
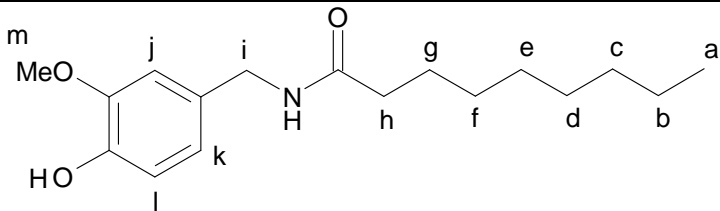


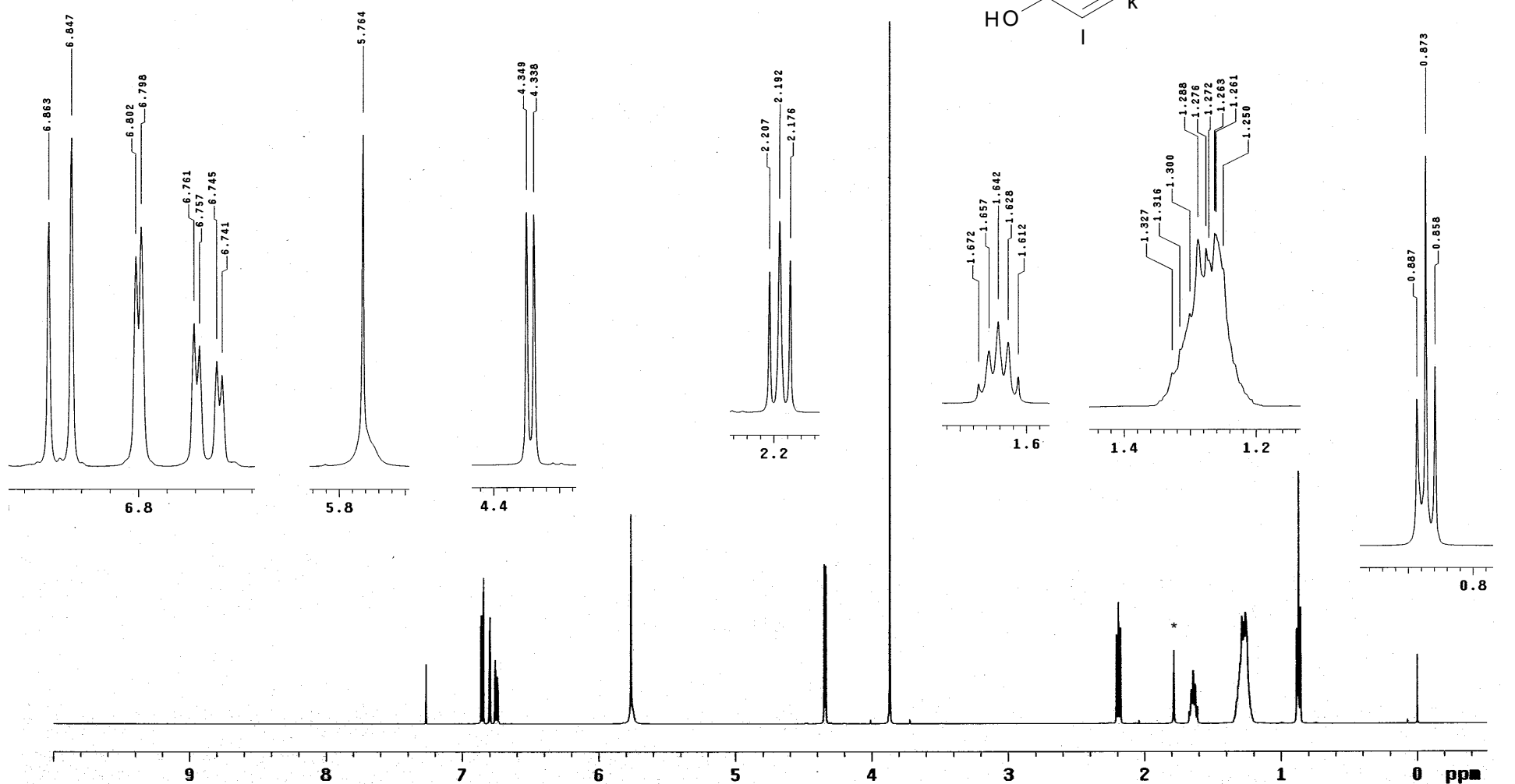
NMR SPECTROMETRY

Contributor's name and address:		Verification Laboratory
Secretariat identification code	25-3-0003r (p1/2)	DSO National Laboratories
Signature		11 Stockport Road
		Singapore 117605
Chemical information:		
Chemical name	Pelargonic acid vanillylamide	
Schedule number		
CAS registry number	2444-46-4	
Chemical structure with numbering of atoms		
Molecular formula	C ₁₇ H ₂₇ NO ₃	
Sample information:		
Sample purity	97%	
Sample concentration	15.6 mg/mL	
Solvent	CDCl ₃	
pH	-	
Source	Sigma Aldrich	
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)	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 = 0.87, Hb – Hf = 1.25 – 1.33, Hg = 1.64, Hh = 2.19, Hi = 4.34, Hj = 6.80, Hk = 6.75, Hl = 6.86, Hm = 3.87	
Coupling constants (Hz)	J(a,b) = 7.05, J(g,h) = 7.69, J(k,l) = 8.01	

25-3-0003r (p2/2)

Pelargonic acid vanillylamide (C₁₇H₂₇NO₃) [2444-46-4]

¹H NMR



Res.Freq: 499.662 MHz
Solvent: CDCl₃
Temperature: 25°C
Concentration: 15.6 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]	J[Hz]	Nuc δ[ppm]	J[Hz]
a: 0.87	J(a,b) = 7.05	k: 6.75	J(k,l) = 8.01
b - f: 1.25 - 1.33		l: 6.86	
g: 1.64	J(g,h) = 7.69	m: 3.87	
h: 2.19			
i: 4.34			
j: 6.80			