438099-15; CD_3OD; 400 MHz

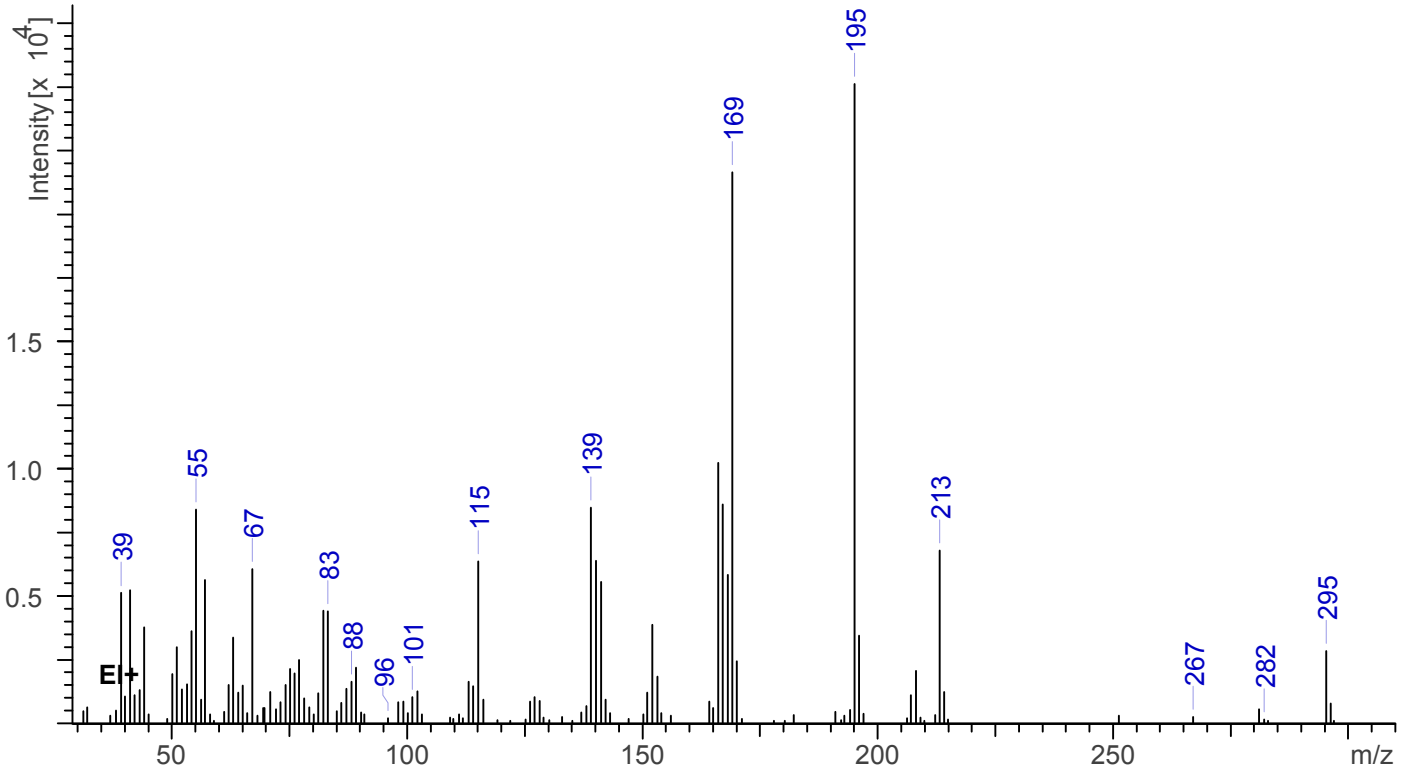


3.2 Gas Chromatography/Mass Spectrometry

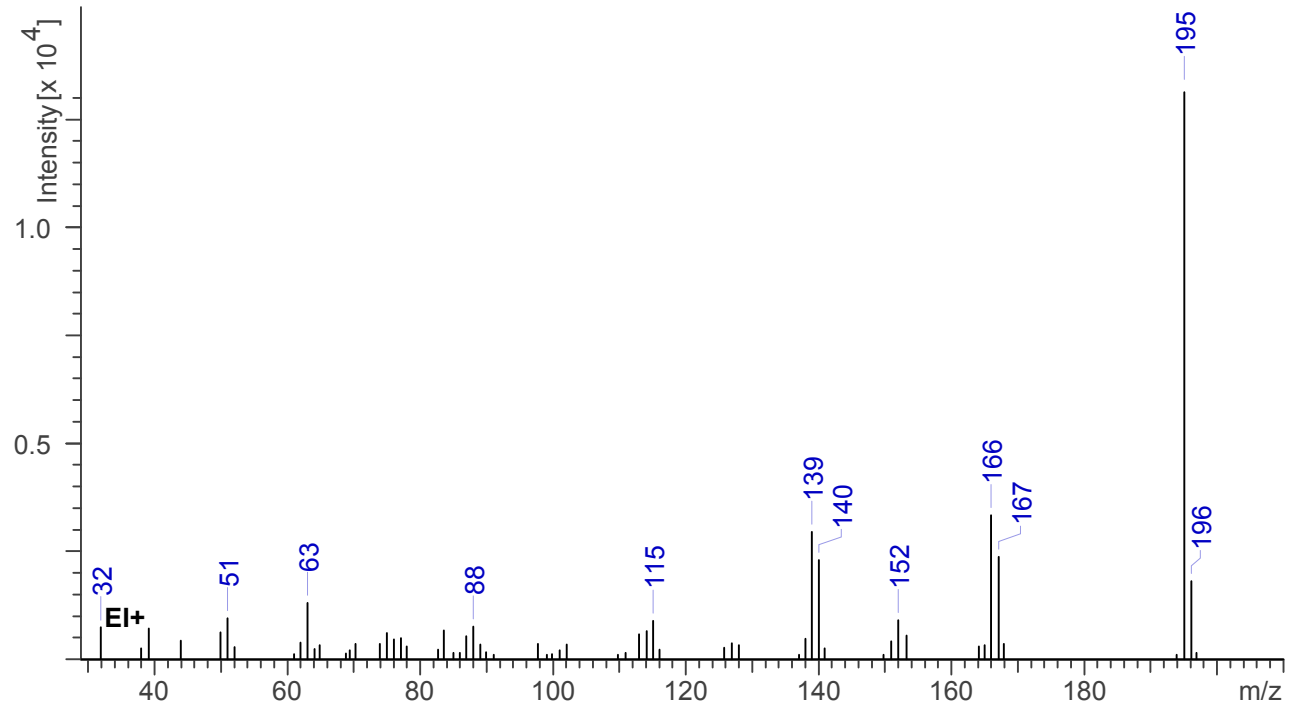
Sample Preparation: Dilute analyte ~1 mg/mL base extracted into chloroform.

Instrument:	Agilent gas chromatograph operated in split mode with MS detector
