

Electronic Supplementary Information

Design, Synthesis and Biological evaluation of 1-(Fluoroalkylidene)-1,1-bisphosphonic Acids against *Trypanosoma cruzi*

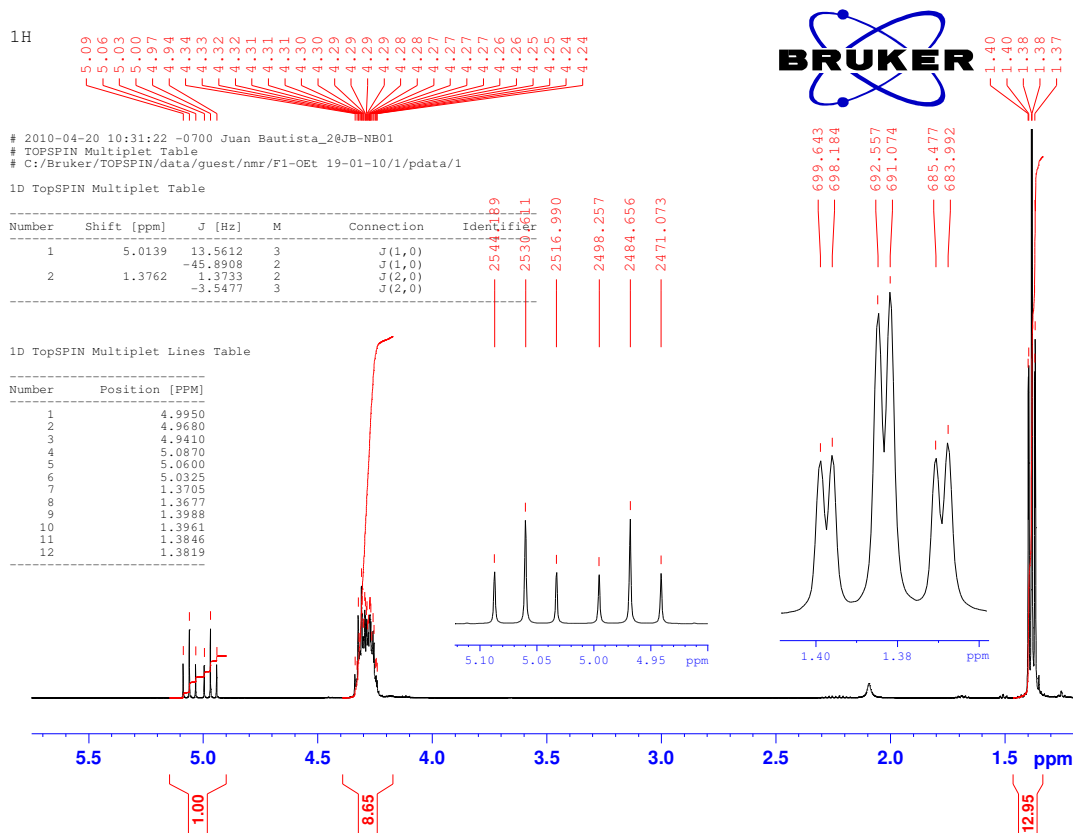
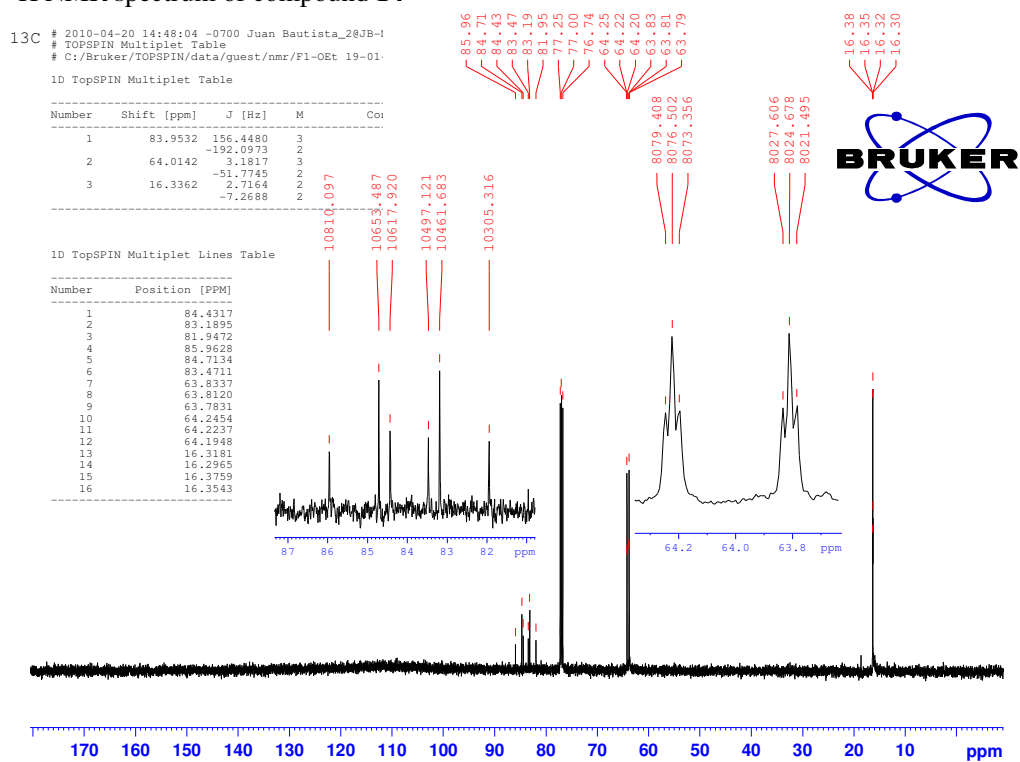
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¹H NMR spectrum of compound 14¹³C NMR spectrum of compound 14

31P F1-(OEt)3



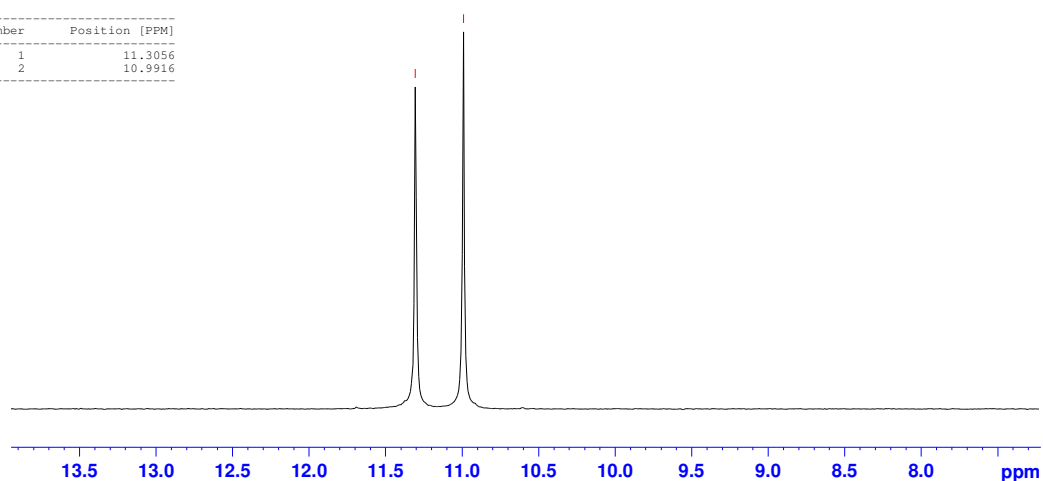
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Number	Position [PPM]
1	11.3056
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³¹P NMR spectrum of compound 14

