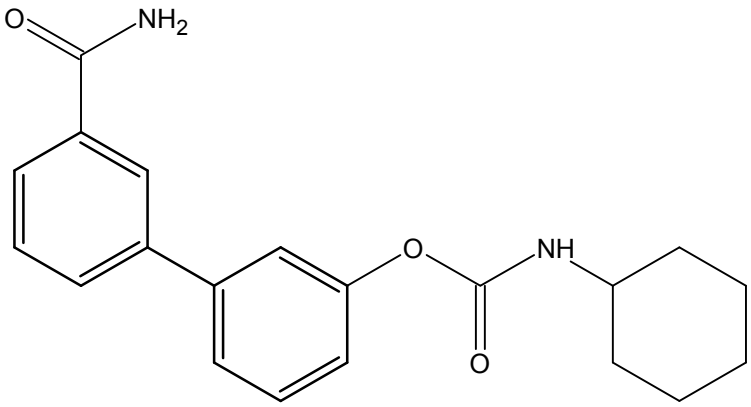
URB-597

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



1. GENERAL INFORMATION

IUPAC Name: 3'-carbamoylbiphenyl-3-yl cyclohexylcarbamate

CAS#: 546141-08-6

Synonyms: KDS-4103

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 (^{o}C)
Base	$C_{20}H_{22}N_2O_3$	338	Not Determined

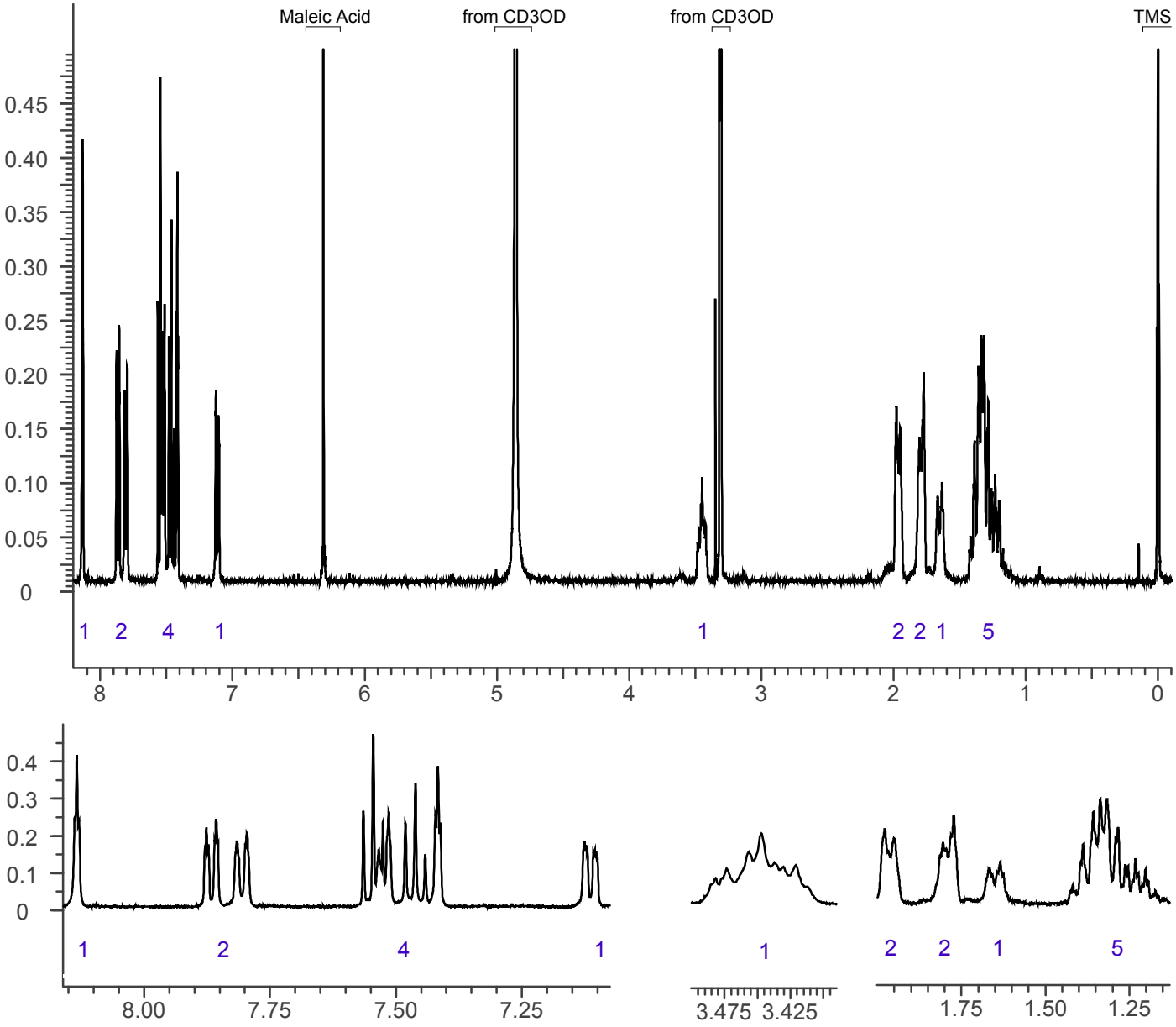
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~15 mg/mL in CD_3OD 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

