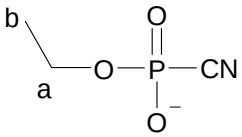
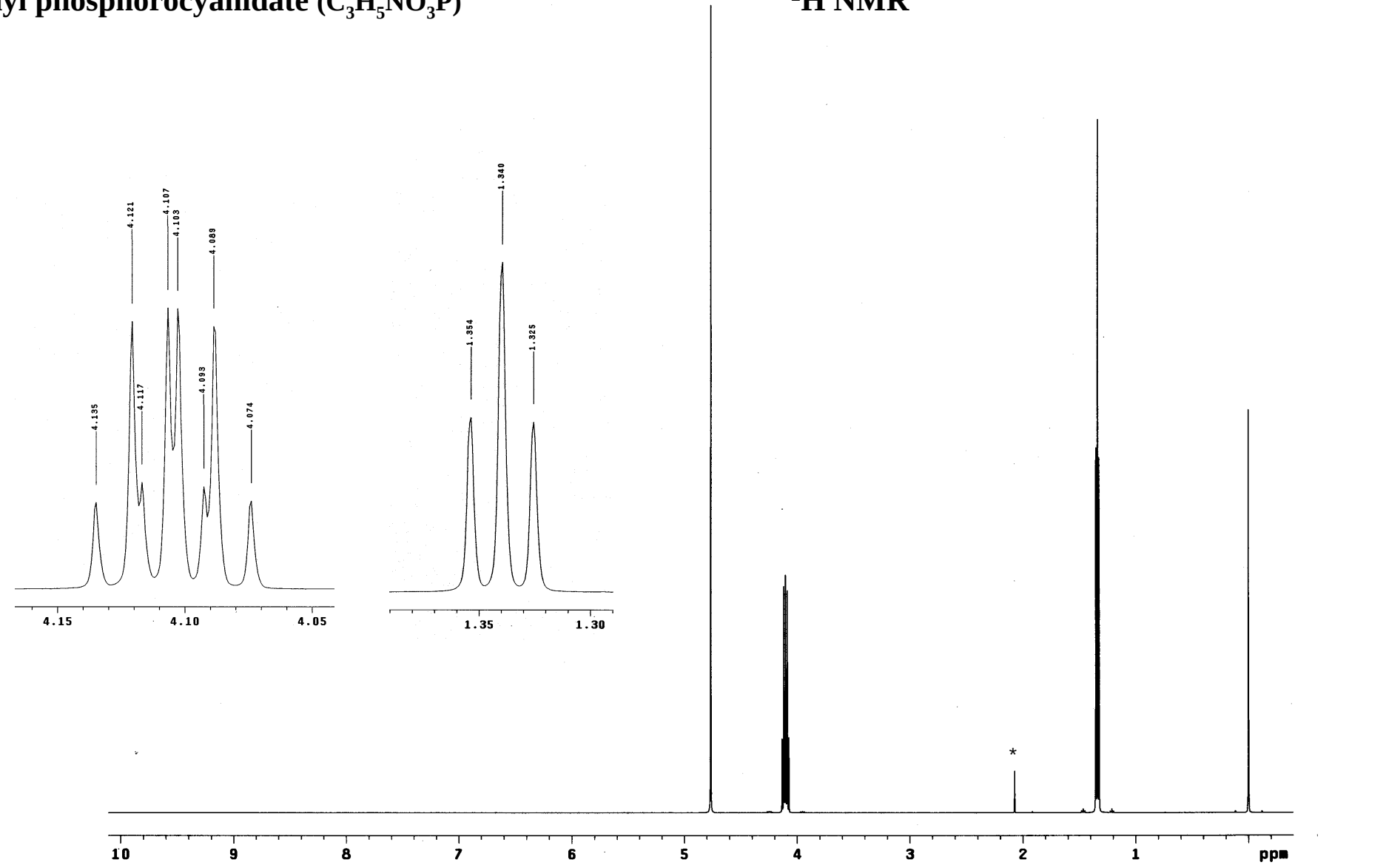
NMR SPECTROMETRY

Contributor's name and address:	Verification Laboratory DSO National Laboratories 11 Stockport Road Singapore 117605
Secretariat identification code	25-3-0009r (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	^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	6 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 = 4.11, Hb = 1.34
Coupling constants (Hz)	J(a,P) = 9.06, J(a,b) = 7.05

Ethyl phosphorocyanidate ($C_3H_5NO_3P$)

^{1}H NMR



Res.Freq: 499.662 MHz
Solvent: D_2O
Temperature: 25°C
Concentration: 30 mg/mL
pH: 8.32

Reference: Sodium 3-(Trimethyl silyl)propionic acid (internal)
Spectral Width: 5252.1 Hz
Data points [FID]: 31480
Data points [Spectrum]: 32768
Pulse width: 4.463 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]
a: 4.11	J(a,P) = 9.06
b: 1.34	J(a,b) = 7.05