PMA120-1H

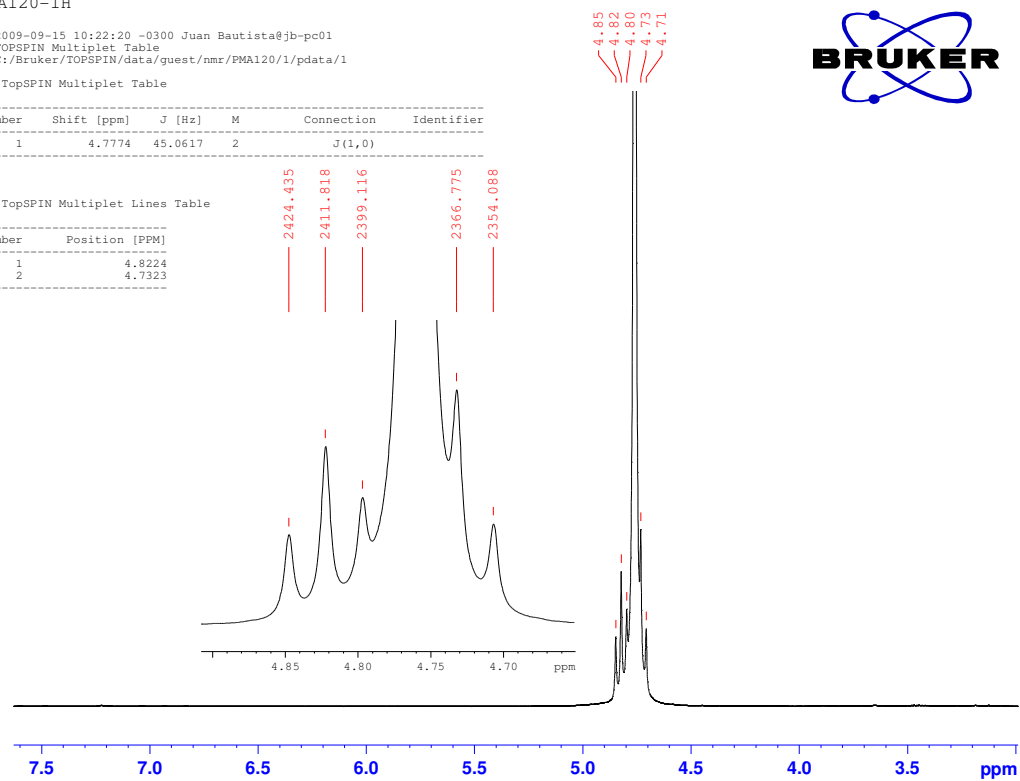
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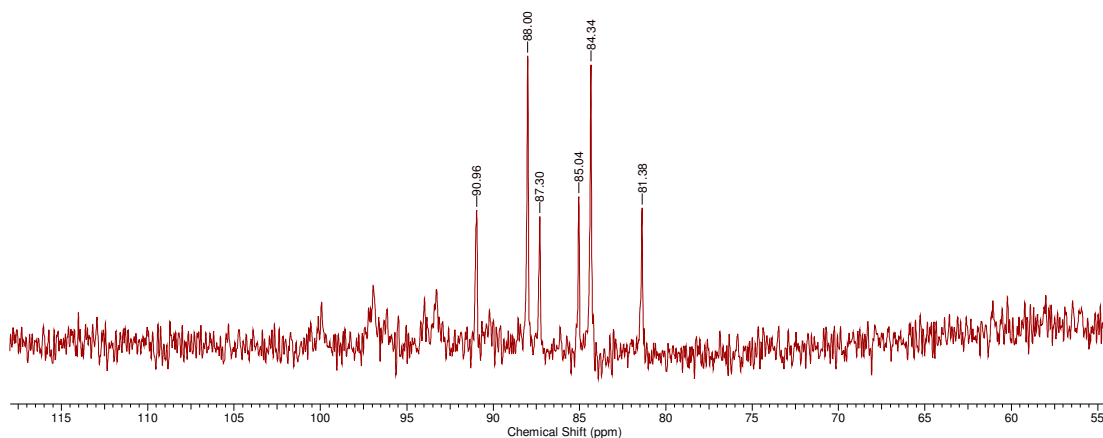
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1	4.7774	45.0617	2		J(1,0)

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1	4.8224
2	4.7323

¹H NMR spectrum of compound 35

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3	85.04	4279.8	0.0126
4	87.30	4393.6	0.0108
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6	90.96	4577.9	0.0114

