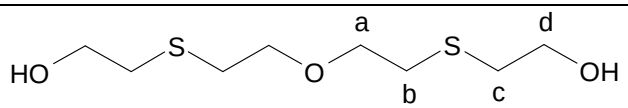
NMR SPECTROMETRY

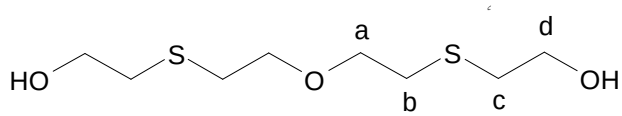
Contributor's name and address:		Verification Laboratory DSO National Laboratories 11 Stockport Road Singapore 117605
Secretariat identification code	25-3-0027r (p1/2)	
Signature		
Chemical information:		
Chemical name	Bis(2-hydroxyethylthioethyl)ether	
Schedule number		
CAS registry number	7426-02-0	
Chemical structure with numbering of atoms		
Molecular formula	$C_8H_{18}O_3S_2$	
Sample information:		
Sample purity	95 %	
Sample concentration	31 mg/mL	
Solvent	D_2O	
pH	-	
Source	In-house synthesis YL30251	
Reference chemical shift (internal)	3-(Trimethylsilyl)propionic-2,2,3,3-d4 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	^1H	
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)	3.462 µs, 45°	
Date of experiment	6 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 = 3.74, Hb = 2.78, Hc = 2.81, Hd = 3.76	
Coupling constants (Hz)	J(a,b) = 6.41, J(c,d) = 6.41	

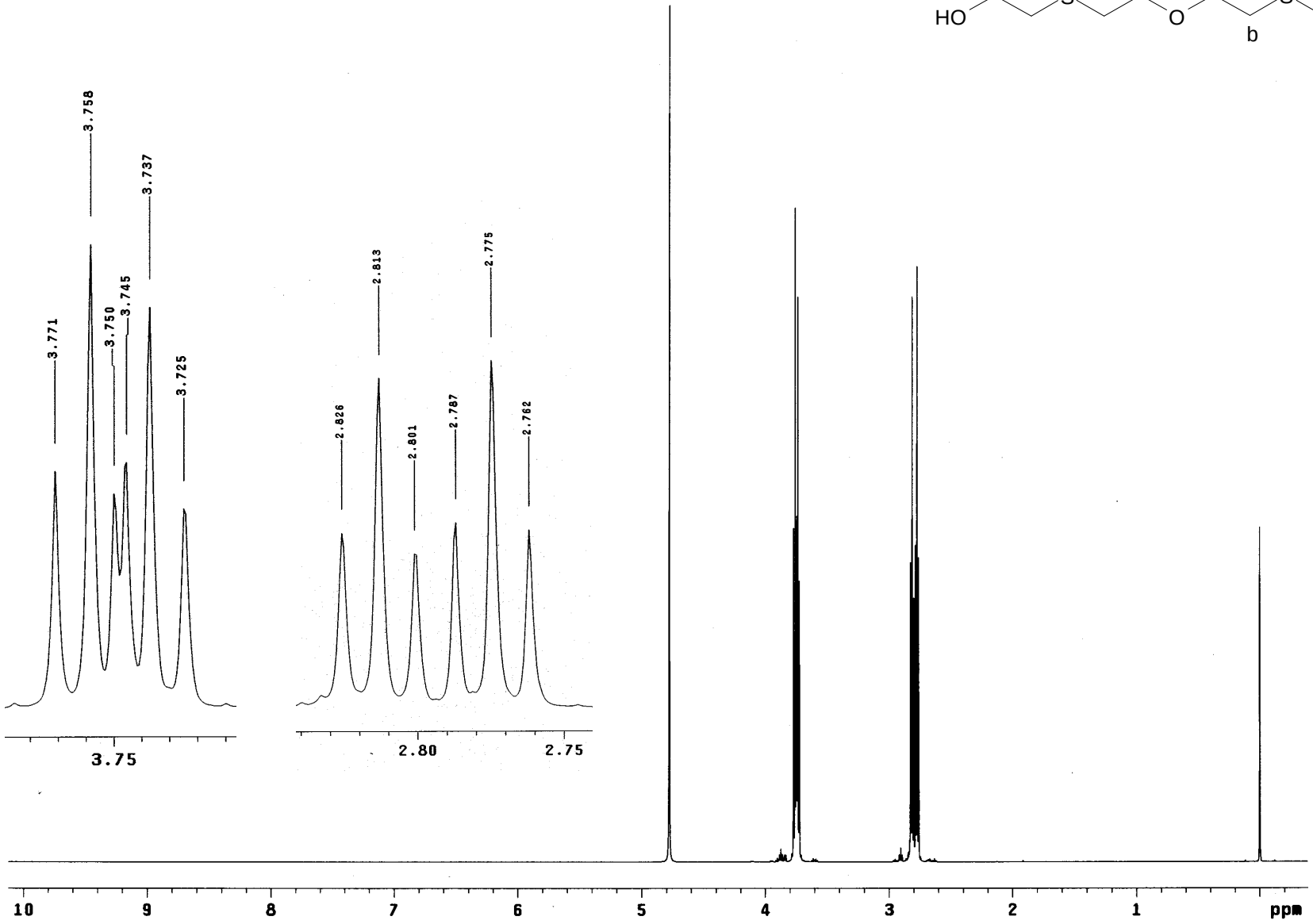
25-3-0027r (p2/2)

Bis(2-hydroxyethythioethyl)ether ($C_8H_{18}O_3S_2$)

[7426-02-0]

^{1}H NMR





Res.Freq: 499.662 MHz
Solvent: D_2O
Temperature: 25°C
Concentration: 31 mg/mL
Reference: TSPA-d_4 (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]	J[Hz]
a: 3.74	J(a,b) = 6.41
b: 2.78	J(c,d) = 6.41
c: 2.81	
d: 3.76	