

Org Lett

Triphenylphosphonium-Stoppered [2]Rotaxanes

Stuart J. Rowan, Stuart J. Cantrill and J. Fraser Stoddart*

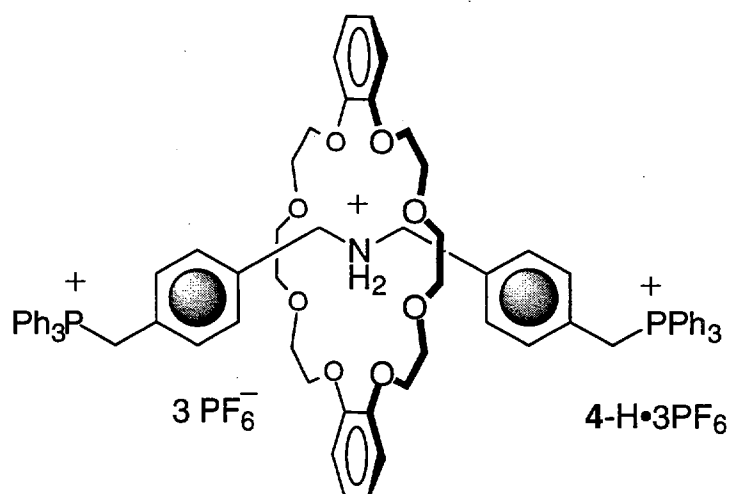
SUPPORTING INFORMATION:

^1H NMR spectra

^{13}C NMR spectra

For **4-H**·3PF₆, **5-H**·2PF₆, **8-H**·3PF₆ and **9-H**·2PF₆

SUPPORTING INFORMATION:



¹H NMR spectra

¹³C NMR spectra

Los Angeles (14th April 1999)

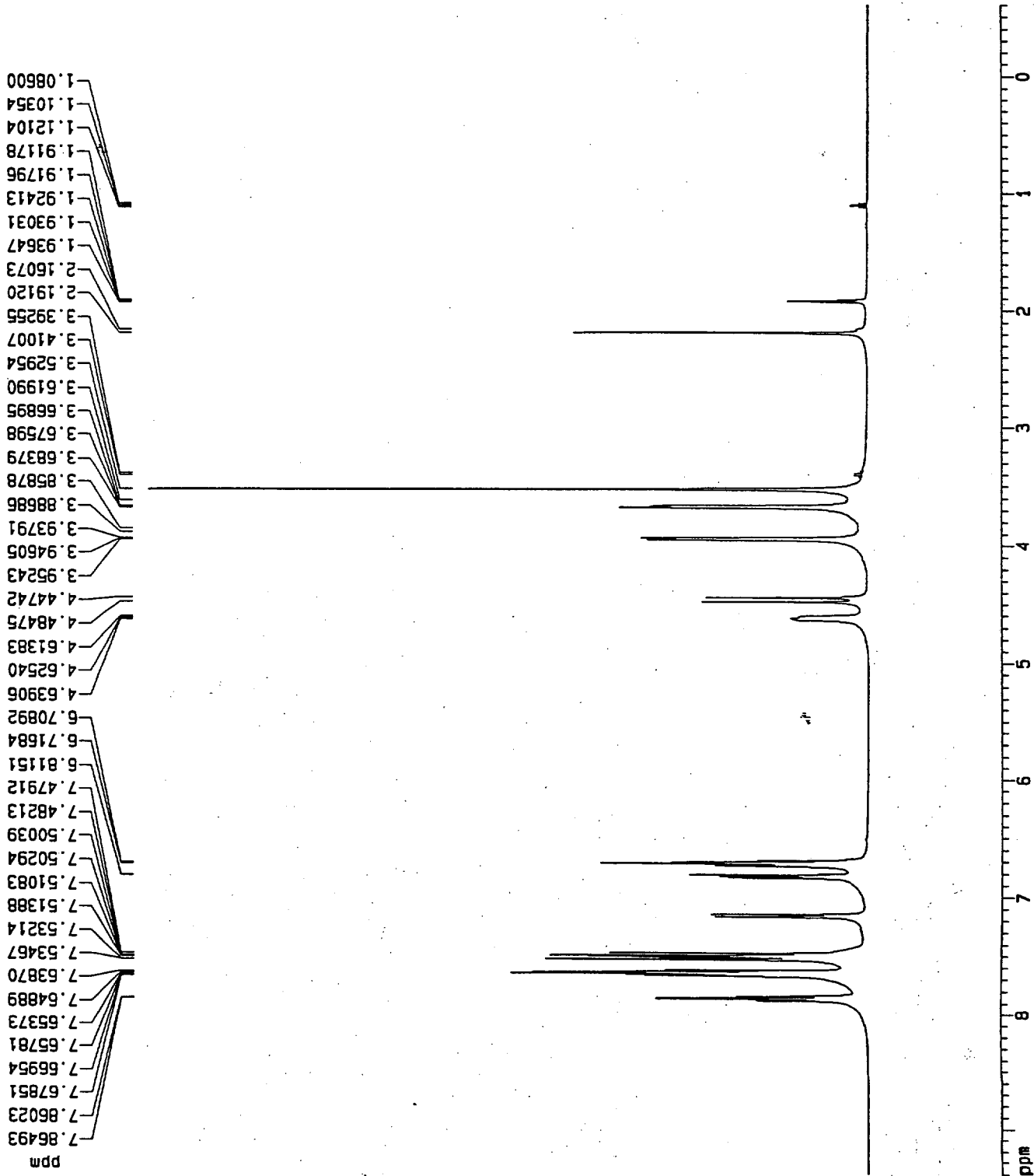
bis phos rotaxane

Current Data Parameters
 NAME bisphosrotaxC
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 990309
 Time 19.31
 INSTRUM arx400
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 PULPROG zg30
 TD 65536
 SOLVENT CD3CN
 NS 8
 DS 0
 SWH 8064.516 Hz
 FIDRES 0.123055 Hz
 AQ 4.0632820 sec
 RG 256
 DW 62.000 usec
 DE 88.57 usec
 TE 300.0 K
 D1 2.0000000 sec
 P1 8.25 usec
 SFO1 400.1324008 MHz
 NUCLEUS 1H