¹³C NMR spectrum of compound 35

PMA120-P31

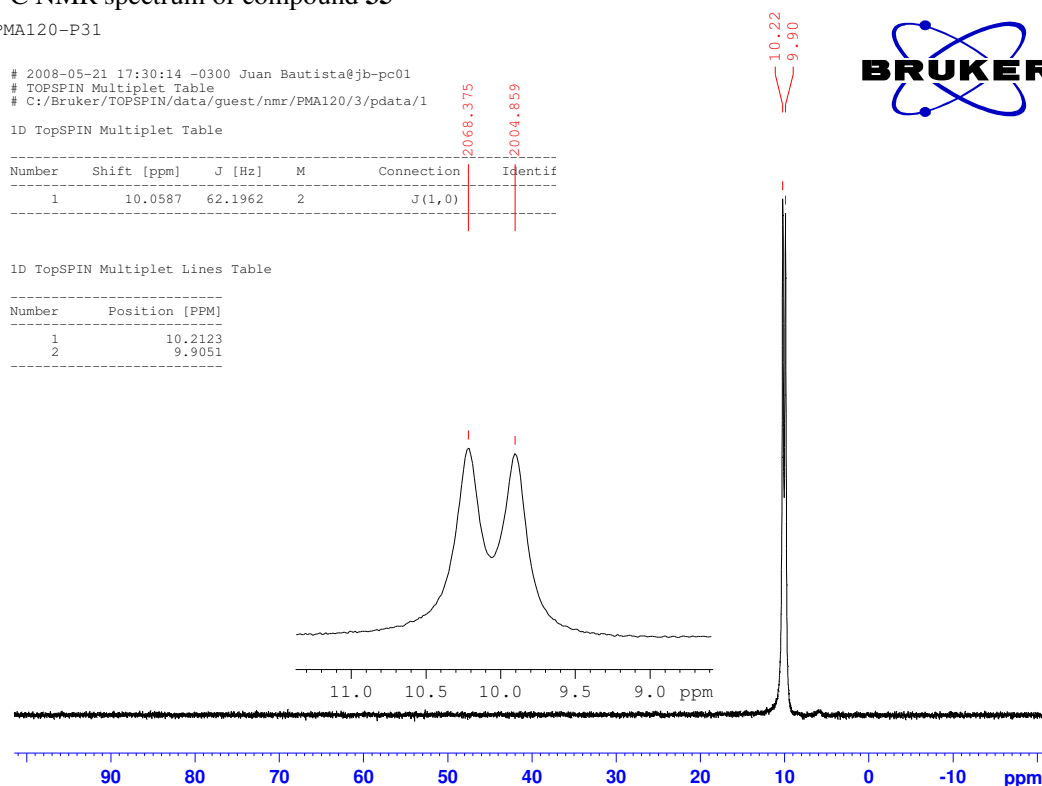
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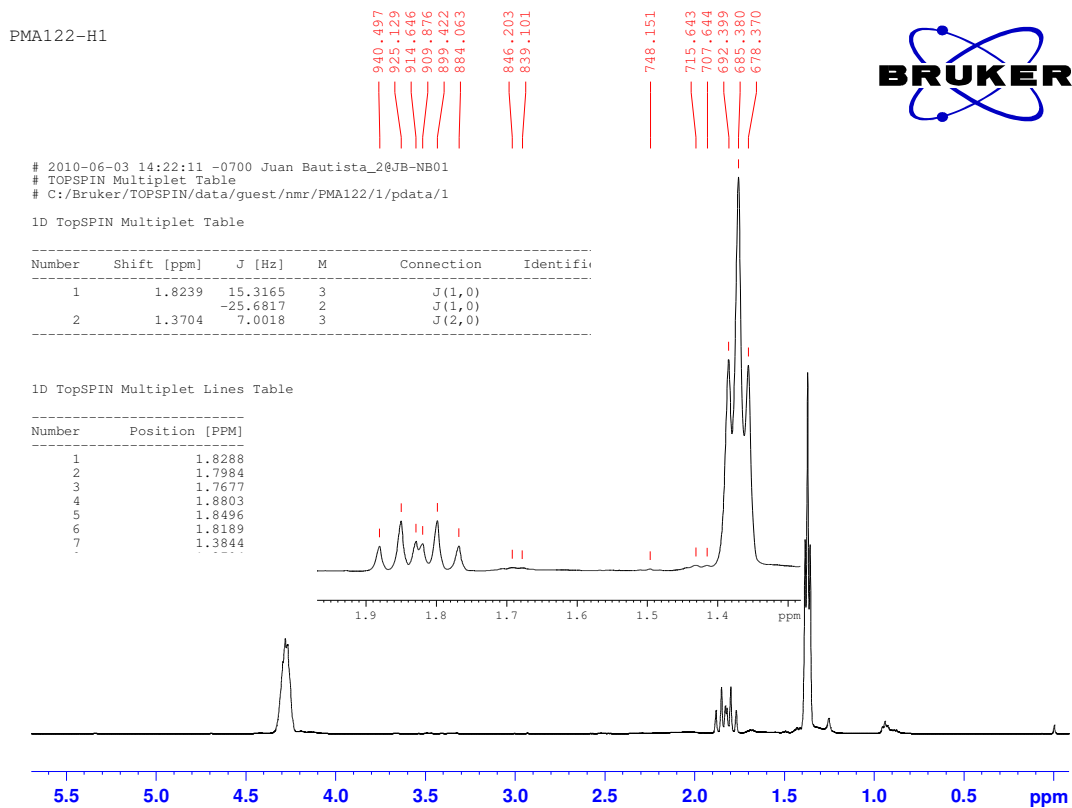
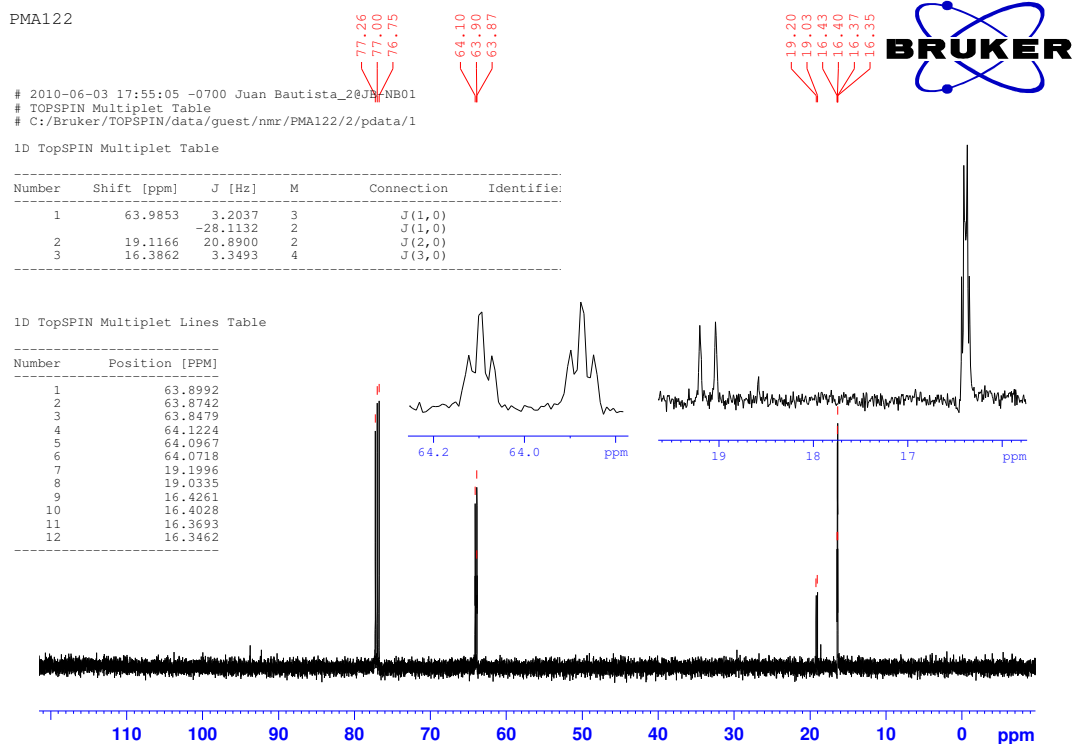
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1	10.0587	62.1962	2	J(1,0)	

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³¹P NMR spectrum of compound 35