^{1}H NMR: URB-597 Lot # ALB-223-1; CD_3OD; 400MHz

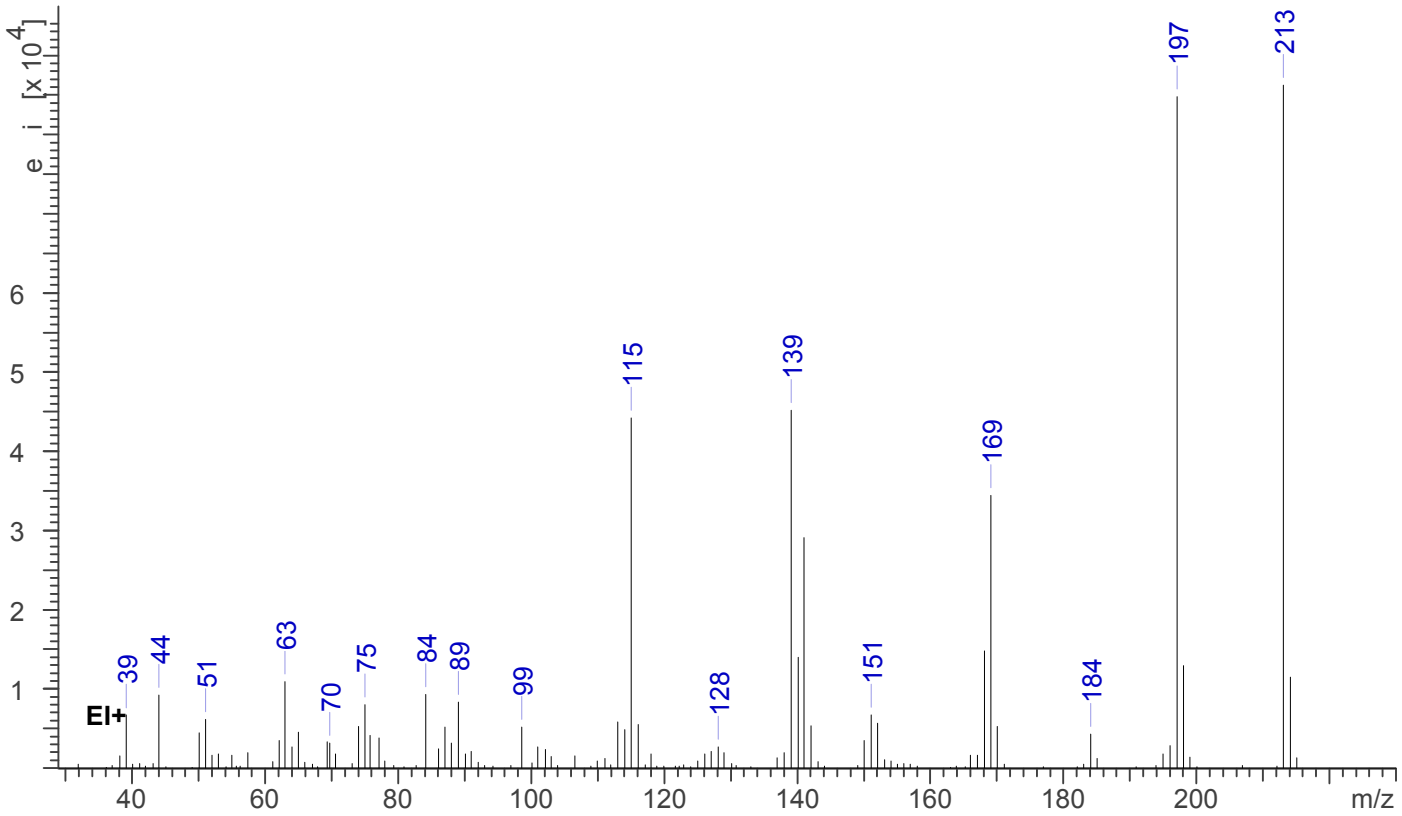


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

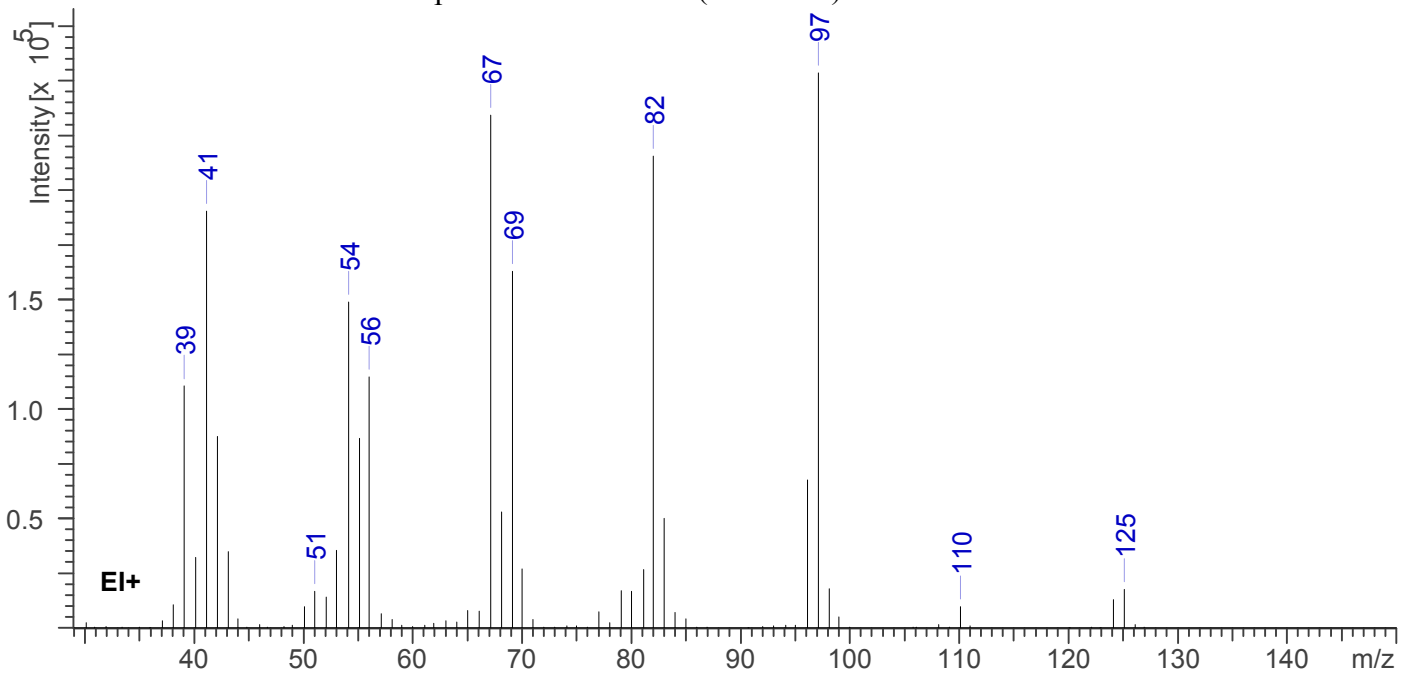
Sample Preparation: Dilute analyte to ~4 mg/mL in chloroform with 5 drops methanol.

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:	MWt 213: 14.926 min; MWt 125: 2.860 min.

