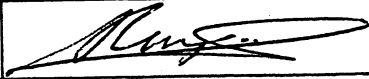
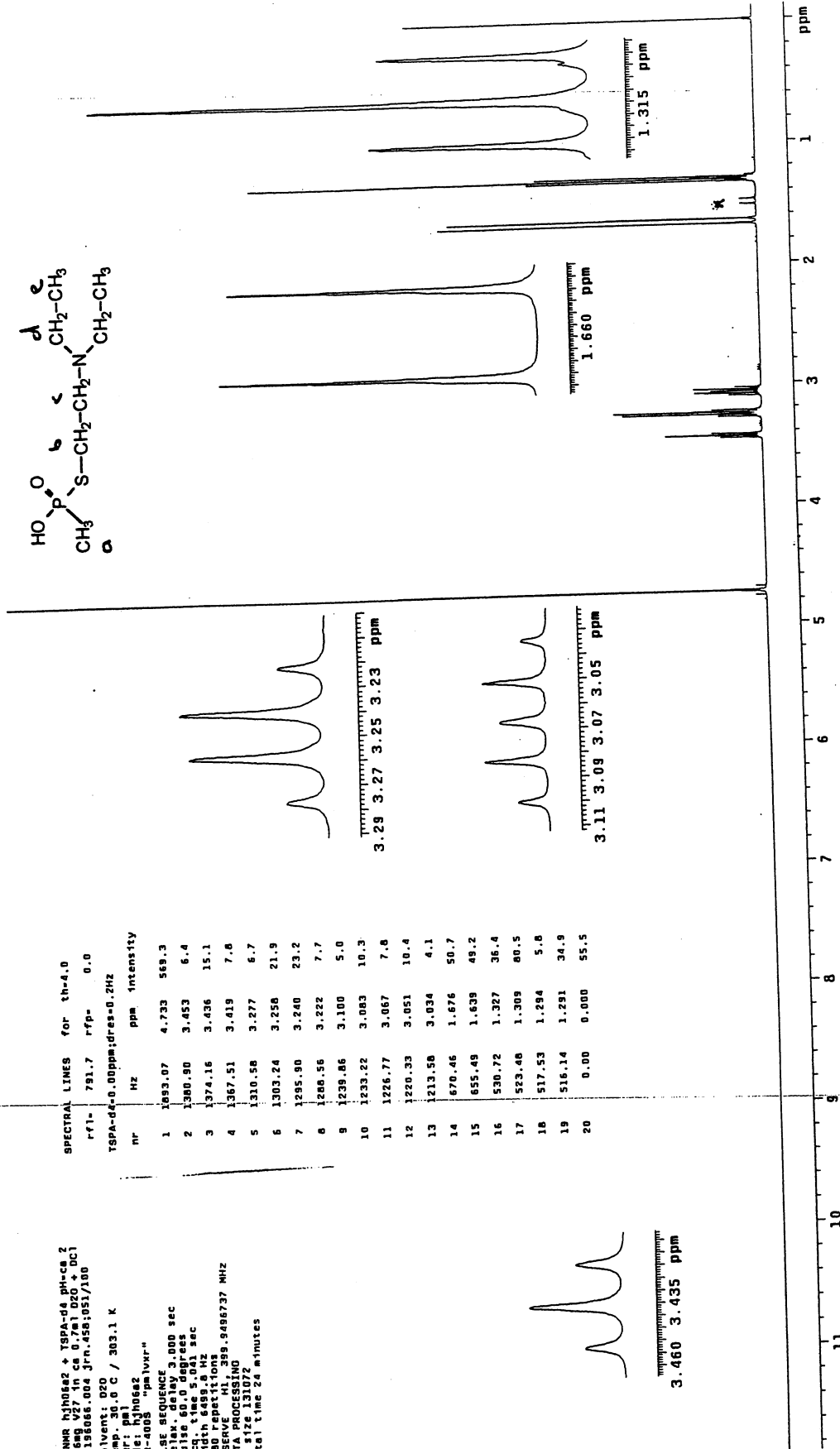
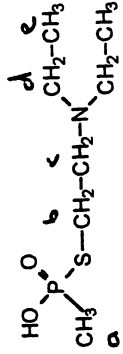


