
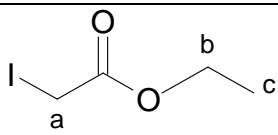


## NMR SPECTROMETRY

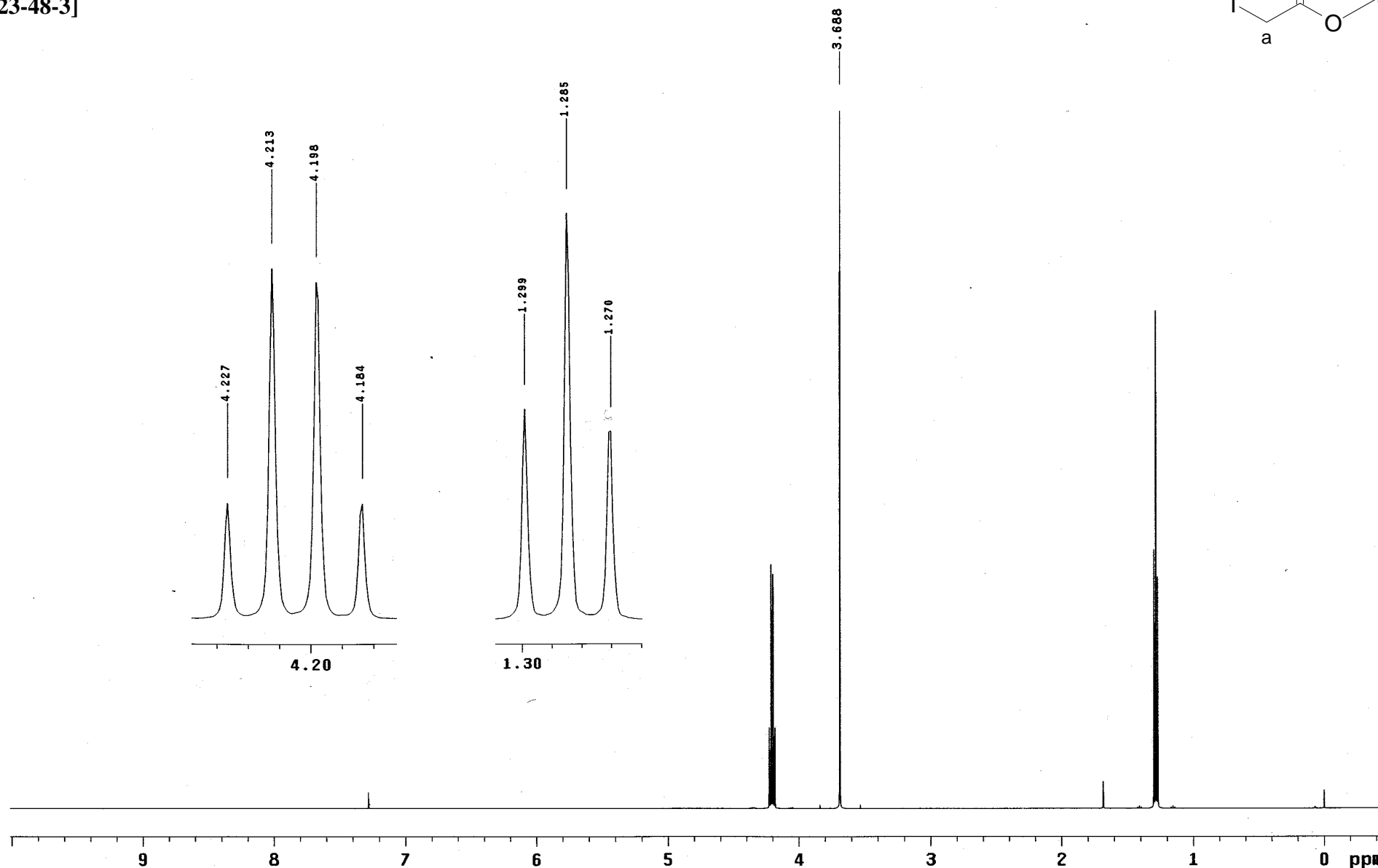
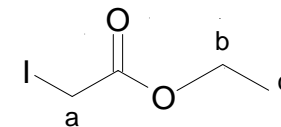
<b>Contributor's name and address:</b>		Verification Laboratory
Secretariat identification code	25-3-0039r (p1/2)	DSO National Laboratories
Signature		11 Stockport Road Singapore 117605
<b>Chemical information:</b>		
Chemical name	Ethyl iodoacetate	
Schedule number		
CAS registry number	623-48-3	
Chemical structure with numbering of atoms		
Molecular formula	C <sub>4</sub> H <sub>7</sub> IO <sub>2</sub>	
<b>Sample information:</b>		
Sample purity	98 %	
Sample concentration	75 mg/mL	
Solvent	CDCl <sub>3</sub>	
pH	-	
Source	Alfa Aesar	
Reference chemical shift (internal)	TMS, 0 ppm	
<b>Instrument information:</b>		
Manufacturer	Varian, Inc.	
Model	Inova 500 MHz	
Spectrometer frequency	500 MHz	
Software version	VNMR version 6.1C	
<b>Experimental information:</b>		
Nucleus measured	<sup>1</sup> 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	11 Apr 2005	
Data points in FID	31480	
Number of scans	16	
Baseline correction	Yes	
<b>Spectral information:</b>		
Chemical shifts (ppm) assigned except for acidic protons	Ha = 3.69, Hb = 4.21, Hc = 1.29	
Coupling constants (Hz)	J(b,c) = 7.05	

25-3-0039r (p2/2)

# Ethyl iodoacetate (C<sub>4</sub>H<sub>7</sub>IO<sub>2</sub>)

[623-48-3]

## <sup>1</sup>H NMR



Res.Freq: 499.662 MHz  
Solvent: CDCl<sub>3</sub>  
Temperature: 25°C  
Concentration: 75 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]	J[Hz]
a: 3.69	
b: 4.21	J(b,c) = 7.05
c: 1.29	