¹H NMR spectrum of compound 26¹³C NMR spectrum of compound 26

PMA122-31P



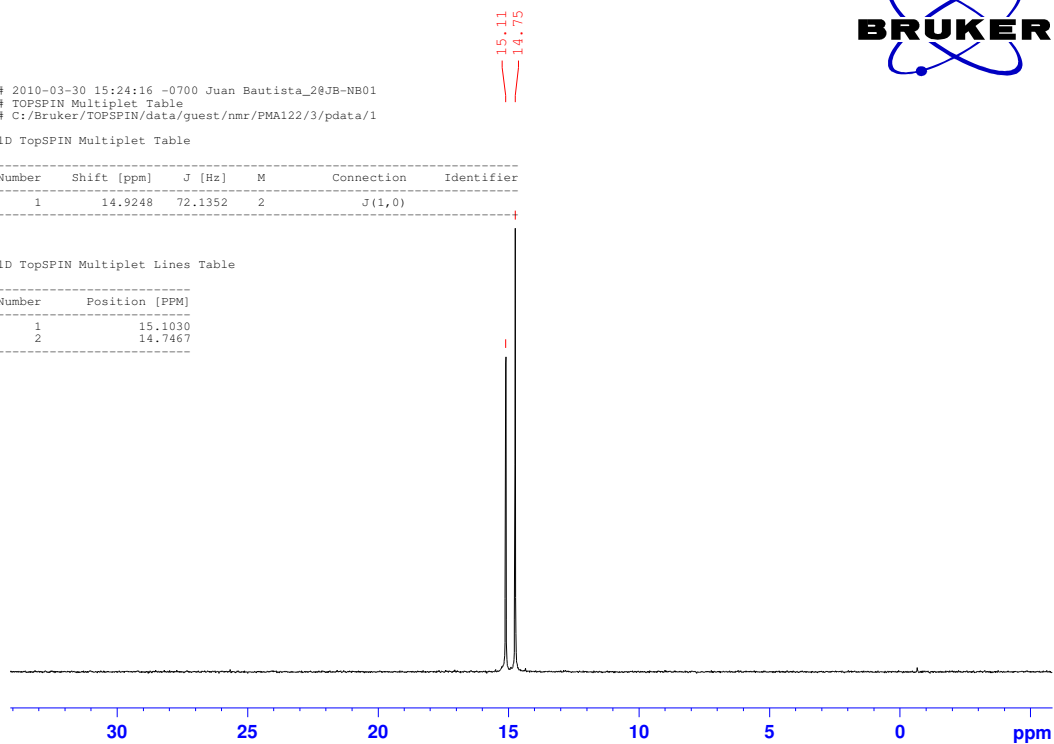
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1	14.9248	72.1352	2	J(1,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	15.1030
2	14.7467

 ^{31}P NMR spectrum of compound **26**

1H

1.71
1.68
1.66
1.66
1.63
1.60



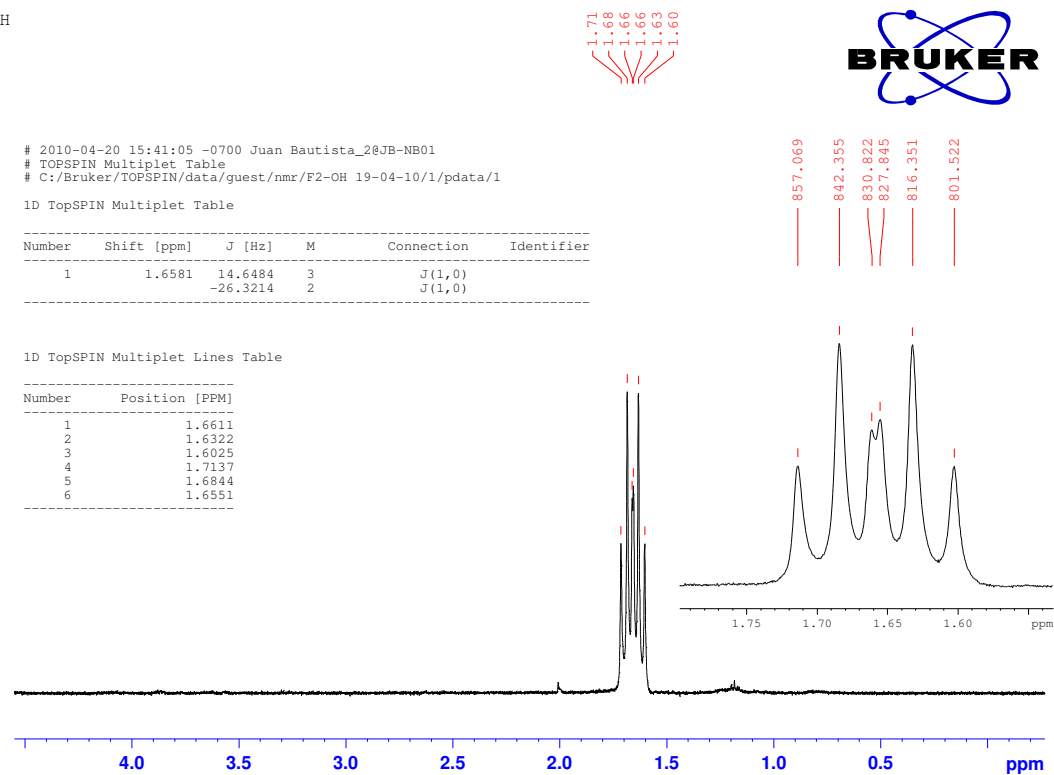
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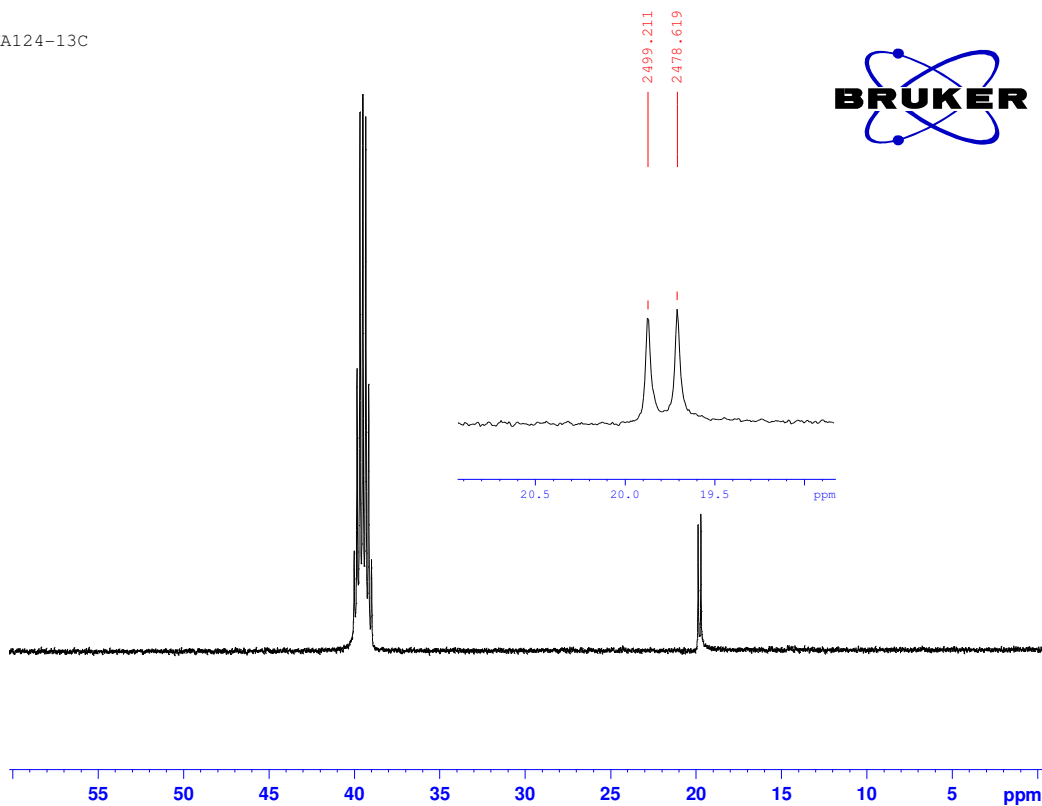
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1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	1.6611
2	1.6322
3	1.6025
4	1.7137
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6	1.6551