F2 - Processing parameters
 SI 65536
 SF 400.1300173 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 20.00 cm
 FIP 9.400 ppm
 F1 3761.22 Hz
 F2P -0.600 ppm
 F2 -240.08 Hz
 PPMCM 0.50000 ppm/cm
 HZCM 200.06500 Hz/cm



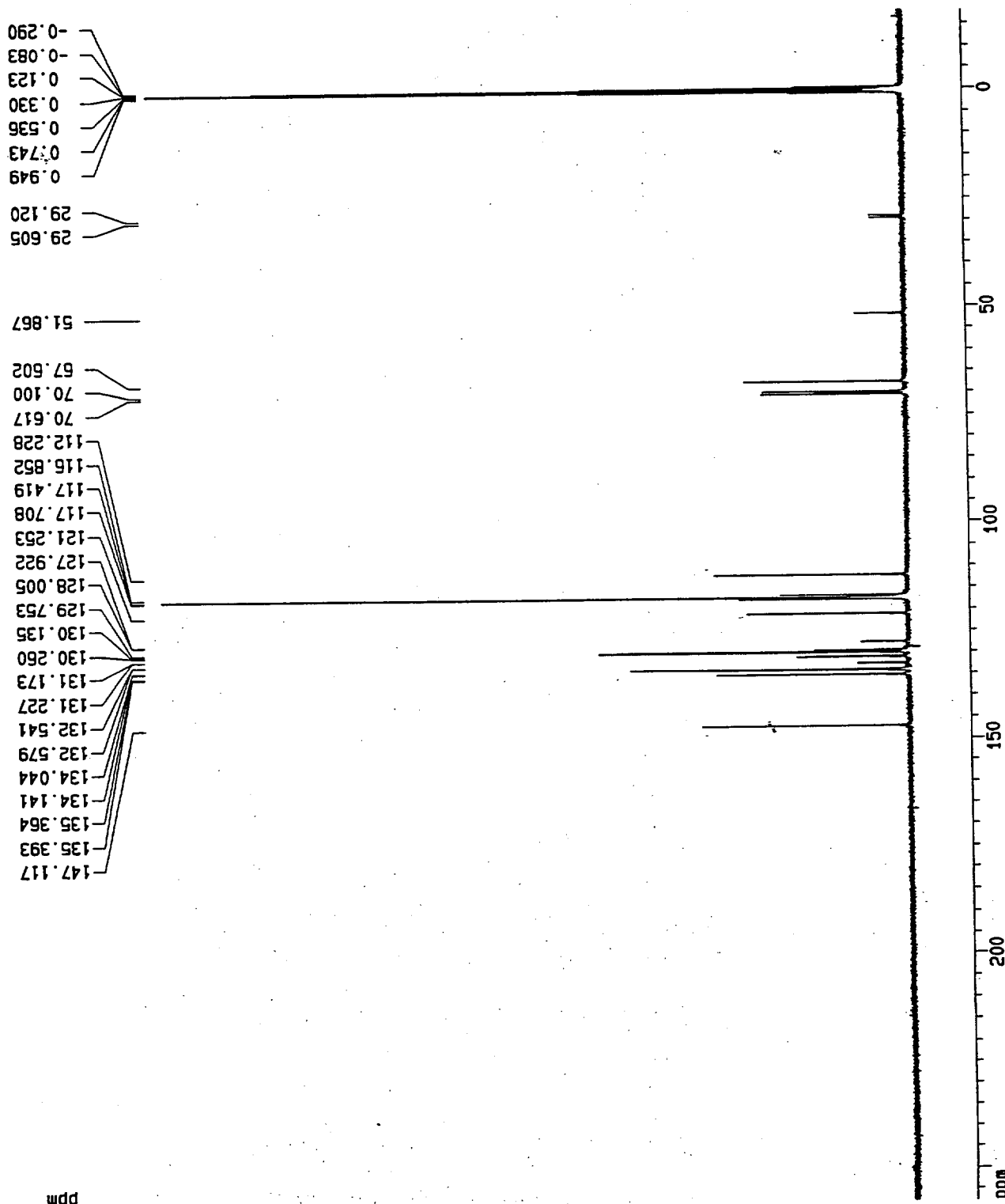
bisphos rotaxane

Current Date Parameters
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 PROCNO 1

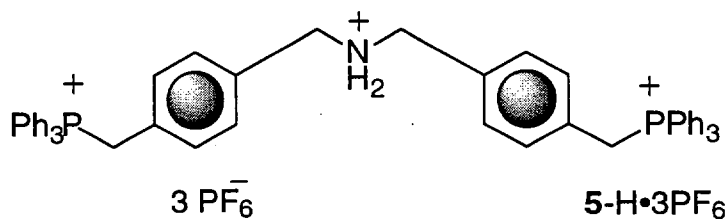
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 SOLVENT CD3CN
 NS 1400
 DS 0
 SMH 27777.777 Hz
 FIDRES 0.423855 Hz
 AQ 1.1796980 sec
 RG 32768
 DH 16.000 usec
 DE 25.71 usec
 TE 300.0 K
 D12 0.0000200 sec
 DL5 23.50 dB
 CPDPRG waltz16
 P31 100.00 usec
 P1 2.0000000 sec
 P1 6.25 usec
 SF01 100.6248445 MHz
 NUCLEUS 13C
 D11 0.0300000 sec