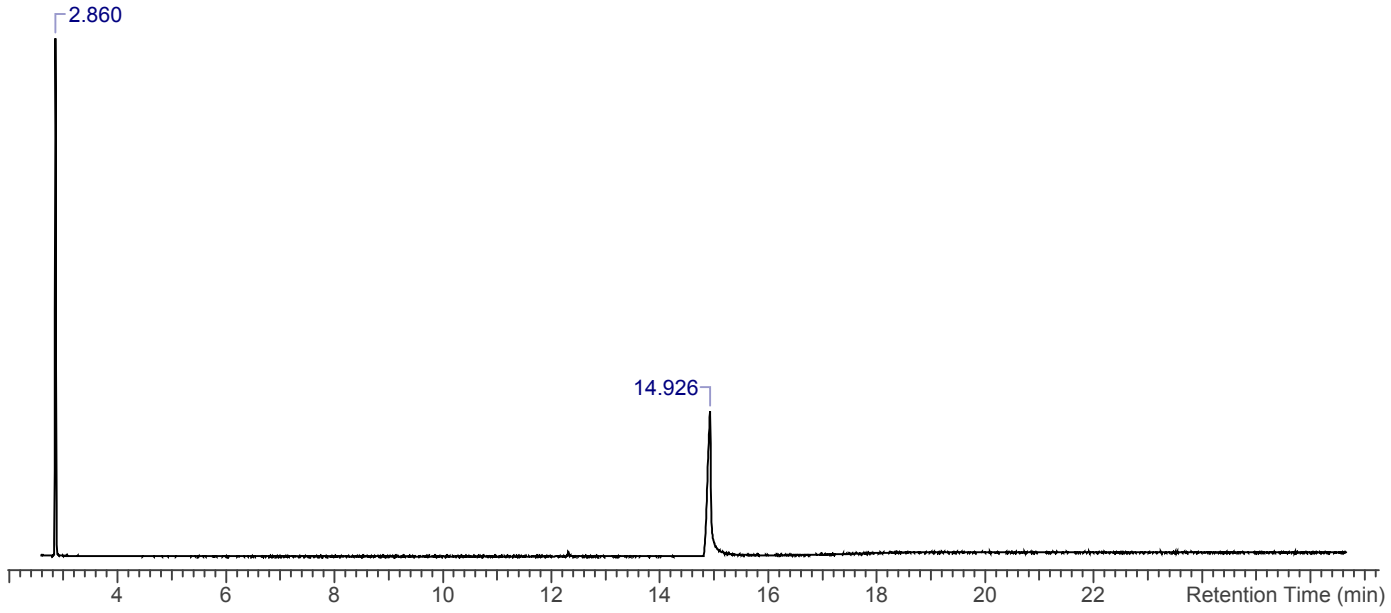
EI Mass Spectrum: URB-597 (MWt 213) Lot # ALB-223-1



EI Mass Spectrum: URB-597 (MWt 125) Lot # ALB-223-1



TIC: URB-597 Lot # ALB-223-1



GC/MS Analytical Observation:

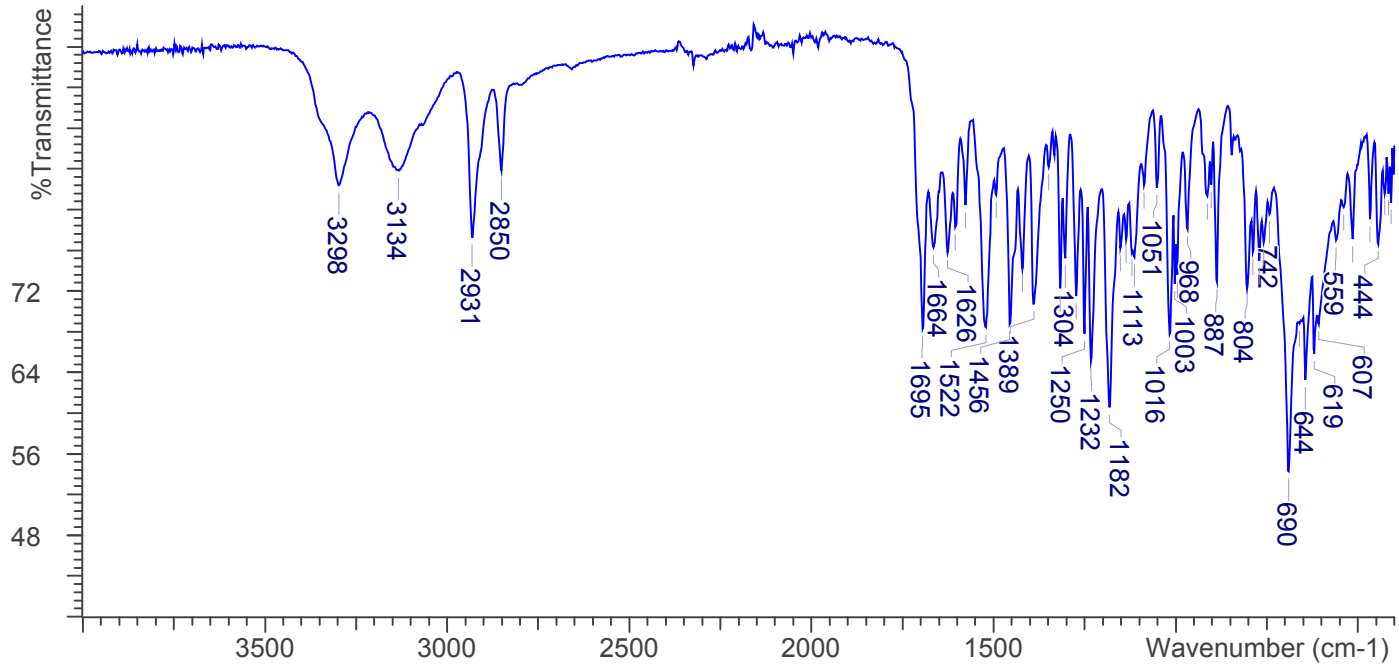
URB-597 is thermally unstable; therefore, no Electron Impact mass spectrum of the complete molecule could be obtained. Instead, the mass spectrum shows the presence of two compounds,one with a molecular weight of 213 and a second with a molecular weight of 125. The combined masses equal the molecular weight of URB-597. The mass spectra of the two compounds are shown above along with the TIC.