 ^1H NMR spectrum of compound **36**

PMA124-13C

¹³C NMR spectrum of compound **36**

PMA124-31P

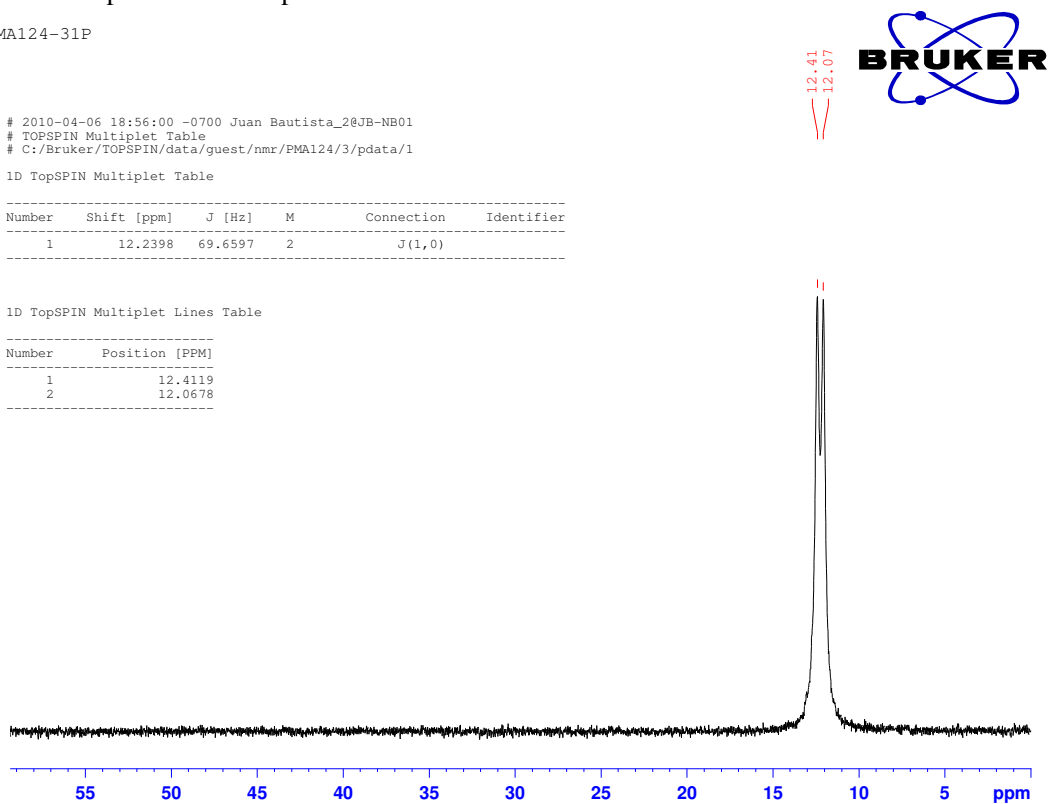
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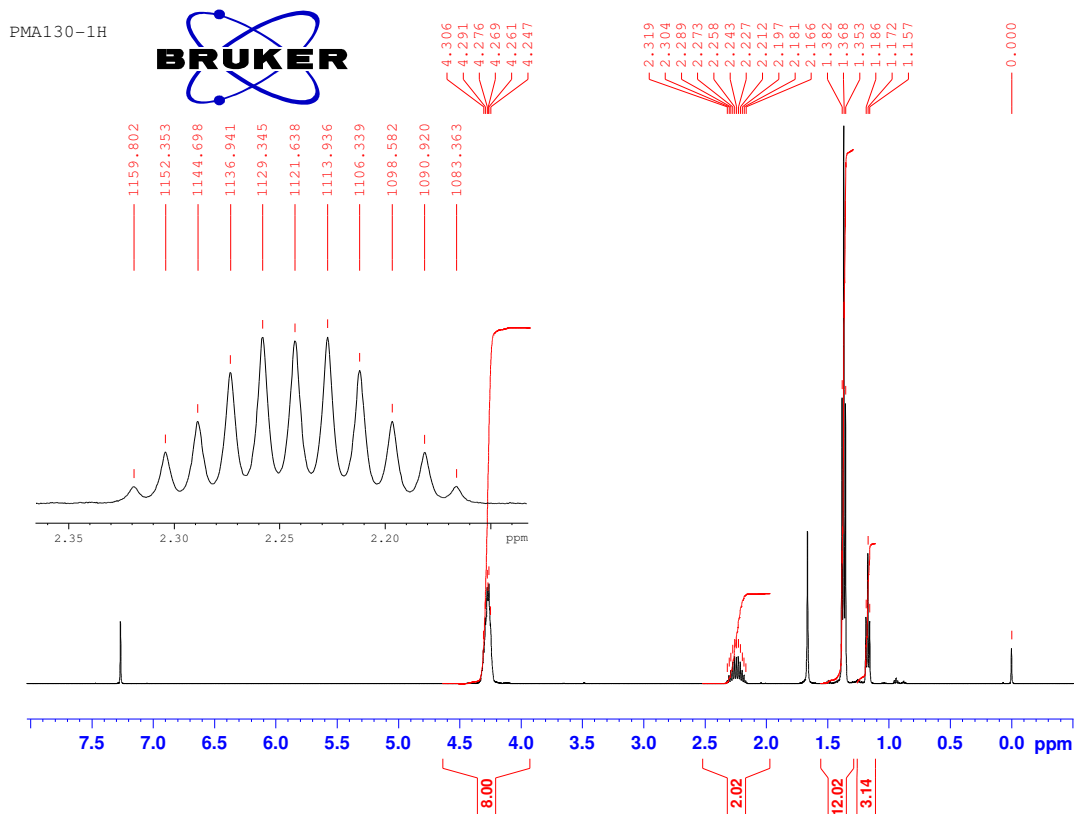
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1D TopSPIN Multiplet Lines Table

