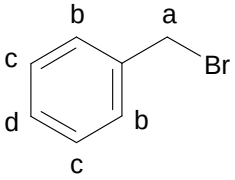
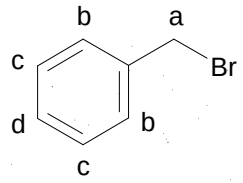
NMR SPECTROMETRY

Contributor's name and address:	Verification Laboratory DSO National Laboratories 11 Stockport Road Singapore 117605
Secretariat identification code	25-3-0013r (p1/2)
Signature	
Chemical information:	
Chemical name	Benzyl bromide
Schedule number	
CAS registry number	100-39-0
Chemical structure with numbering of atoms	
Molecular formula	C_7H_7Br
Sample information:	
Sample purity	>98 %
Sample concentration	50 mg/mL
Solvent	$CDCl_3$
pH	-
Source	Fluka
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)	3.462 μs, 45°
Date of experiment	1 Jun 2005
Data points in FID	31480
Number of scans	16
Baseline correction	Yes
Spectral information:	
Chemical shifts (ppm) assigned except for acidic protons	Ha = 4.48, Hb = 7.37 – 7.39, Hc = 7.31 – 7.35, Hd = 7.26 – 7.30
Coupling constants (Hz)	-

Benzyl bromide (C_7H_7Br)

[100-39-0]

^{1}H NMR



Res.Freq: 499.662 MHz
Solvent: $CDCl_3$
Temperature: 25°C
Concentration: 50 mg/mL
Reference: TMS (internal)

Spectral Width: 5252.1 Hz
Data points [FID]: 31480
Data points [Spectrum]: 32768
Pulse width: 3.462 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:	4.48
b:	7.37 – 7.39
c:	7.31 – 7.35
d:	7.26 – 7.30