F2 - Processing parameters
 SI 65536
 SF 100.6127710 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 258.043 ppm
 F1 25962.42 Hz
 F2P -18.043 ppm
 F2 -1815.36 Hz
 PPMCH 13.80430 ppm/cm
 HZCM 1388.88679 Hz/cm



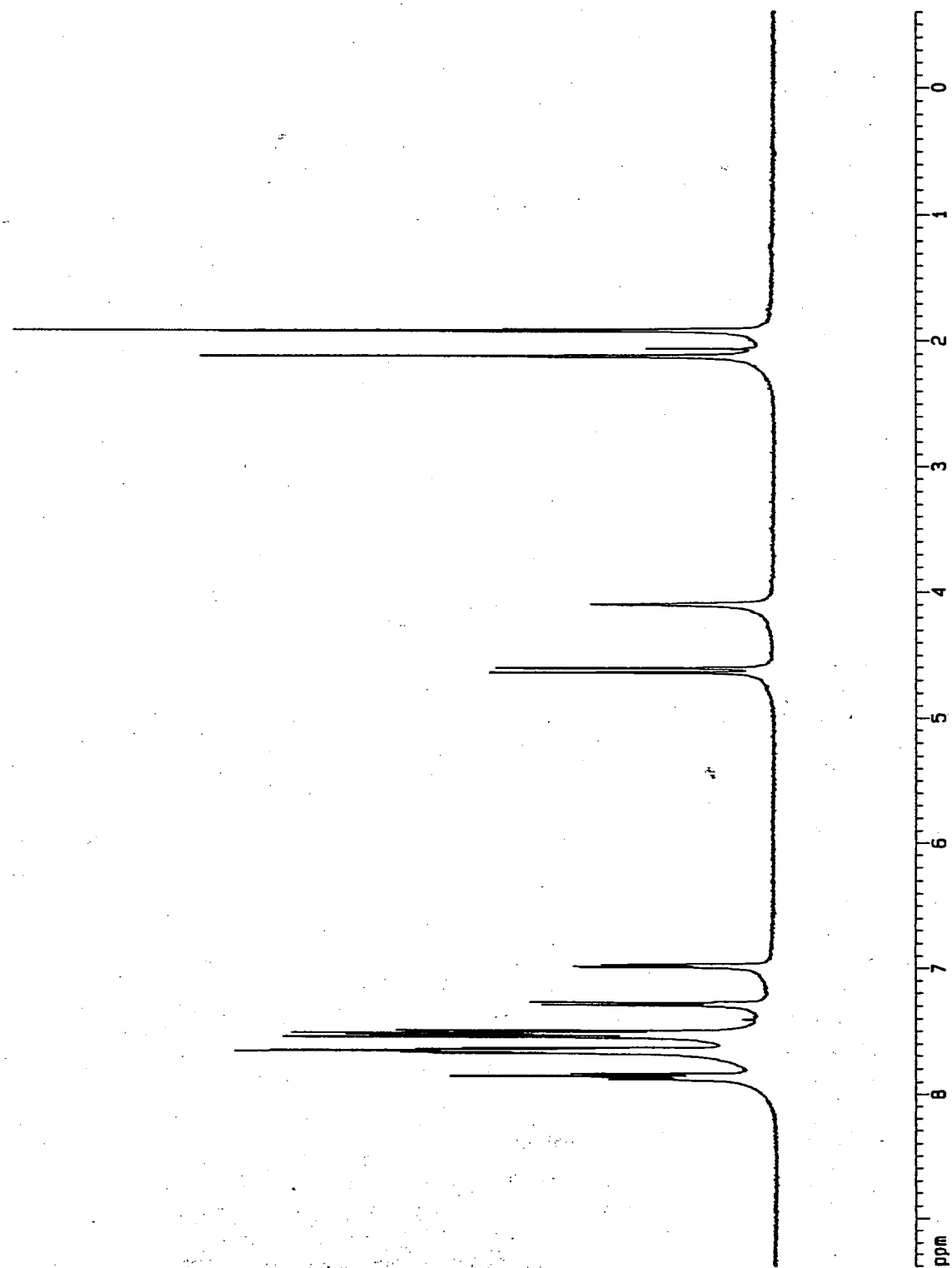
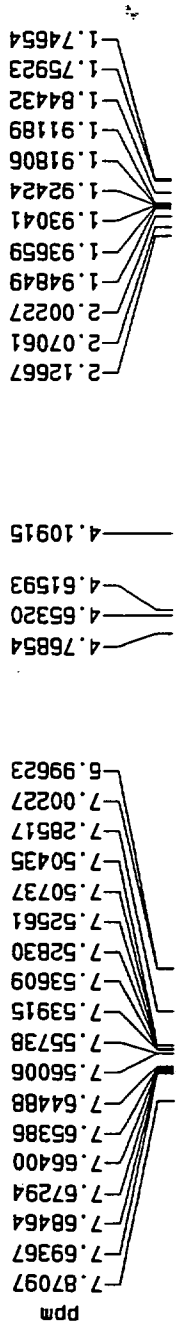
SUPPORTING INFORMATION:



^1H NMR spectra

^{13}C NMR spectra

bisphos thread in CD3CN



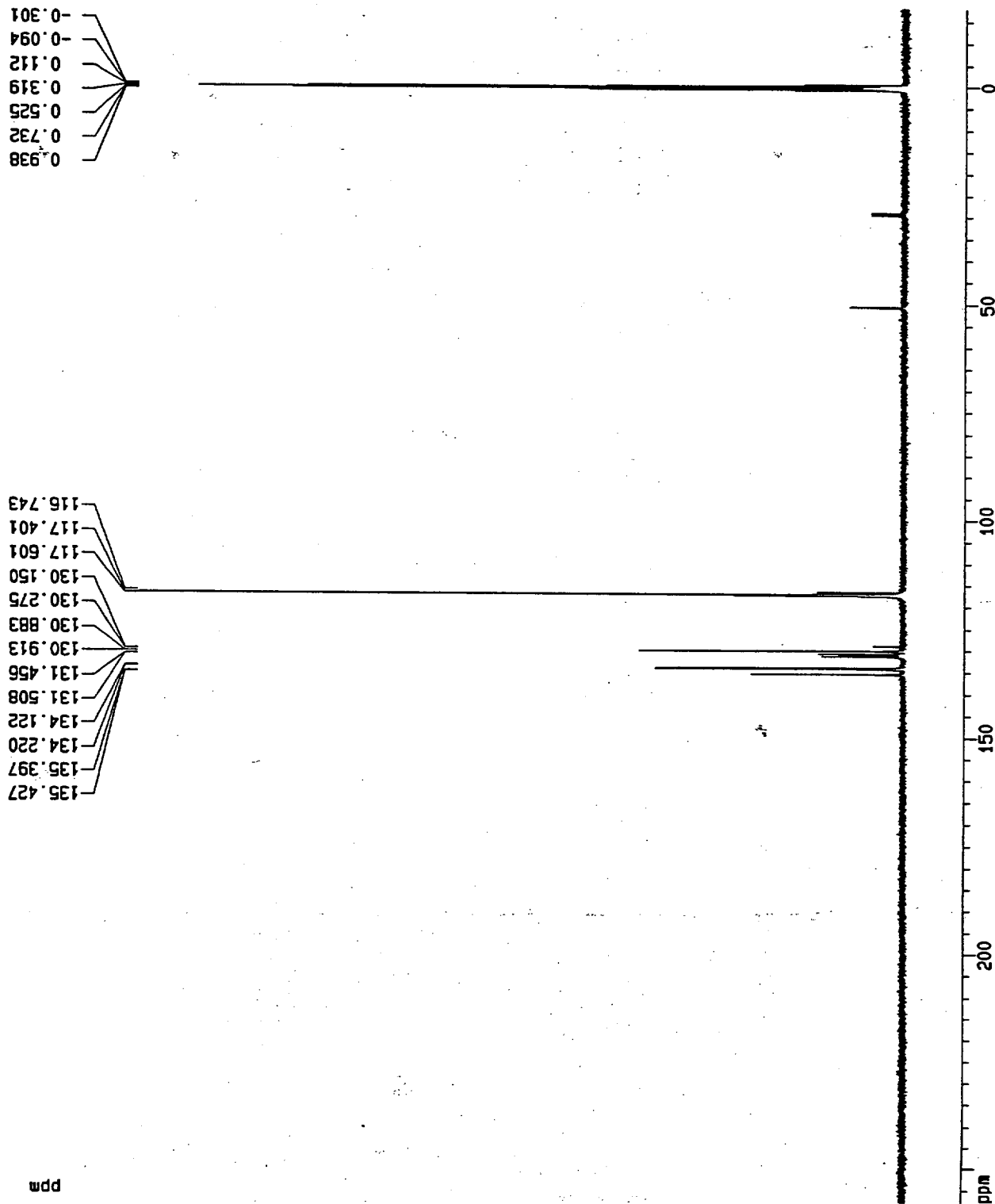
Current Data Parameters
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 PROCNO 1

F2 - Acquisition Parameters
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 Time 12:57
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 PULPROG zg30
 TD 65536
 SOLVENT CD3CN
 NS 16
 DS 0
 SMH 8064.516 Hz
 FIDRES 0.123055 Hz
 AQ 4.0632820 sec
 RG 4096
 DW 62.000 usec
 DE 88.57 usec
 TE 300.0 K
 D1 2.0000000 sec
 P1 8.25 usec
 SFO1 400.1324008 MHz
 NUCLEUS 1H

F2 - Processing parameters
 SI 65536
 SF 400.1300173 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 9.400 ppm
 F1 3761.22 Hz
 F2P -0.600 ppm
 F2 -240.08 Hz
 PPMCM 0.50000 ppm/cm
 HZCM 200.06500 Hz/cm

bis phos thread



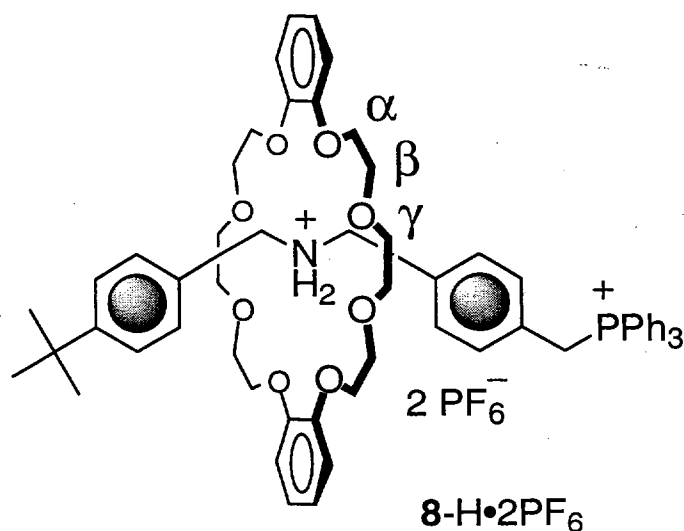
Current Data Parameters
 NAME BisphosthreadC
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
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 PULPROG zgpg30
 TD 65536
 SOLVENT CD3CN
 NS 1000
 DS 0
 SWH 2777.777 Hz
 FIDRES 0.423855 Hz
 AQ 1.179690 sec
 RG 32768
 DH 18.000 usec
 DE 25.71 usec
 TE 300.0 K
 D12 0.0000200 sec
 DL5 23.50 dB
 CPDPRG waltz16
 P31 100.00 usec
 D1 2.0000000 sec
 P1 6.25 usec
 SF01 100.6248445 MHz
 NUCLEUS 13C
 D11 0.0300000 sec

