
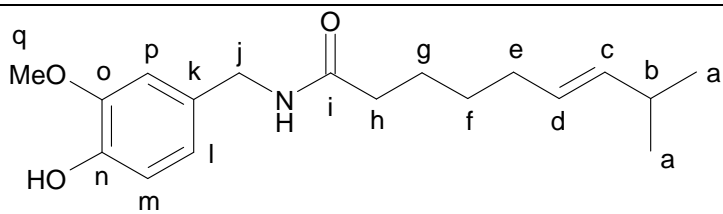
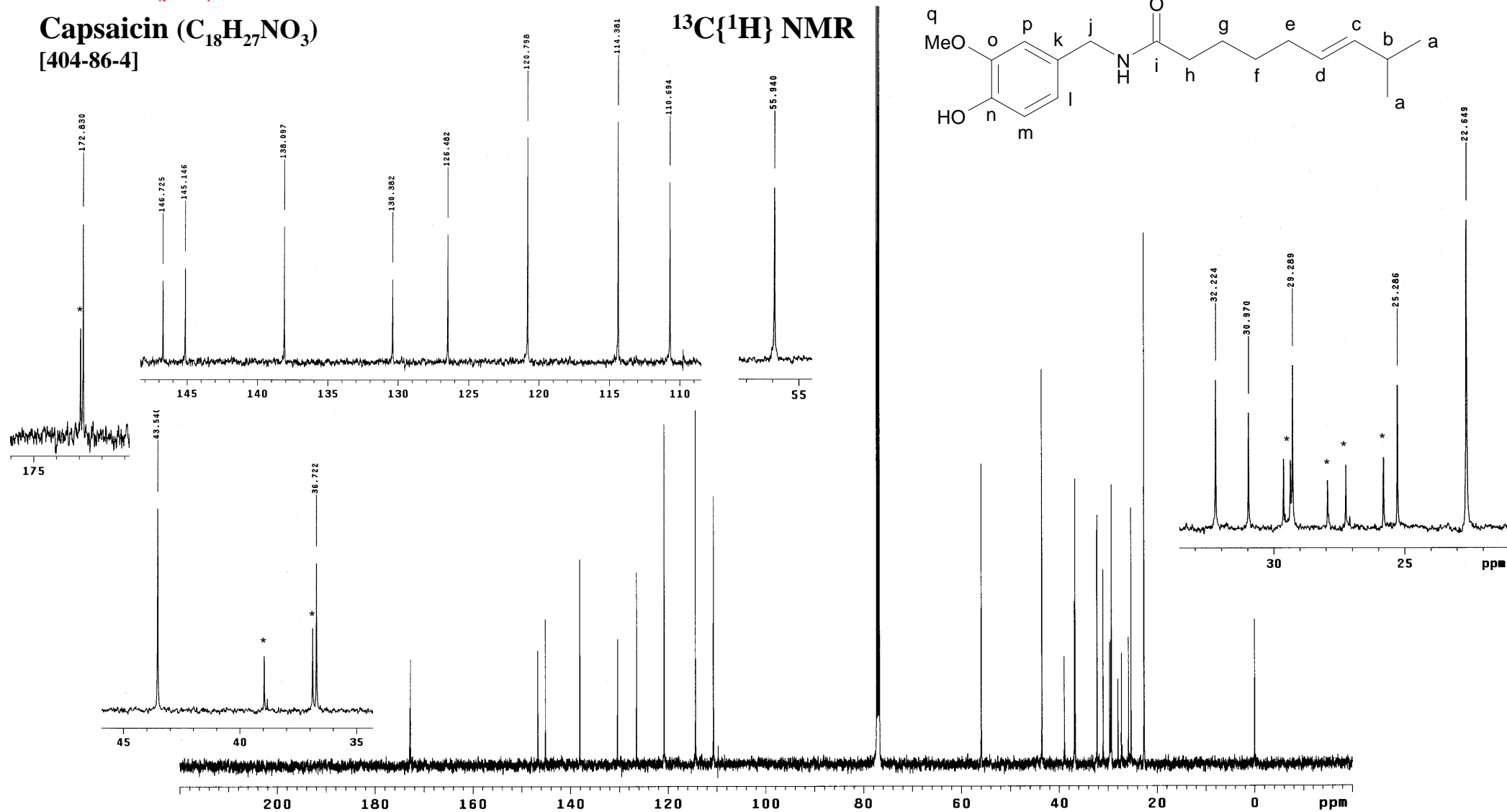


NMR SPECTROMETRY

Contributor's name and address:		Verification Laboratory
Secretariat identification code	25-3-0002r (p1/2)	DSO National Laboratories
Signature		11 Stockport Road
		Singapore 117605
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 (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)	4.125 μs, 45°	
Date of experiment	18 Apr 2005	
Data points in FID	35108	
Number of scans	720	
Baseline correction	Yes	
Spectral information:		
Chemical shifts (ppm) assigned except for acidic protons	Ca = 22.65, Cb = 30.97, Cc = 138.10, Cd = 126.48, Ce = 32.22, Cf = 29.29, Cg = 25.29, Ch = 36.72, Ci = 172.83, Cj = 43.54, Ck = 130.38, Cl = 120.80, Cm = 114.38, Cn = 146.72, Co = 145.14, Cp = 110.69, Cq = 55.94	
Coupling constants (Hz)	-	

Capsaicin (C₁₈H₂₇NO₃)
[404-86-4]



Res.Freq: 125.653 MHz

Solvent: CDCl₃

Temperature: 25°C

Concentration: 21 mg/mL

Reference: TMS (internal)

Spectral Width: 35133.9 Hz

Data points [FID]: 35108

Data points [Spectrum]: 65536

Pulse width: 4.125 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: 22.65

b: 30.97

c: 138.10

d: 126.48

e: 32.22

f: 29.29

Nuc δ[ppm]

g: 25.29

h: 36.72

i: 172.83

j: 43.54

k: 130.38

l: 120.80

Nuc δ[ppm]

m: 114.38

n: 146.72

o: 145.14

p: 110.69

q: 55.94