NMR SPECTROMETRY

Contributor's name and address:	S.H. van Krimpen TNO Prins Maurits Laboratory P.O. Box 45 2280 AA Rijswijk The Netherlands
Secretariat identification code	6-3-268
Signature	
Chemical information:	
Chemical name	S-2-diethylaminoethyl methylphosphonothiolate
CAS register number (optional)	
Chemical structure with numbering of atoms	see spectrum
Molecular formula (optional)	C7H18NO2PS
Sample information:	
Sample purity (optional)	
Sample concentration (optional)	17.6 mg/0.7ml
Solvent	D2O+DCI
pH (if relevant)	ca 2
Source (optional)	TNO-PML
Reference-chemical shift (internal/external)	TSPA-d4 internal
Instrument information:	
Manufacturer	Varian
Model	VXR-400S
Spectrometer frequency ¹ H	400
Data system (optional)	Sun OS
Software version (optional)	VNMR 5.1A
Experimental information:	
Nucleus measured	¹ H
Sample temperature	30 °C
Spectral width (Hz)	6499.8
Data points in Fourier transformed spectrum	128K
Repetition time (optional)	8 s
Pulse angle (µs and degrees) (optional)	16.4/60
Line width of a certain line (e.g. TMS) (optional)	0.2 Hz
Window function (e.g. line broadening) (optional)	not used
Date of experiment (optional)	7 August 96
Data points in FID (optional)	64K

1H-NMR INHRES2 & TSPA-d4 ph-ca 2
 314.466 V27 in ca 0.7ml D2O + DCI
 21419066.004 J-n.458;051/180
 solvent: D2O
 Temp: 30.0 C / 303.1 K
 User: h1hose2
 File: h1hose2
 VNR-4005 "pm1ver"
 PULSE SEQUENCE
 Relax. delay 3.000 sec
 Aq 9.00 sec
 Aq1sc 9.00 sec
 Width 6489.6 Hz
 180 Repeats:10
 OBSERVE HL 399.9486737 MHz
 PRG1: zgpg30
 PR2: 131372
 Total time 24 minutes

SPECTRAL LINES	for	th=4.0
rfl-	Hz	rfp= 0.0
TSPA-d4=0.00ppm;dr=0.2HZ		
nr	Hz	ppm intensity
1	1093.07	4.733 569.3
2	1380.90	3.453 6.4
3	1374.16	3.436 15.1
4	1367.51	3.419 7.8
5	1310.58	3.277 6.7
6	1303.24	3.250 21.9
7	1285.90	3.240 23.2
8	1286.56	3.222 7.7
9	1239.86	3.100 5.0
10	1233.22	3.083 10.3
11	1226.77	3.067 7.8
12	1220.39	3.051 10.4
13	1213.58	3.034 4.1
14	670.46	1.676 50.7
15	655.49	1.639 49.2
16	530.72	1.327 36.4
17	523.48	1.309 80.5
18	517.53	1.294 5.8
19	516.14	1.291 34.9
20	0.00	0.000 55.5



a: 1.66 ppm
 b: 3.07 ppm
 c: 3.44 ppm
 d: 3.25 ppm
 e: 1.31 ppm

J(cd): 6.7 Hz
 J(de): 7.3 Hz
 J(aP): 15.0 Hz
 J(bP): 12.9 Hz

S-2-diethylaminoethyl methylphosphonothiolate

Concentration 16.7 mg/0.7 ml D₂O + DCI
 Reference TSPA-d4 internal; resolution: 0.2 Hz
 pH= ca 2