
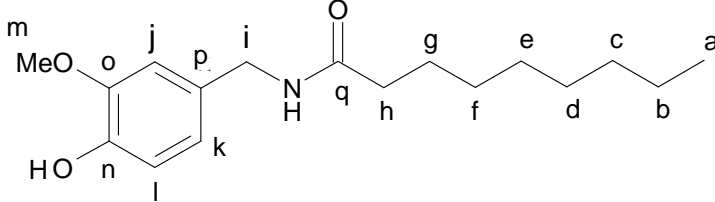


NMR SPECTROMETRY

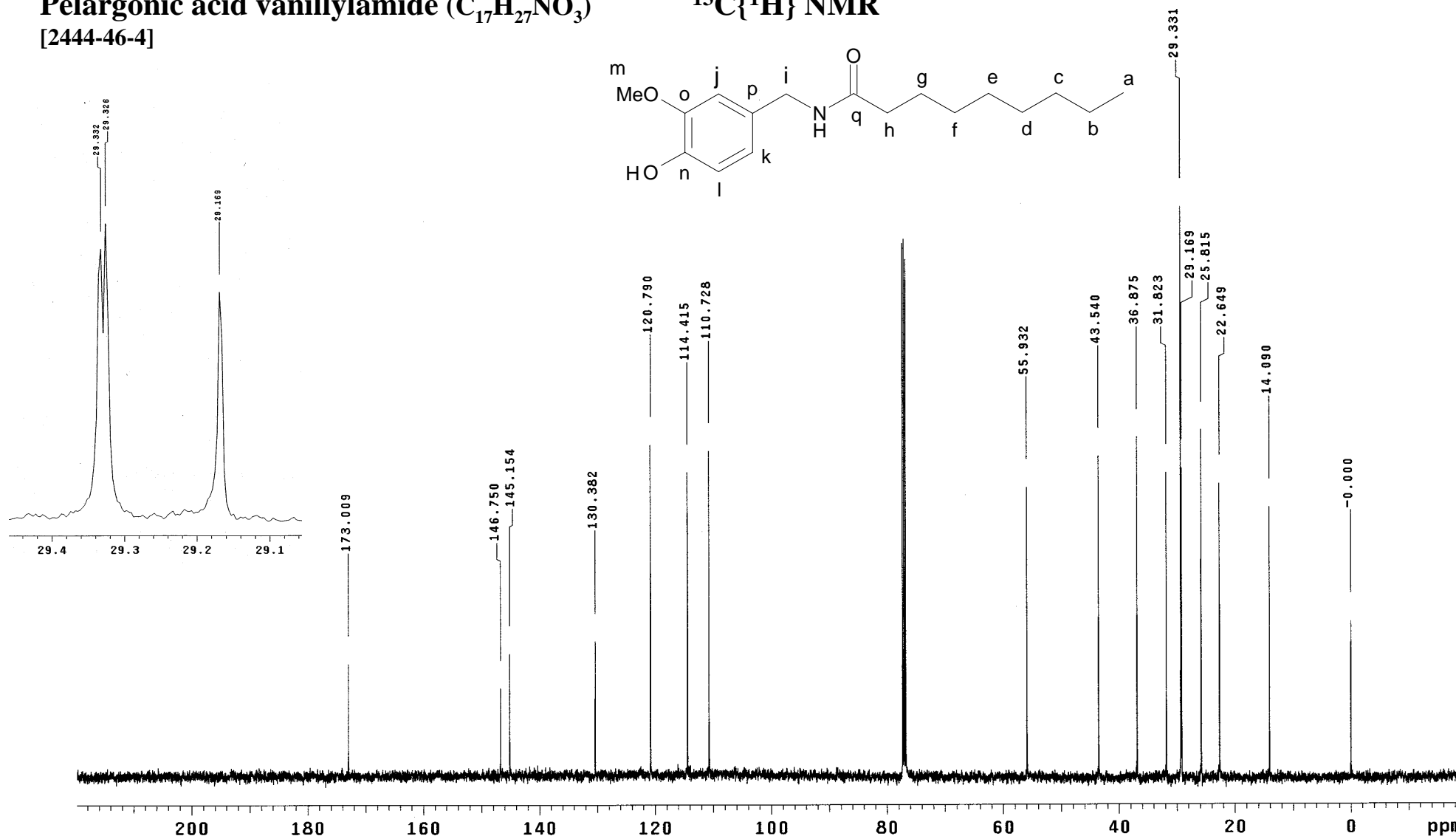
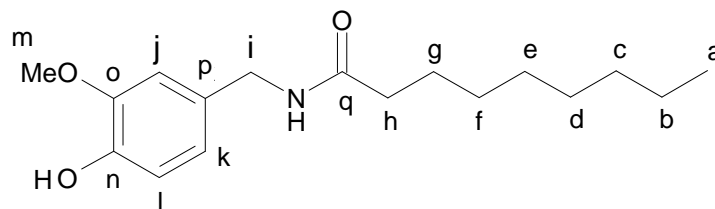
Contributor's name and address:		Verification Laboratory
Secretariat identification code	25-3-0004r (p1/2)	DSO National Laboratories
Signature		11 Stockport Road Singapore 117605
Chemical information:		
Chemical name	Pelargonic acid vanillylamide	
Schedule number		
CAS registry number	2444-46-4	
Chemical 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	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	1 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 = 14.09, Cb = 22.65, Cc = 31.82, Cd, Ce, Cf = 29.16 – 29.33, Cg = 25.82, Ch = 36.88, Ci = 43.54, Cj = 110.73, Ck = 120.79, Cl = 114.42, Cm = 55.93, Cn = 146.75, Co = 145.15, Cp = 130.38, Cq = 173.01	
Coupling constants (Hz)	-	

25-3-0004r (p2/2)

Pelargonic acid vanillylamide ($C_{17}H_{27}NO_3$)

[2444-46-4]

$^{13}C\{^1H\}$ NMR



Res.Freq: 125.653 MHz

Solvent: $CDCl_3$

Temperature: 25°C

Concentration: 15.6 mg/mL

Reference: TMS (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: 14.09

b: 22.65

c: 31.82

d,e,f: 29.16 – 29.33

g: 25.82

Nuc δ [ppm]

h: 36.88

i: 43.54

j: 110.73

k: 120.79

l: 114.42

Nuc δ [ppm]

m: 55.93

n: 146.75

o: 145.15

p: 130.38

q: 173.01