F2 - Processing parameters
 SI 65536
 SF 100.6127710 MHz
 HDW EM
 SS8 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 258.043 ppm
 F1 25962.42 Hz
 F2 -18.043 ppm
 F2 -1915.36 Hz
 PPMCM 13.80430 ppm/cm
 HZCM 1388.88879 Hz/cm

SUPPORTING INFORMATION:



¹H NMR spectra

¹³C NMR spectra

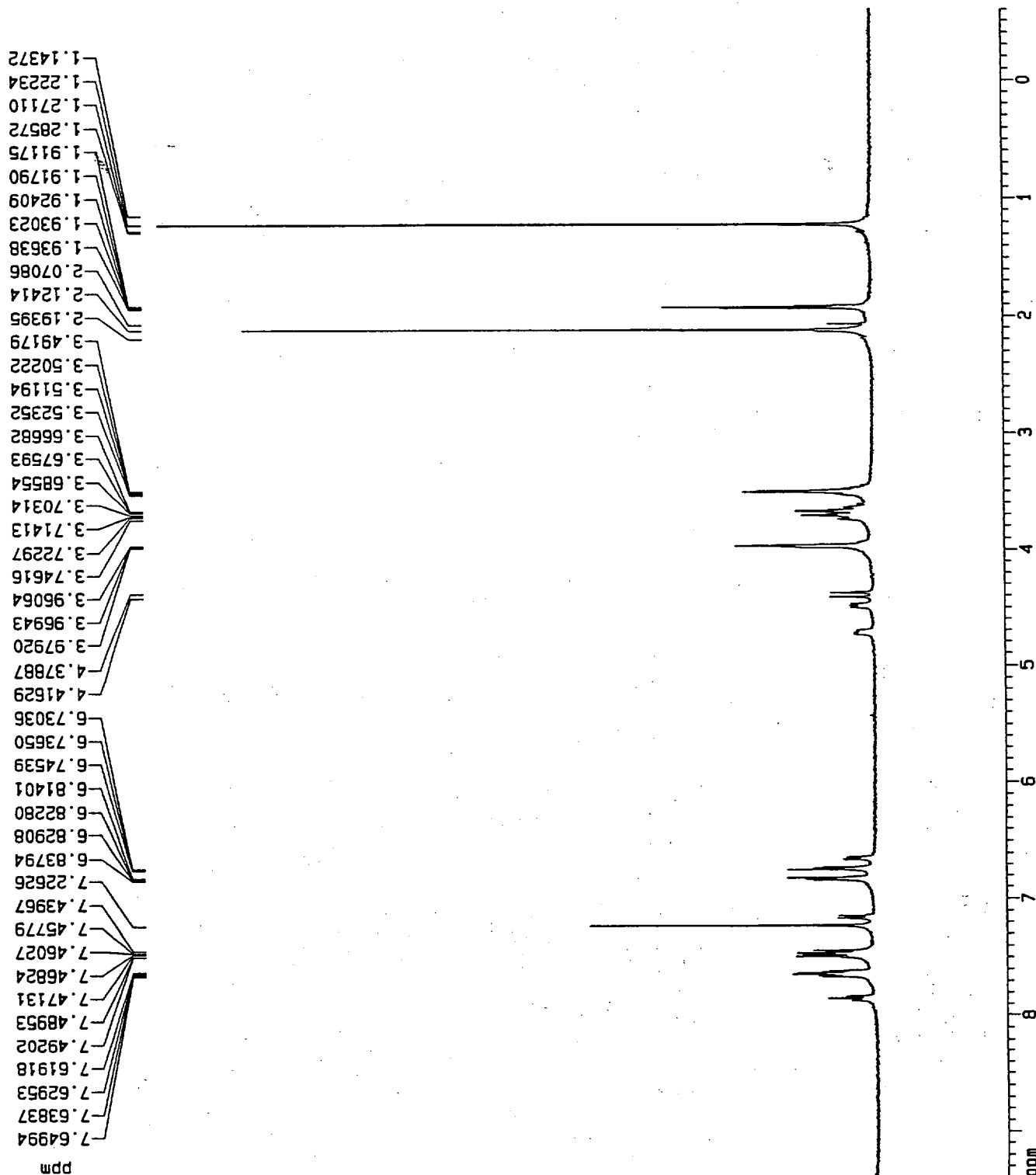
monphos rotax 24C8 in CD3CN

Current Data Parameters
 NAME monphosrot24c
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 PROCNO 1

F2 - Acquisition Parameters
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 Time 14.25
 INSTRUM arx400
 PROBHD 5 mm QNP 1H
 PULPROG zg30
 TD 65536
 SOLVENT CD3CN
 NS 16
 DS 0
 SWH 8064.516 Hz
 FIDRES 0.123055 Hz
 AQ 4.0632820 sec
 RG 2048
 DW 62.000 usec
 DE 88.57 usec
 TE 300.0 K
 D1 2.0000000 sec
 P1 8.25 usec
 SFO1 400.1324008 MHz
 NUCLEUS 1H

