
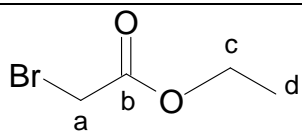


NMR SPECTROMETRY

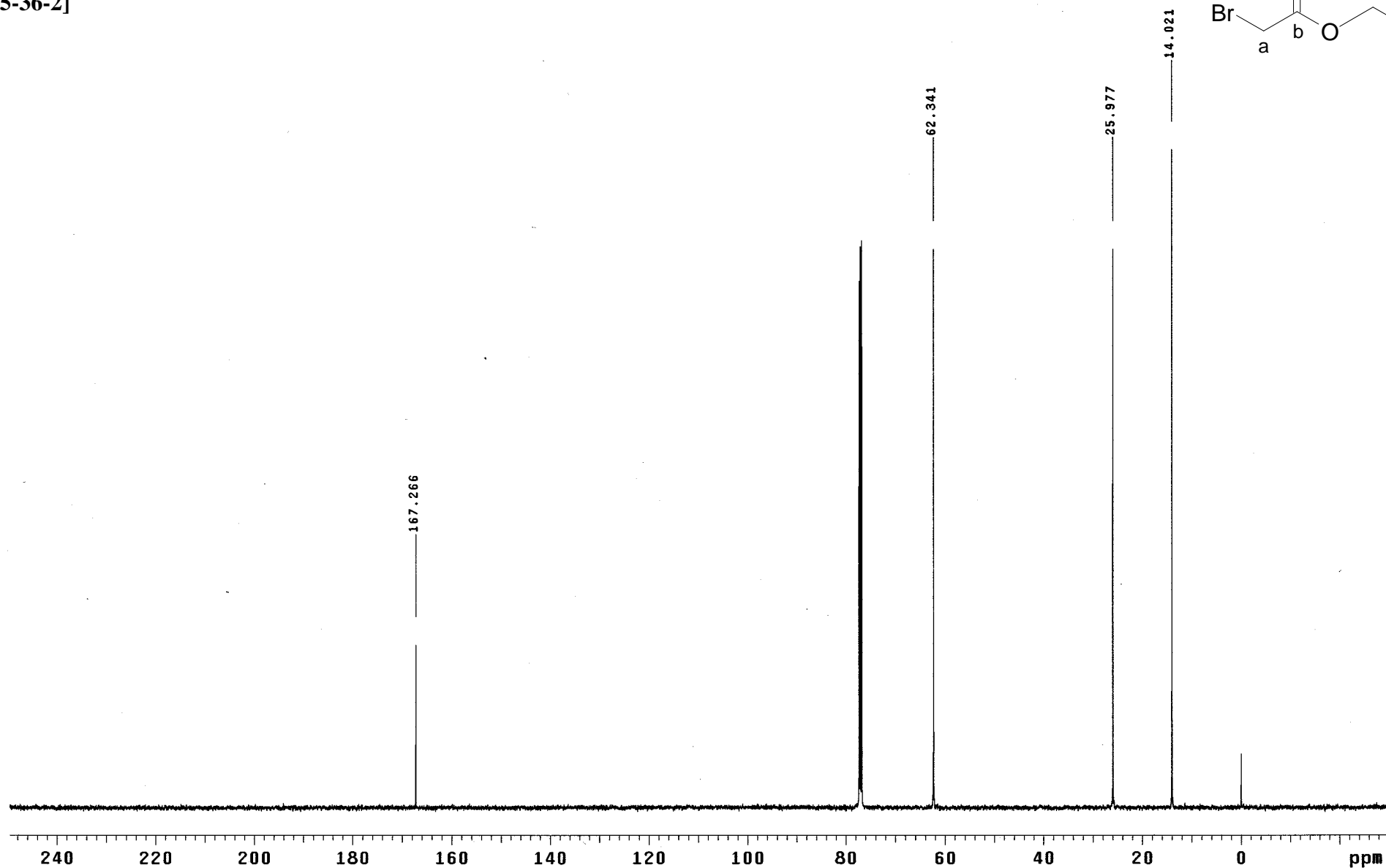
Contributor's name and address:		Verification Laboratory
Secretariat identification code	25-3-0038r (p1/2)	DSO National Laboratories
Signature		11 Stockport Road Singapore 117605
Chemical information:		
Chemical name	Ethyl bromoacetate	
Schedule number		
CAS registry number	105-36-2	
Chemical structure with numbering of atoms		
Molecular formula	C ₄ H ₇ BrO ₂	
Sample information:		
Sample purity	>98 %	
Sample concentration	75 mg/mL	
Solvent	CDCl ₃	
pH	-	
Source	Merck	
Reference chemical shift (internal)	TMS, 0 ppm	
Instrument information:		
Manufacturer	Varian, Inc.	
Model	Inova 500 MHz	
Spectrometer frequency	500 MHz	
Software version	VNMR version 6.1C	
Experimental information:		
Nucleus measured	¹³ C{ ¹ H}	
Sample temperature	25 °C	
Spectral width (Hz)	35133.9	
Data points in Fourier transformed spectrum	65536	
Repetition time	2.5 s	
Pulse angle (μs and degrees)	4.125 μs, 45°	
Date of experiment	13 Apr 2005	
Data points in FID	35108	
Number of scans	720	
Baseline correction	Yes	
Spectral information:		
Chemical shifts assigned except for acidic protons	Ca = 25.98, Cb = 167.27, Cc = 62.34, Cd = 14.02	
Coupling constants	-	

25-3-0038r (p2/2)

Ethyl bromoacetate (C₄H₇BrO₂)

[105-36-2]

¹³C{¹H} NMR



Res.Freq: 125.653 MHz
Solvent: CDCl₃
Temperature: 25°C
Concentration: 75 mg/mL

Reference: TMS (internal)
Spectral Width: 35133.9 Hz
Data points [FID]: 35108
Data points [Spectrum]: 65536

Pulse width: 4.125 μs, 45°
Number of Scans: 720
Line broadening: 2
Rep. time: 2.5 s

Resolution: 1.07 Hz (TMS)
Baseline correction: Yes
Instrument: Varian INOVA 500

Nuc δ[ppm]	Nuc δ[ppm]
a: 25.98	d: 14.02
b: 167.27	
c: 62.34	