
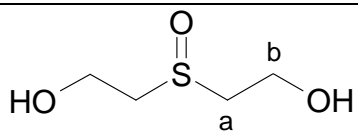


NMR SPECTROMETRY

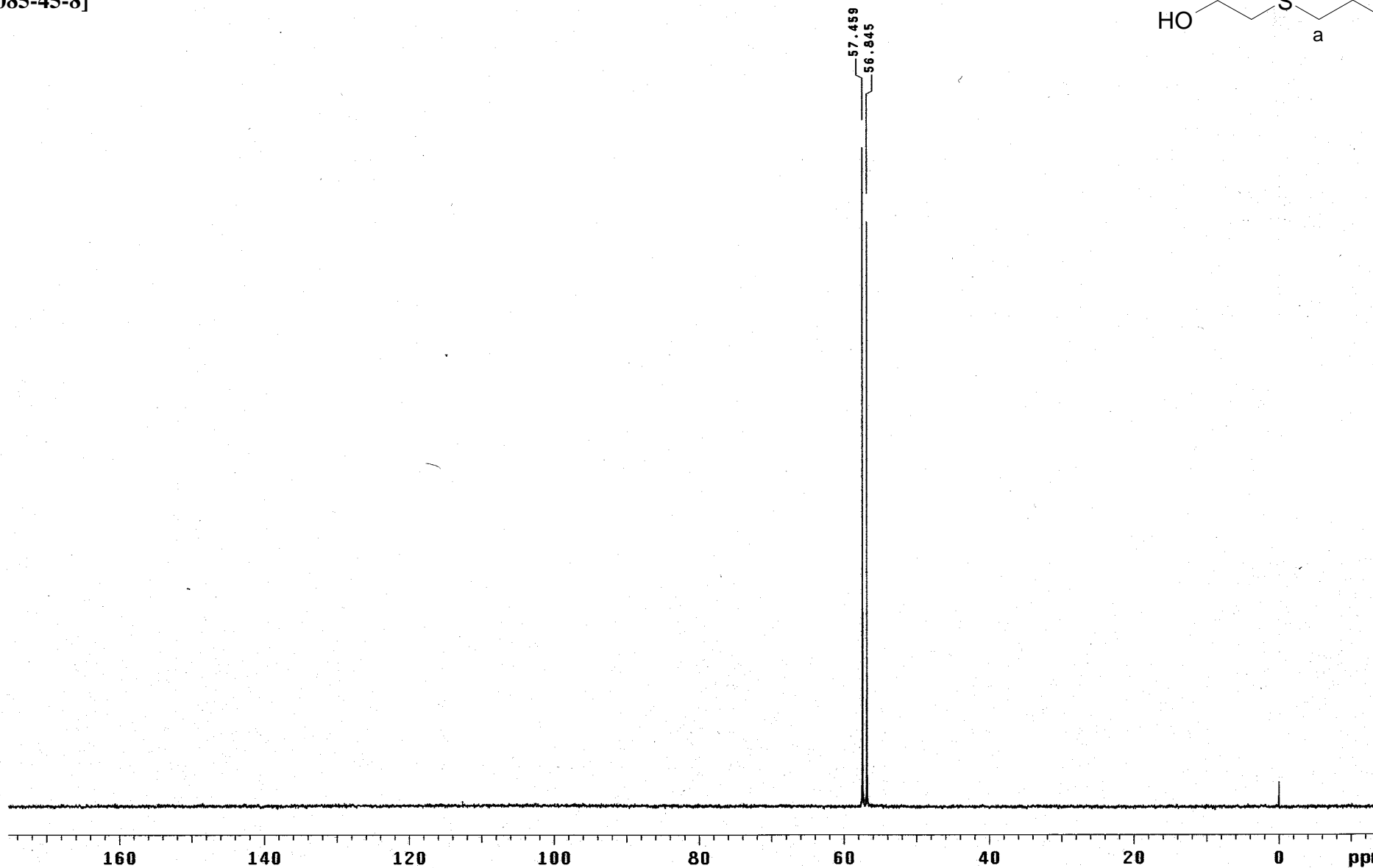
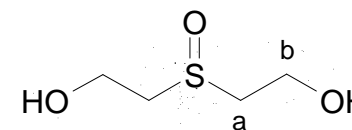
Contributor's name and address:		Verification Laboratory
Secretariat identification code	25-3-0032r (p1/3)	DSO National Laboratories
Signature		11 Stockport Road Singapore 117605
Chemical information:		
Chemical name	Bis(2-hydroxyethyl)sulfoxide	
Schedule number		
CAS registry number	3085-45-8	
Chemical structure with numbering of atoms		
Molecular formula	C ₄ H ₁₀ O ₃ S	
Sample information:		
Sample purity	99 %	
Sample concentration	50 mg/mL	
Solvent	D ₂ O	
pH	-	
Source	In-house synthesis CL02177	
Reference chemical shift (internal)	3-(Trimethylsilyl)propionic-2,2,3,3-d ₄ acid, 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)	6.463 μs, 45°	
Date of experiment	3 Jun 2005	
Data points in FID	35062	
Number of scans	720	
Baseline correction	Yes	
Spectral information:		
Chemical shifts (ppm) assigned except for acidic protons	Ca = 56.85, Cb = 57.46	
Coupling constants (Hz)	-	

25-3-0032r (p2/3)

Bis(2-hydroxyethyl)sulfoxide (C₄H₁₀O₃S)

[3085-45-8]

¹³C{¹H} NMR



Res.Freq: 125.653 MHz
Solvent: D₂O
Temperature: 25°C
Concentration: 50 mg/mL

Reference: TSPA-d4 (internal)
Spectral Width: 35133.9 Hz
Data points [FID]: 35062
Data points [Spectrum]: 65536

Pulse width: 6.463 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]
a: 56.85
b: 57.46

25-3-0032r (p3/3)

Bis(2-hydroxyethyl)sulfoxide (C₄H₁₀O₃S)

[3085-45-8]