Column:	DB-1 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) 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 µL injected
MS Parameters:	Mass scan range: 30-550 amu Threshold: 100 Tune file: stune.u Acquisition mode: scan
Retention Time:	URB-602: 16.766 minutes; possible breakdown at 9.330 minutes

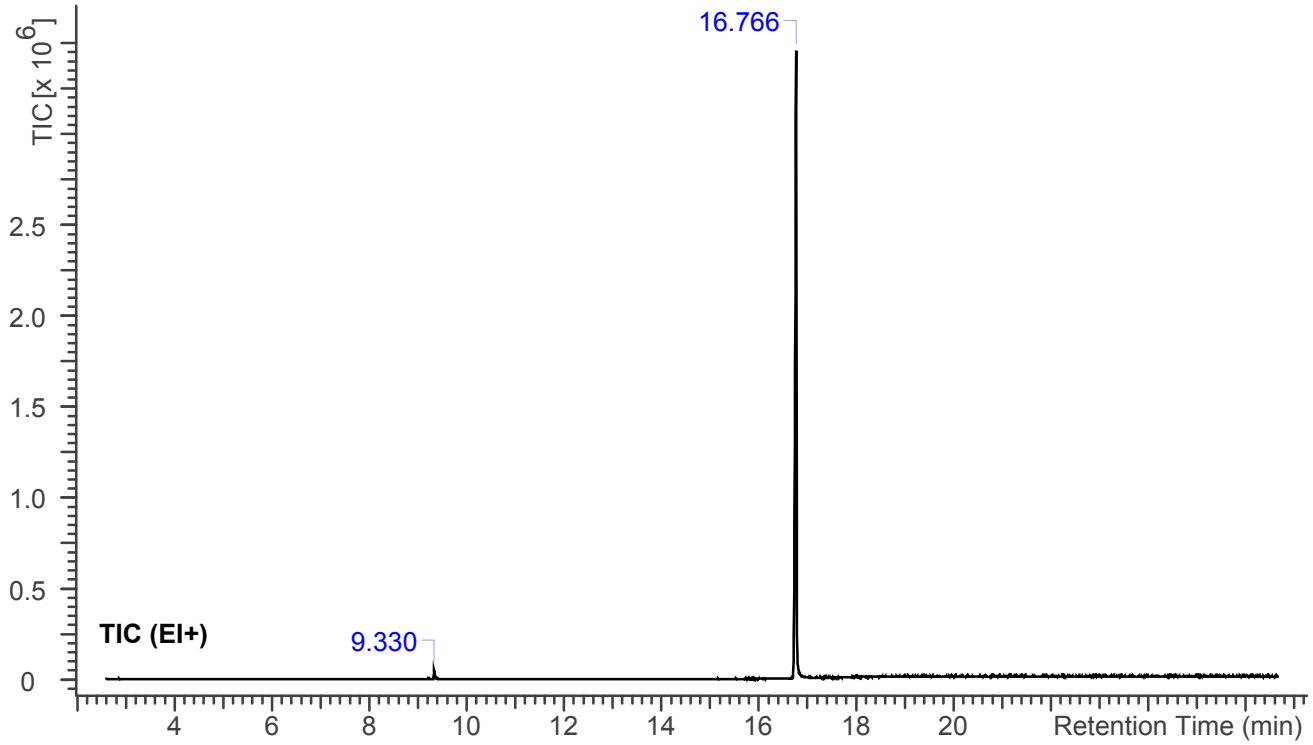
EI Mass Spectrum: URB-602 Lot 0438099-15



