
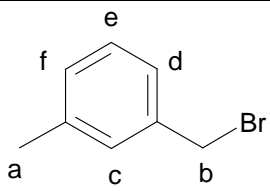


NMR SPECTROMETRY

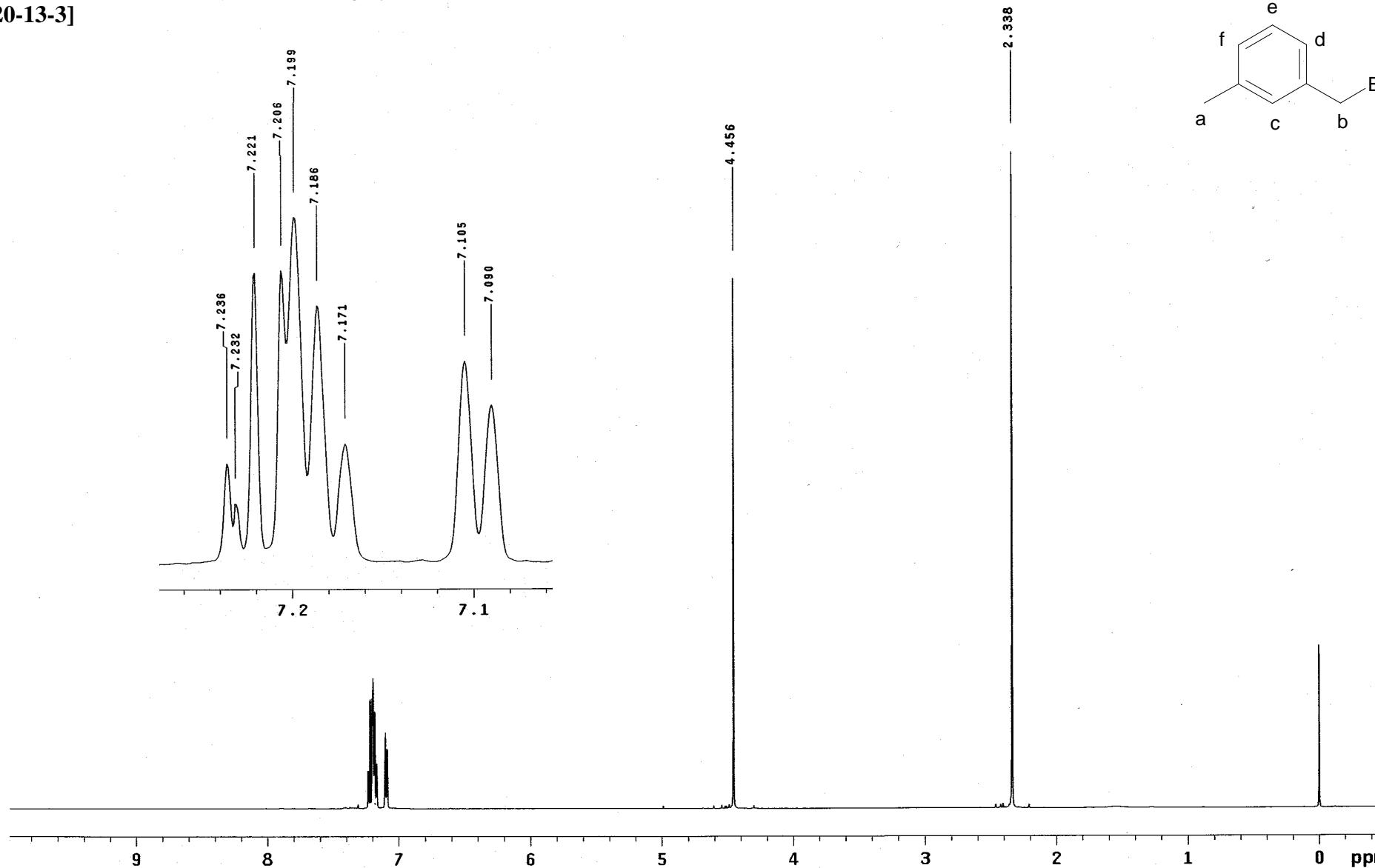
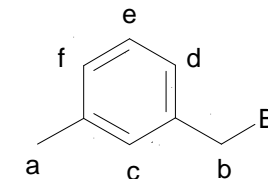
Contributor's name and address:		Verification Laboratory
Secretariat identification code	25-3-0017r (p1/2)	DSO National Laboratories
Signature		11 Stockport Road Singapore 117605
Chemical information:		
Chemical name	3-Methylbenzyl bromide	
Schedule number		
CAS registry number	620-13-3	
Chemical structure with numbering of atoms		
Molecular formula	C ₈ H ₉ Br	
Sample information:		
Sample purity	97 %	
Sample concentration	69 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	¹ H	
Sample temperature	25 °C	
Spectral width (Hz)	5252.1	
Data points in Fourier transformed spectrum	32768	
Repetition time	12 s	
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 assigned except for acidic protons	Ha = 2.34; Hb = 4.46; Hc, Hd, He = 7.17 – 7.24; Hf = 7.09 – 7.11	
Coupling constants	-	

25-3-0017r (p2/2)

3-Methyl benzyl bromide (C₈H₉Br)

[620-13-3]

¹H NMR



Res.Freq: 499.662 MHz
Solvent: CDCl₃
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: 2.34
b: 4.46
c, d, e: 7.17 – 7.24
f: 7.09 – 7.11