F2 - Processing parameters
 SI 65536
 SF 400.1300173 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 9.400 ppm
 F1 3761.22 Hz
 F2P -0.600 ppm
 F2 -240.08 Hz
 PPMCM 0.50000 ppm/cm
 HZCM 200.06500 Hz/cm



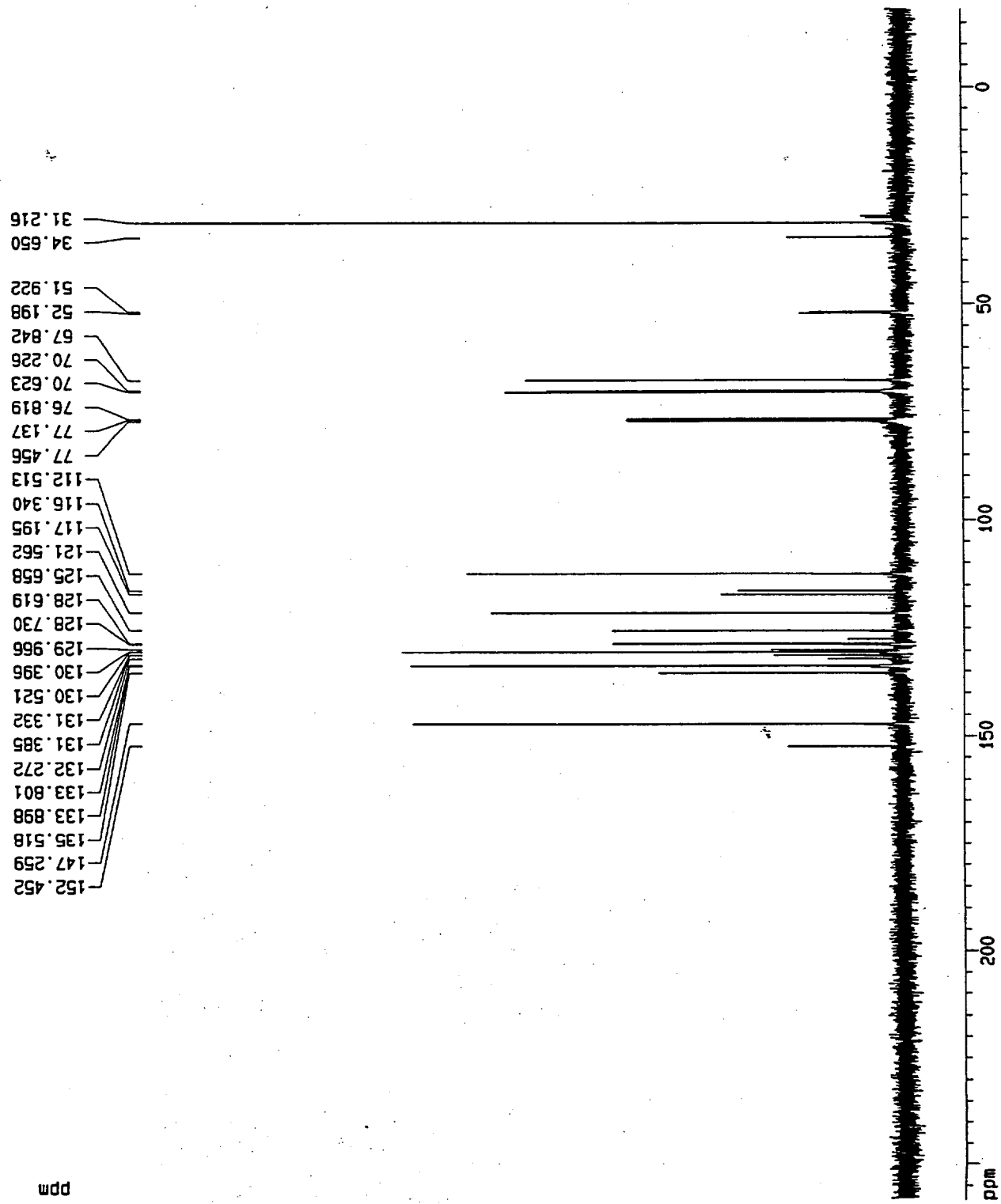
monophos rotaxane

Current Data Parameters
 NAME Monophosrotax
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 990313
 Time 16.21
 INSTRUM arx400
 PROBHD 5 mm QNP 1H
 PULPROG zgpg
 TD 65536
 SOLVENT CDCl3
 NS 200
 DS 0
 SMH 27777.777 Hz
 FIDRES 0.423855 Hz
 AQ 1.1796980 sec
 RG 32768
 DM 18.000 usec
 DE 25.71 usec
 TE 300.0 K
 D12 0.0000200 sec
 DL5 23.50 dB
 CPDPRG waltz16
 P31 100.00 usec
 D1 2.0000000 sec
 P1 6.25 usec
 SF01 100.6248445 MHz
 NUCLEUS 13C
 D11 0.0300000 sec

