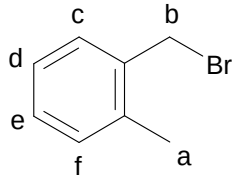
NMR SPECTROMETRY

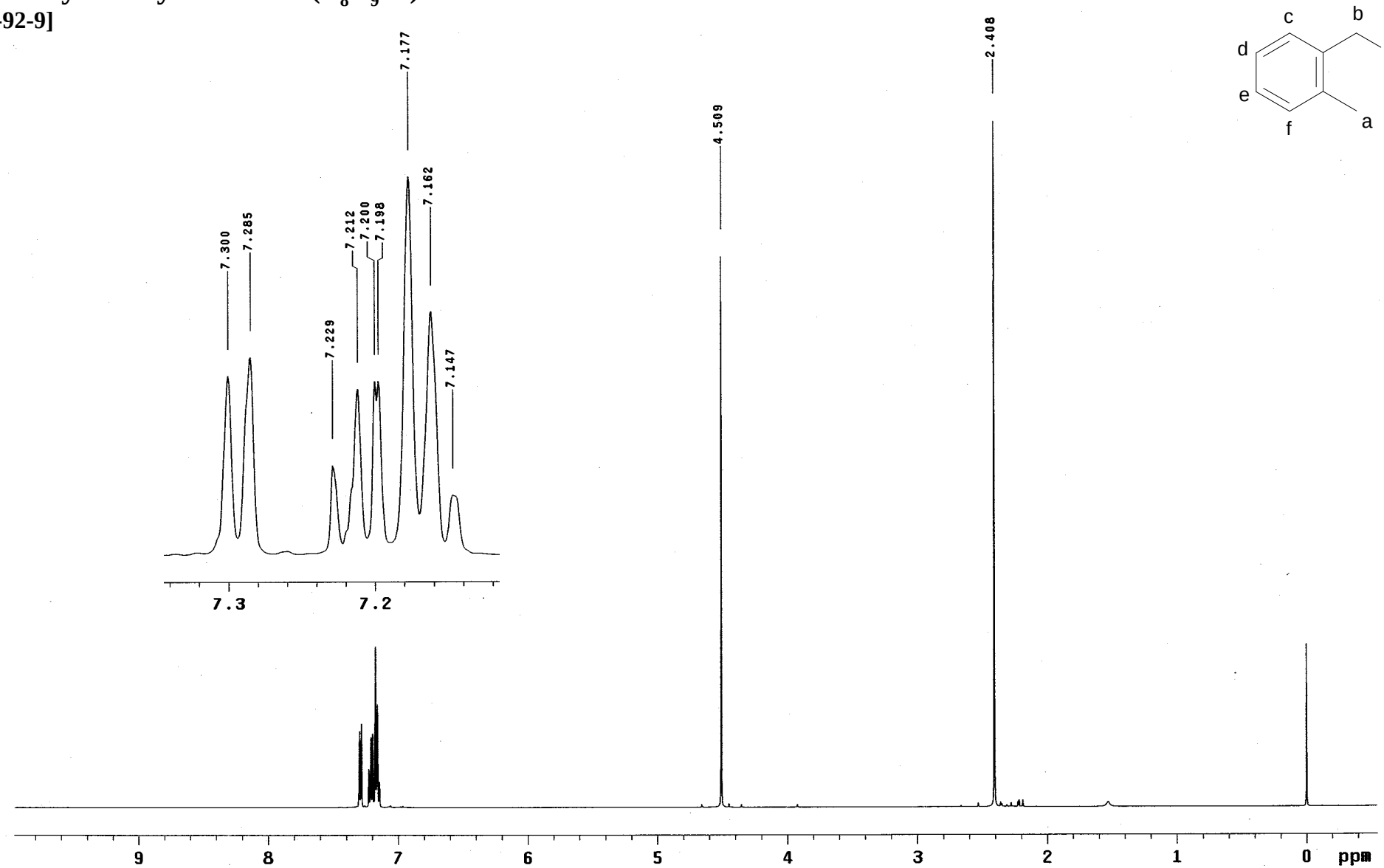
Contributor's name and address:		Verification Laboratory DSO National Laboratories 11 Stockport Road Singapore 117605
Secretariat identification code	25-3-0015r (p1/2)	
Signature		
Chemical information:		
Chemical name	2-Methylbenzyl bromide	
Schedule number		
CAS registry number	89-92-9	
Chemical structure with numbering of atoms		
Molecular formula	C_8H_9Br	
Sample information:		
Sample purity	98 %	
Sample concentration	69 mg/mL	
Solvent	$CDCl_3$	
pH	-	
Source	Aldrich	
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	^1H	
Sample temperature	25 °C	
Spectral width (Hz)	5252.1	
Data points in Fourier transformed spectrum	32768	
Repetition time	12s	
Pulse angle (µs and degrees)	4.463 µs, 45°	
Date of experiment	14 Apr 2005	
Data points in FID	31480	
Number of scans	16	
Baseline correction	Yes	
Spectral information:		
Chemical shifts (ppm) assigned except for acidic protons	Ha = 2.41; Hb = 4.51; Hc = 7.28 – 7.30; Hd, He, Hf = 7.14 – 7.23	
Coupling constants (Hz)		

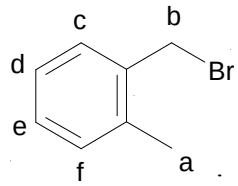
25-3-0015r (p2/2)

2-Methyl benzyl bromide (C_8H_9Br)

[89-92-9]

^{1}H NMR





Res.Freq: 499.662 MHz
Solvent: $CDCl_3$
Temperature: 25°C
Concentration: 69 mg/mL
Reference: TMS (internal)

Spectral Width: 5252.1 Hz
Data points [FID]: 31480
Data points [Spectrum]: 32768
Pulse width: 4.463 µs, 45°
Number of Scans: 16

Line broadening: no
Rep. time: 12 s
Resolution: 0.3 Hz (TMS)
Baseline correction: Yes
Instrument: Varian INOVA 500

Nuc δ[ppm]
a: 2.41
b: 4.51
c: 7.28 – 7.30
d, e, f: 7.14 – 7.23