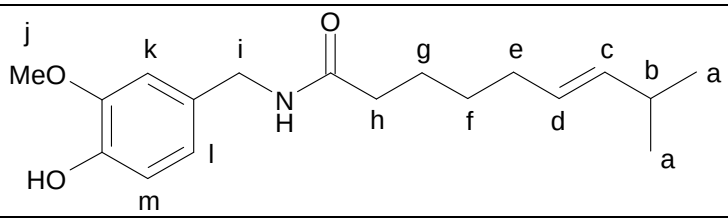
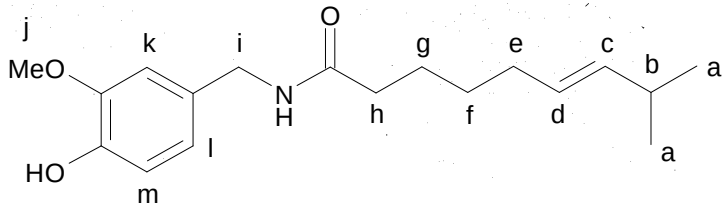
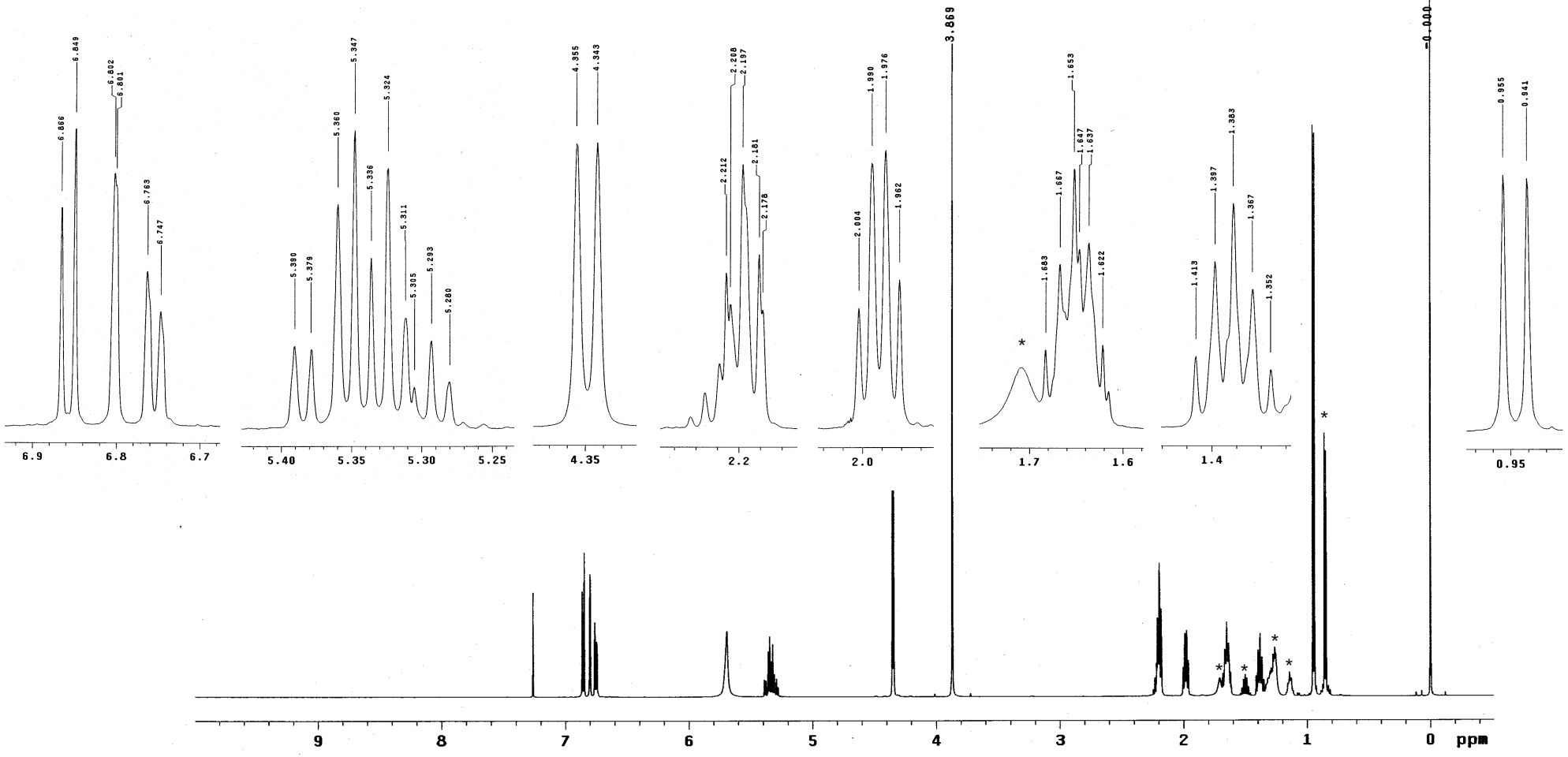
Contributor's name and address:	Verification Laboratory DSO National Laboratories 11 Stockport Road Singapore 117605
Secretariat identification code	25-3-0001r (p1/2)
Signature	
Chemical information:	
Chemical name	Capsaicin
Schedule number	
CAS registry number	404-86-4
Chemical structure with numbering of atoms	
Molecular formula	$C_{18}H_{27}NO_3$
Sample information:	
Sample purity	natural
Sample concentration	21 mg/mL
Solvent	$CDCl_3$
pH	-
Source	TCI (Tokyo Kasei)
Reference chemical shift	TMS (internal), 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	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 = 0.95, Hb = 2.21, Hc = 5.37, Hd = 5.31, He = 1.98, Hf = 1.38, Hg = 1.65, Hh = 2.20, Hi = 4.35 , Hj = 3.87, Hk = 6.80, Hl = 6.75, Hm = 6.86
Coupling constants (Hz)	J(a,b) = 6.73, J(b,c) = 5.93, J(c,d) = 15.39, J(d,e) = 6.09, J(g,h) = 7.69, J(l,m) = 8.01

Capsaicin ($C_{18}H_{27}NO_3$)

[404-86-4]

^{1}H NMR





Res.Freq: 499.662 MHz	Pulse width: 3.462 µs, 45°	**Nuc δ[ppm]**	**J[Hz]**	**Nuc δ[ppm]**	**J[Hz]**
Solvent: $CDCl_3$	Number of Scans: 16	a: 0.95	J(a,b) = 6.73	h: 2.20	
Temperature: 25°C	Line broadening: no	b: 2.21	J(b,c) = 5.93	i: 4.35	
Concentration: 21 mg/mL	Rep. time: 12 s	c: 5.37	J(c,d) = 15.39	j: 3.87	
Reference: TMS (internal)	Resolution: 0.3 Hz (TMS)	d: 5.31	J(d,e) = 6.09	k: 6.80	
Spectral Width: 5252.1 Hz	Baseline correction: Yes	e: 1.98		l: 6.75	J(l,m) = 8.01
Data points [FID]: 31480	Instrument: Varian INOVA 500	f : 1.38		m: 6.86	
Data points [Spectrum]: 32768		g: 1.65	J(g,h) = 7.69		