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2	12.0678

³¹P NMR spectrum of compound **36**

¹H NMR spectrum of compound 27

PMA130-13C

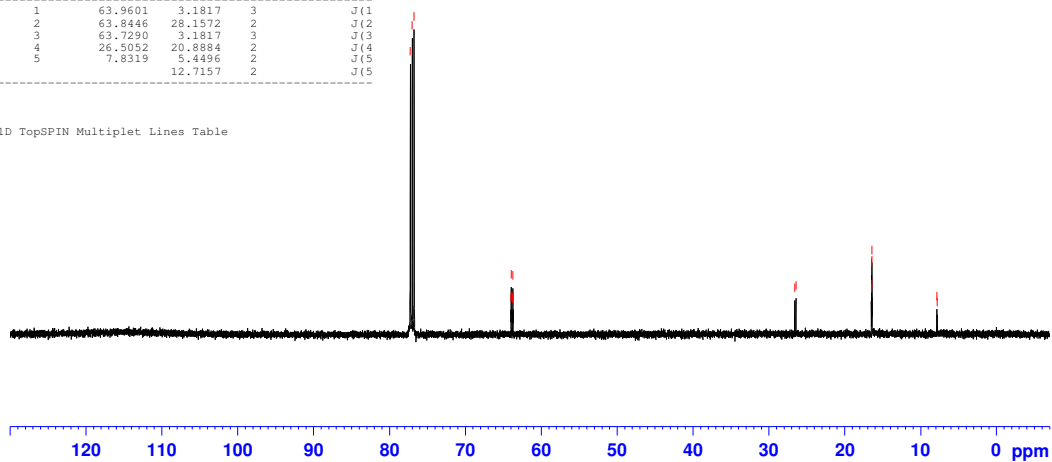


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1	63.9601	3.1817	3	J(1)
2	63.8446	28.1572	2	J(2)
3	63.7290	3.1817	3	J(3)
4	26.5052	20.8884	2	J(4)
5	7.8319	5.4496	2	J(5)
		12.7157	2	J(5)