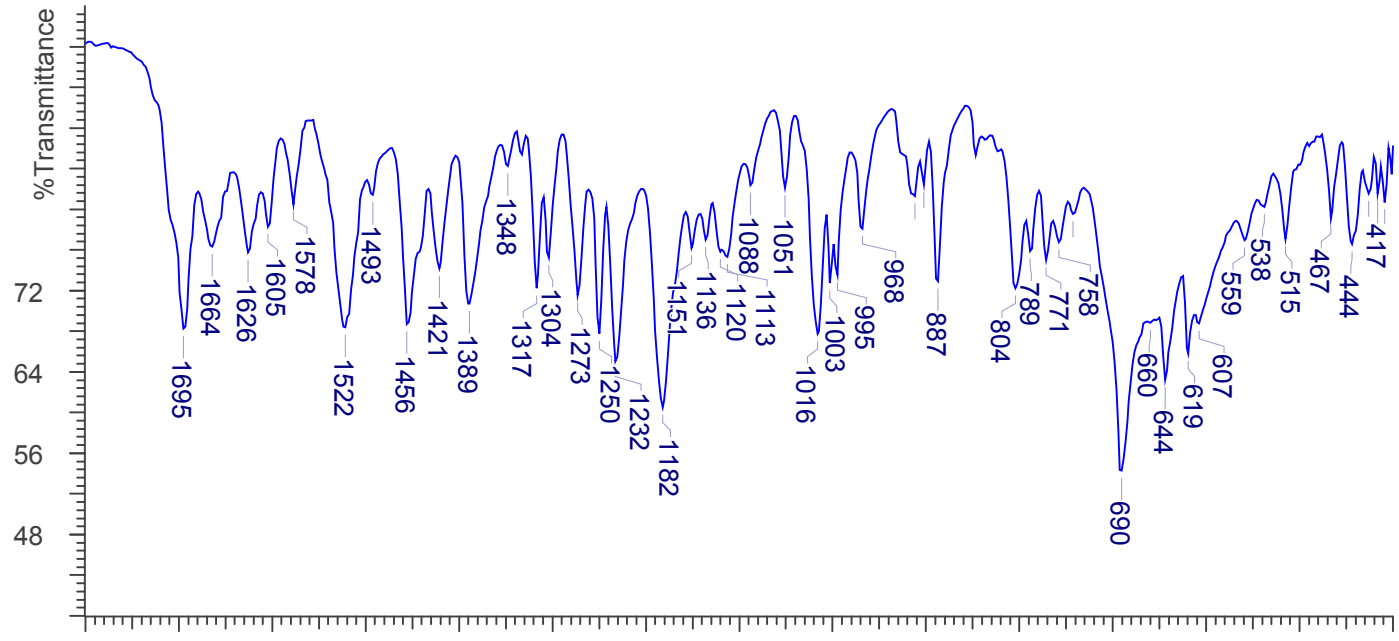
3.3 INFRARED SPECTROSCOPY (FTIR)

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-597 Lot # ALB-223-1





4. ADDITIONAL RESOURCES

Forendex

Wikipedia