EI Mass Spectrum: URB-602 possible breakdown Lot 0438099-15



TIC: URB-602 Lot 0438099-15



GC/MS Analytical Observation:

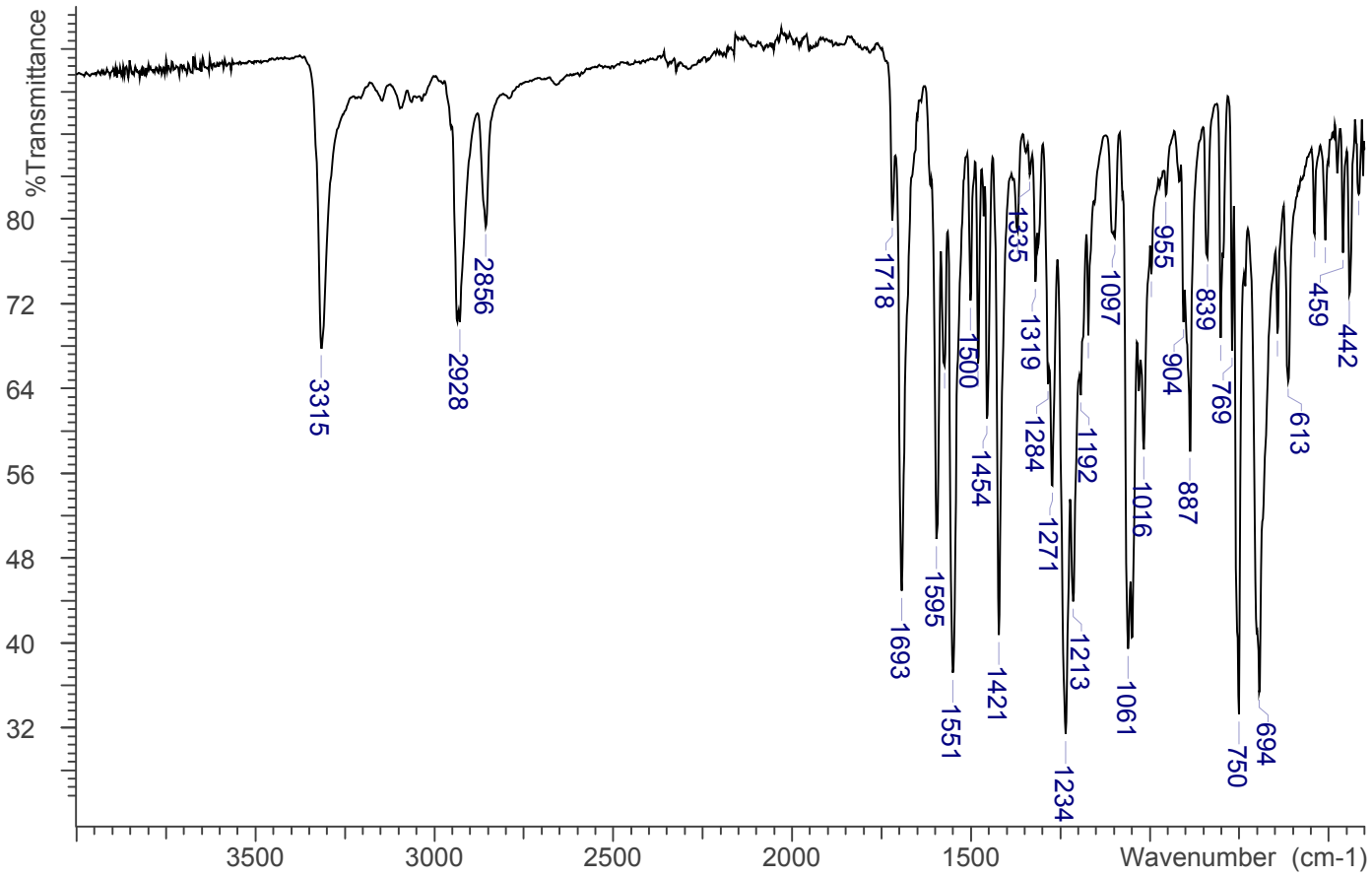
The GC/MS TIC of URB-602 shows two peaks (shown above). The major peak, having a retention time of 16.766 minutes, is URB-602 while the other peak, with a retention time of 9.330 minutes is most likely a breakdown product resulting from cleavage of the cyclohexanol group on the molecule.

