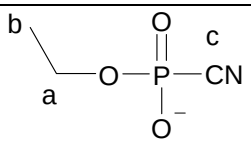
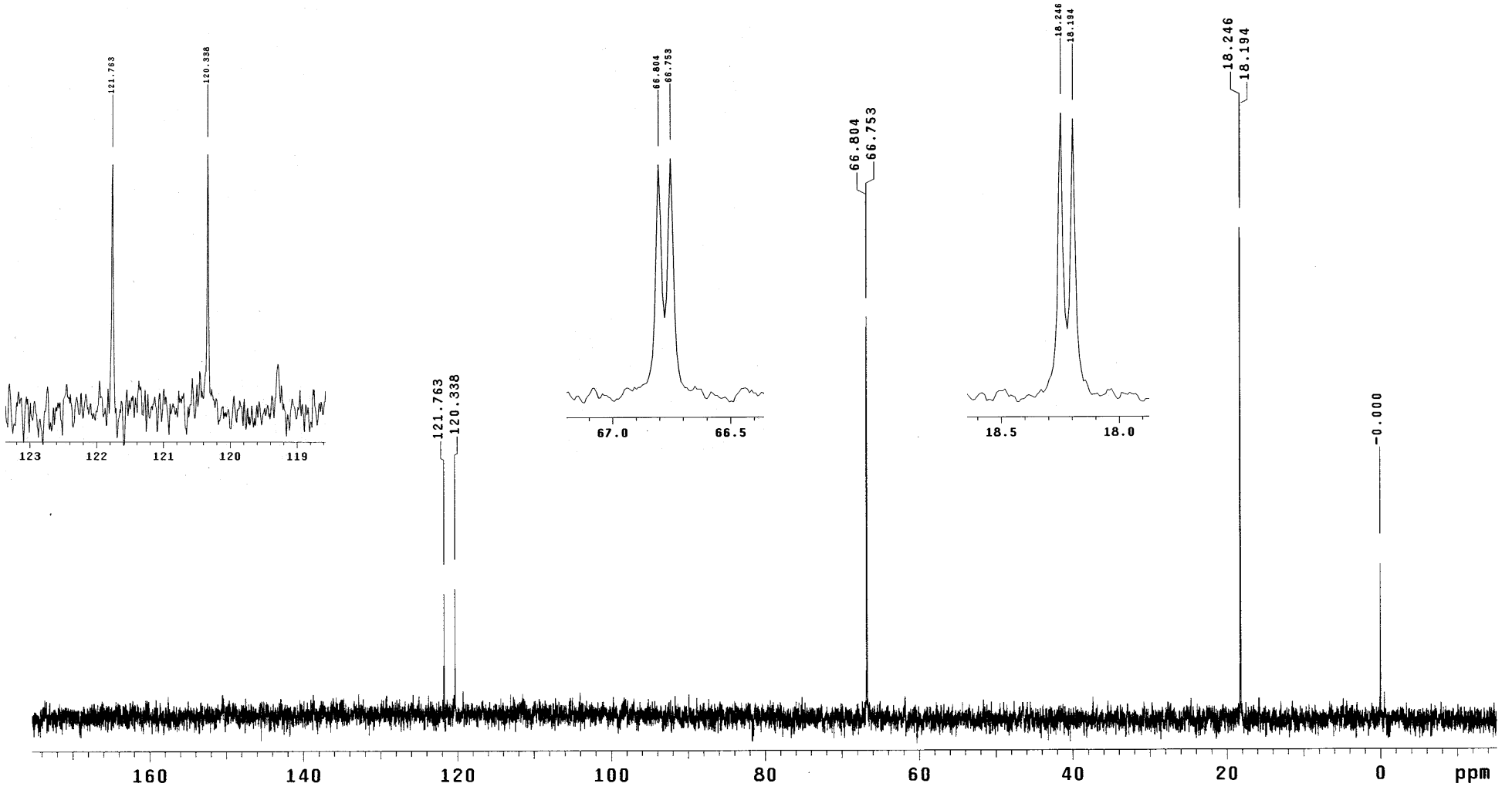
NMR SPECTROMETRY

Contributor's name and address:	Verification Laboratory DSO National Laboratories 11 Stockport Road Singapore 117605
Secretariat identification code	25-3-0010r (p1/2)
Signature	
Chemical information:	
Chemical name	Ethyl phosphorocyanidate
Schedule number	
CAS registry number	
Chemical structure with numbering of atoms	
Molecular formula	$C_3H_5NO_3P$
Sample information:	
Sample purity	96 %
Sample concentration	30 mg/mL
Solvent	D_2O
pH	8.32
Source	In-house synthesis YL30772
Reference chemical shift (internal)	3-(Trimethylsilyl)propionic acid, sodium salt, 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	$^{13}C\{^1H\}$
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	6 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 = 66.78, Cb = 18.22, Cc = 121.05
Coupling constants (Hz)	J(a,P) = 6.43, J(b,P) = 6.43, J(c,P) = 179.06

Ethyl phosphorocyanidate ($C_3H_5NO_3P$) $^{13}C\{^1H\}$ NMR



Res.Freq: 125.653 MHz
Solvent: D2O
Temperature: 25°C
Concentration: 30 mg/mL
pH: 8.32

Reference: Sodium 3-(Trimethyl silyl)propionic acid (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
Baseline correction: Yes
Instrument: Varian INOVA 500

Nuc	δ[ppm]	J[Hz]
a	66.78	J(a,P) = 6.43
b	18.22	J(b,P) = 6.43
c	121.05	J(c,P) = 179.06