1D TopSPIN Multiplet Lines Table

¹³C NMR spectrum of compound 27

PMA130-31P

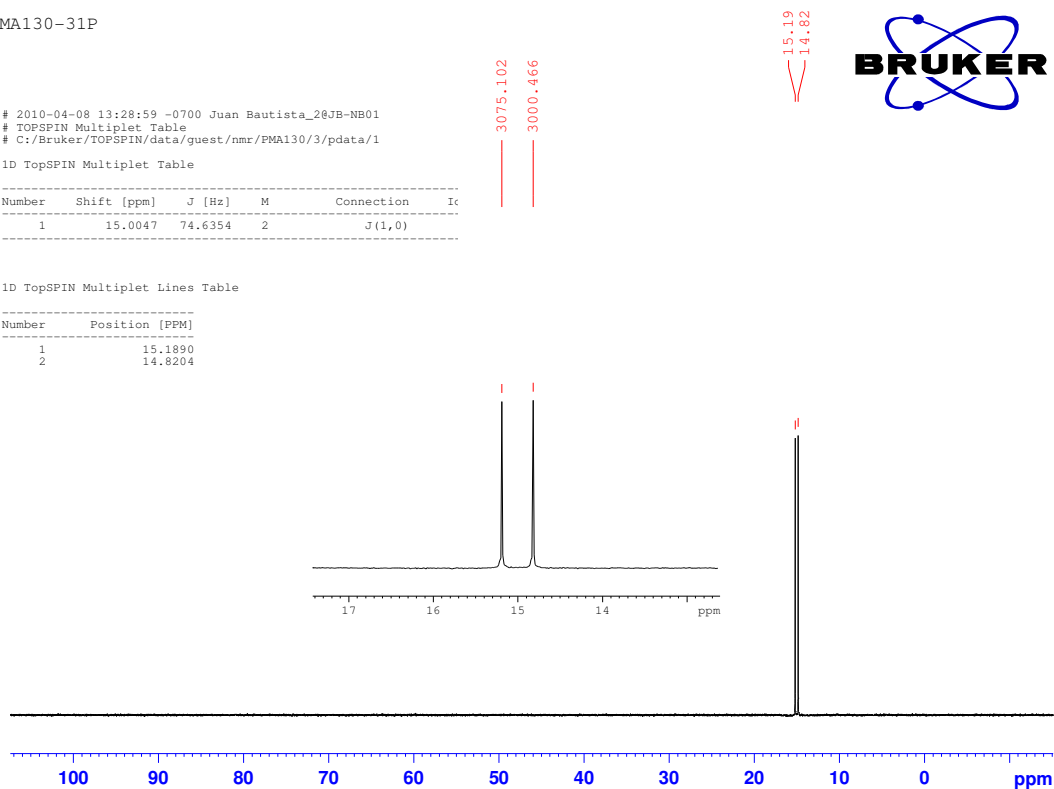
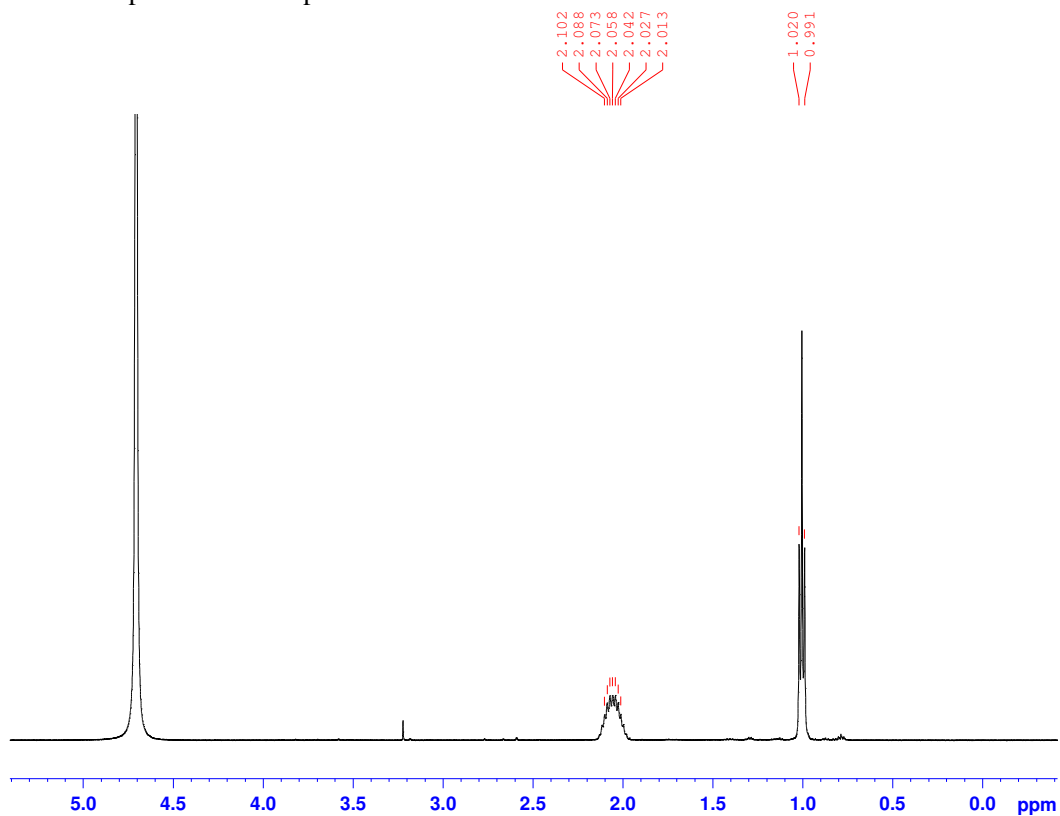
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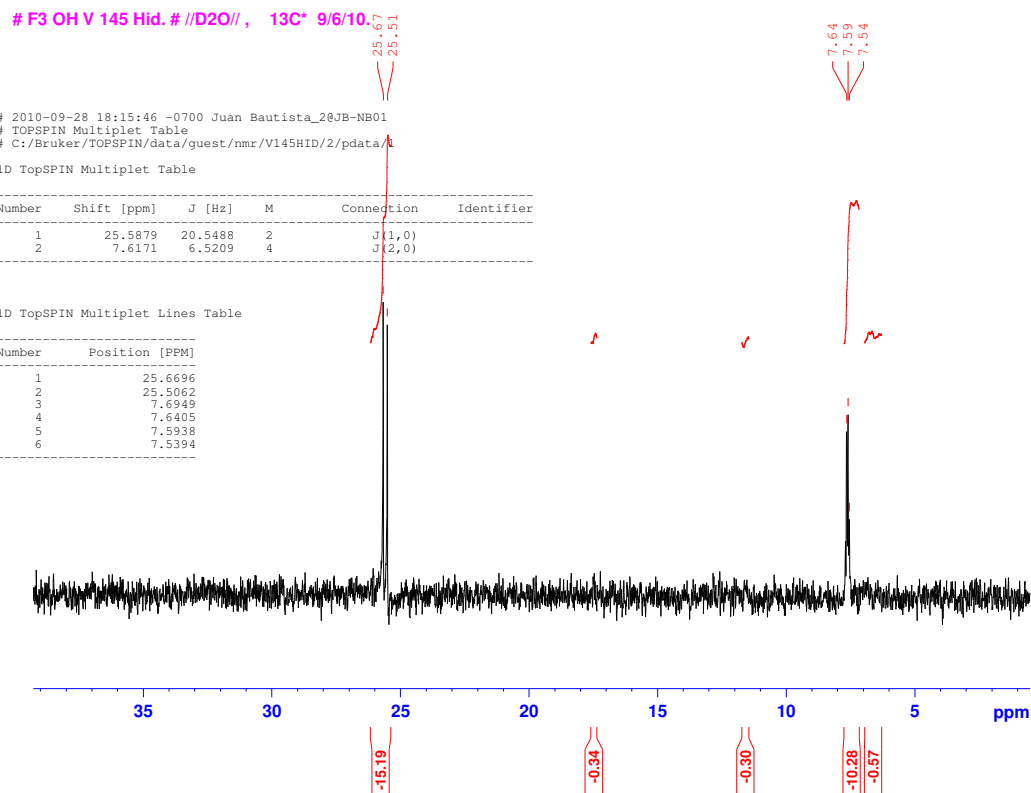
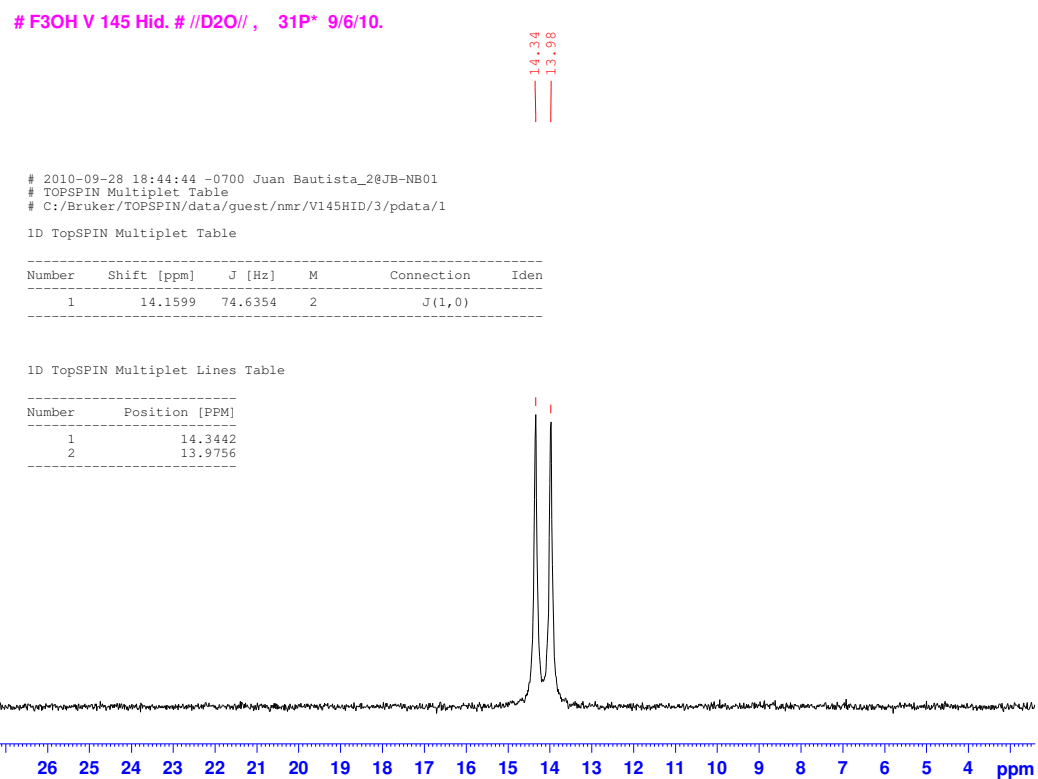
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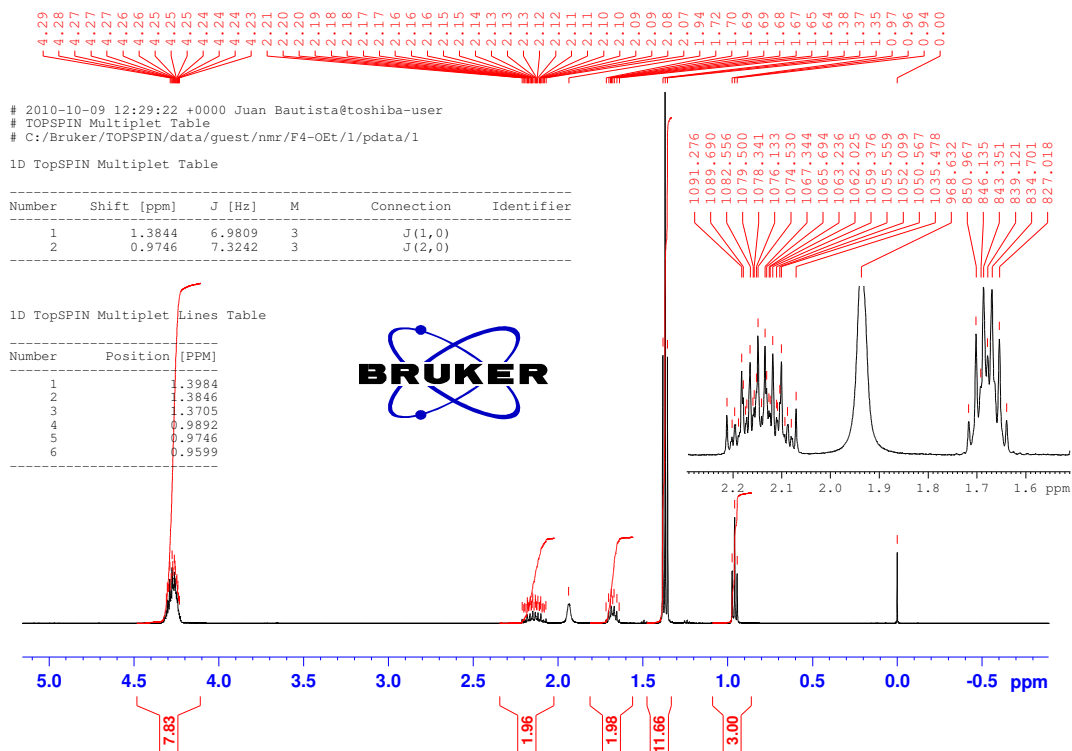
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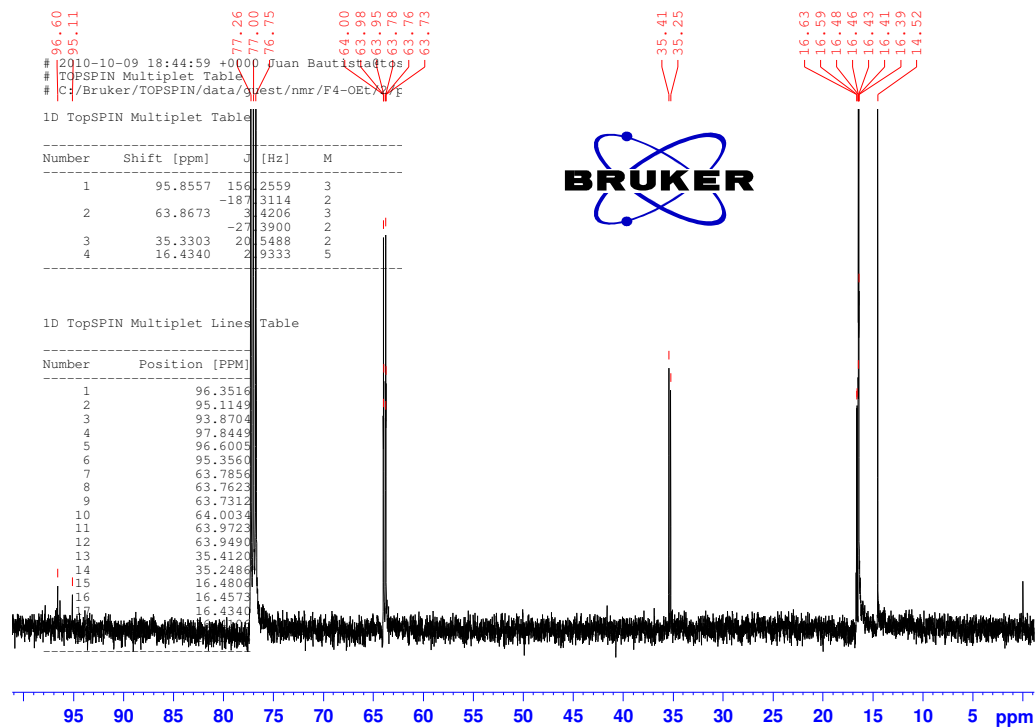
³¹P NMR spectrum of compound **27**¹H NMR spectrum of compound **37**