3.3 INFRARED SPECTROSCOPY (FTIR)

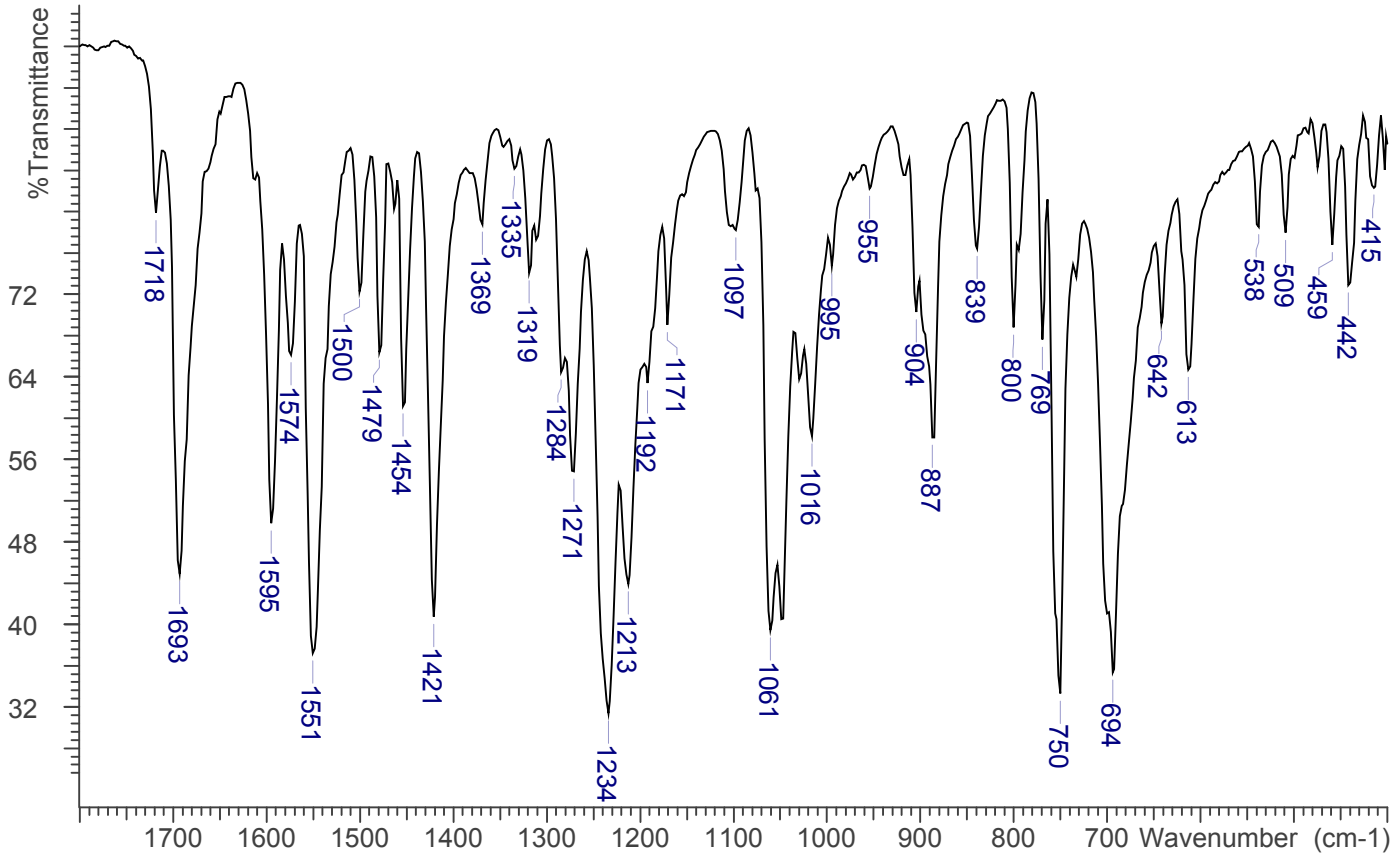
Insrument: FTIR with diamond ATR attachment (3 bounce)

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): URB-602 Lot # 0438099-15



FTIR ATR (Diamond, 3 Bounce): URB-602 Lot # 0438099-15



4. *ADDITIONAL RESOURCES*

Forendex

Wikipedia