F2 - Processing parameters
 SI 65536
 SF 100.6127710 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 258.043 ppm
 F1 25962.42 Hz
 F2P -18.043 ppm
 F2 -1815.36 Hz
 PPRCM 13.80430 ppm/cm
 HZCM 1388.88879 Hz/cm



mono phos rotax HMQC

Current Data Parameter
 NAME Monophosrotax
 EXPNO 3
 PROCNO 1

F2 - Acquisition Paramet

Date_ 990313
 Time 15.10
 INSTRUM nvt400
 PROBRD 5 mm QNP 1H
 PULPROG zgpg30
 TD 1024
 SOLVENT CDCl3
 NS 16
 DS 16
 SS 4000.000 MHz
 SFO1 3.906250 MHz
 FIDRES 0.1280000 sec
 AQ 90
 RG 90
 DM 125.000 uSFC
 DE 158.25 uSFC
 TE 300.0 K
 CNSTZ 135.0000000
 D1 0.2980010 sec
 D11 0.0300000 sec
 P1 8.25 uSFC
 P2 0.0037037 sec
 D2 1.00 dB
 D3 15.90 uSFC
 P3 12.90 uSFC
 F4 100.622652 MHz
 SFO2 13C
 DECNOC 0.22750001 sec
 D7 6.25 uSFC
 P3 0.0000030 sec
 D13 0.0000040 sec
 D15 23.60 dB
 SFO1 400.1320226 MHz
 NUCLEUS 1H
 CPDPRG gprp
 P31 90.00 uSFC
 L3 128
 INO 0.00002495 sec

F1 - Acquisition paramet

NO 2
 TD 256
 SFO1 100.6229 MHz
 FIDRES 79.611610 Hz
 SN 200.000 ppm

F2 - Processing paramet

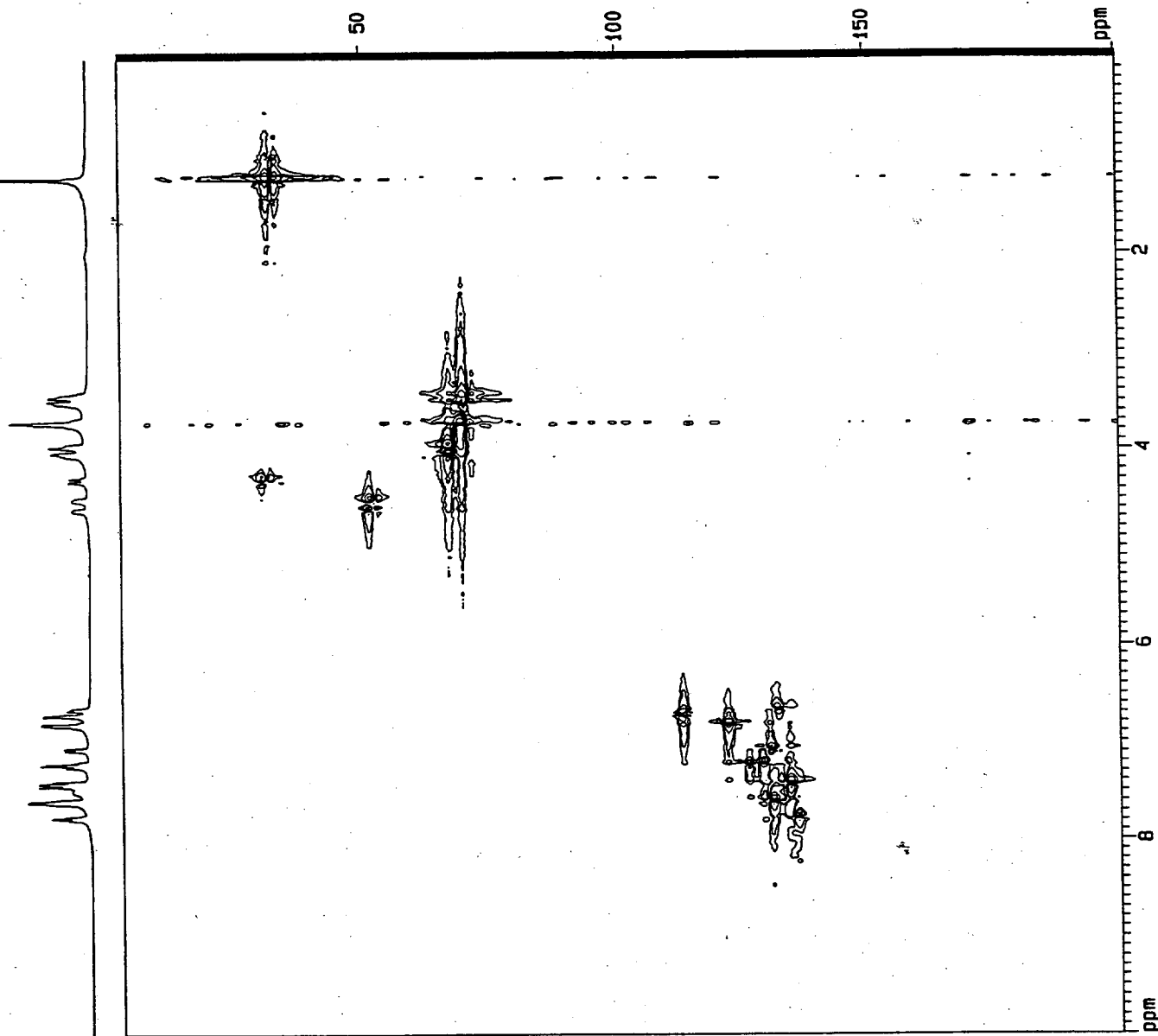
SI 1024
 SF 400.1300173 MHz
 DSINE 2
 LB 0.00 Hz
 GB 0
 PC 1.00

F1 - Processing paramet

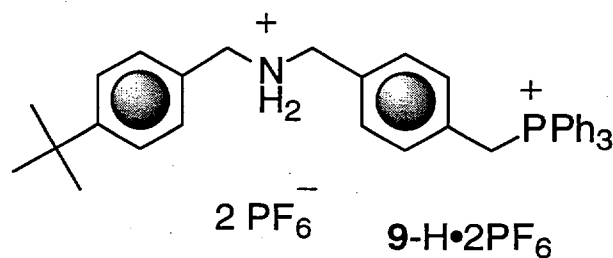
SI 512
 MC2 Steles-TPP1
 SF 100.6127710 MHz
 DSINE 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameter

CR2 15.00 cm
 CK1 15.00 cm
 F2PLO 10.010 ppm
 F2LO 4005.33 Hz
 F2PHI 0.004 ppm
 F2HI 1.43 Hz
 F1PLO 200.336 ppm
 F1LO 20156.83 Hz
 F1PHI 1.000 ppm
 F1HI 400.81 Hz
 F1PHI 0.56710 ppm/c1
 F2PPOH 2661.92708 Hz/c1
 F2PHI 131.26518 ppm/c1
 F1PPOH 1337.06128 Hz/c1



SUPPORTING INFORMATION:

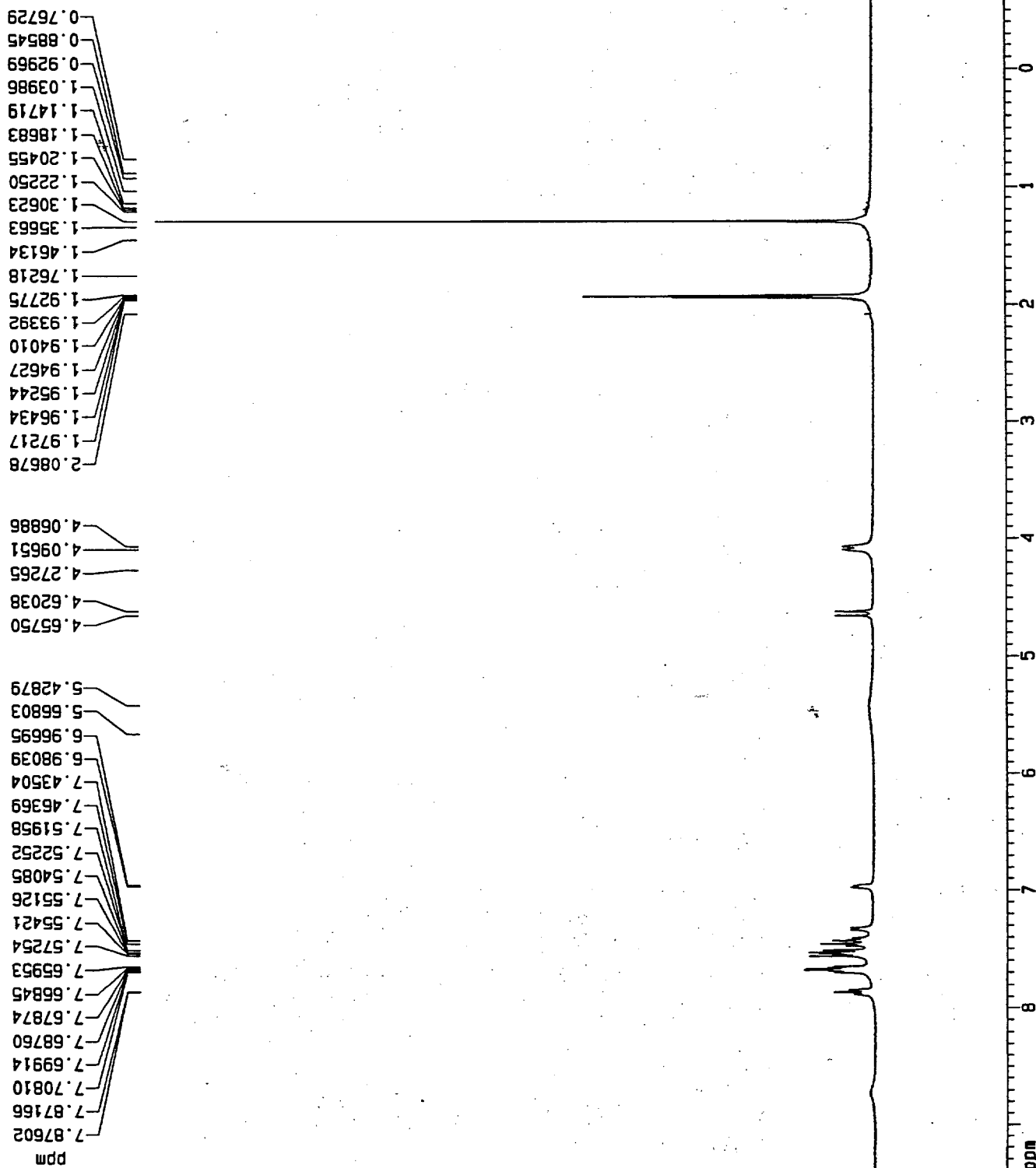


^1H NMR spectra

^{13}C NMR spectra

Los Angeles (14th April 1999)

monophos thread in CD3CN



Current Data Parameters
 NAME monophosthread
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 990210
 Time 19.34
 INSTRUM arx400
 PROBHD 5 mm QNP 1H
 PULPROG zg30
 TO 65536
 SOLVENT CD3CN
 NS 16
 OS 0
 SMH 8064.516 Hz
 FIDRES 0.123055 Hz
 AQ 4.0632820 sec
 RG 8192
 DM 62.000 usec
 DE 88.57 usec
 TE 300.0 K
 D1 2.0000000 sec
 P1 8.25 usec
 SFO1 400.132408 MHz
 NUCLEUS 1H

F2 - Processing parameters
 SI 65536
 SF 400.1300109 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 9.400 ppm
 F1 3761.22 Hz
 F2P -0.600 ppm
 F2 -240.08 Hz
 PPMCM 0.50000 ppm/cm
 HZCM 200.06500 Hz/cm