 ^{13}C NMR spectrum of compound **37** ^{31}P NMR spectrum of compound **37**

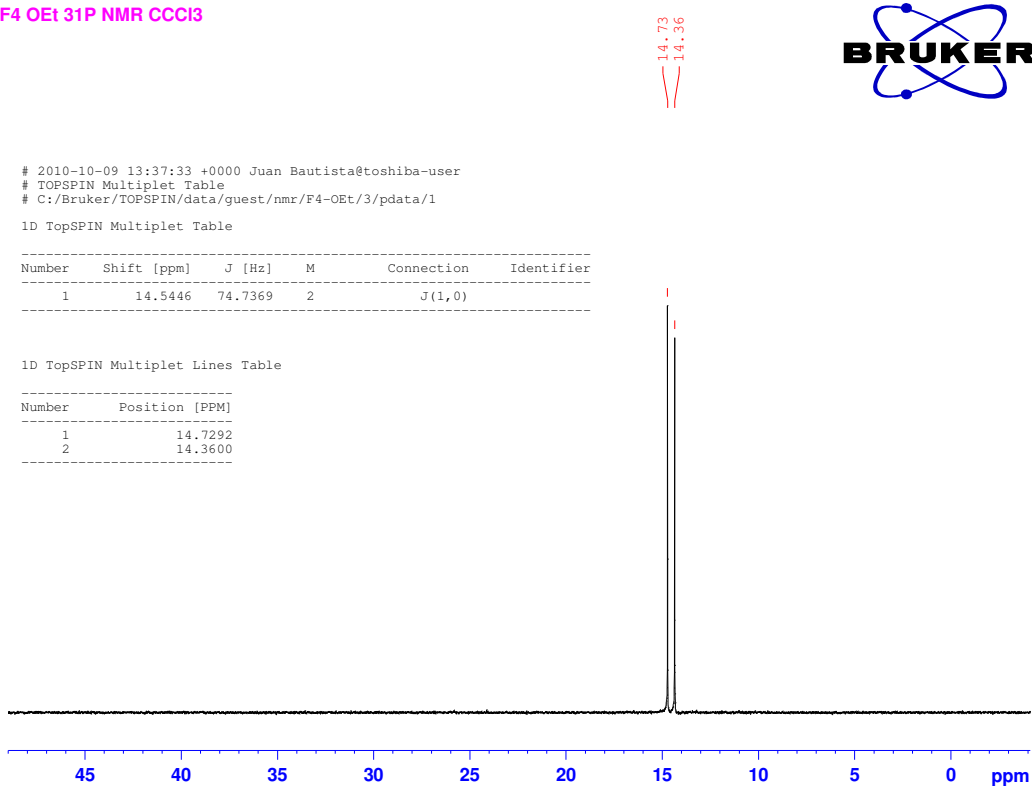
F4 OEt 1H NMR CDCl3

¹H NMR spectrum of compound 28

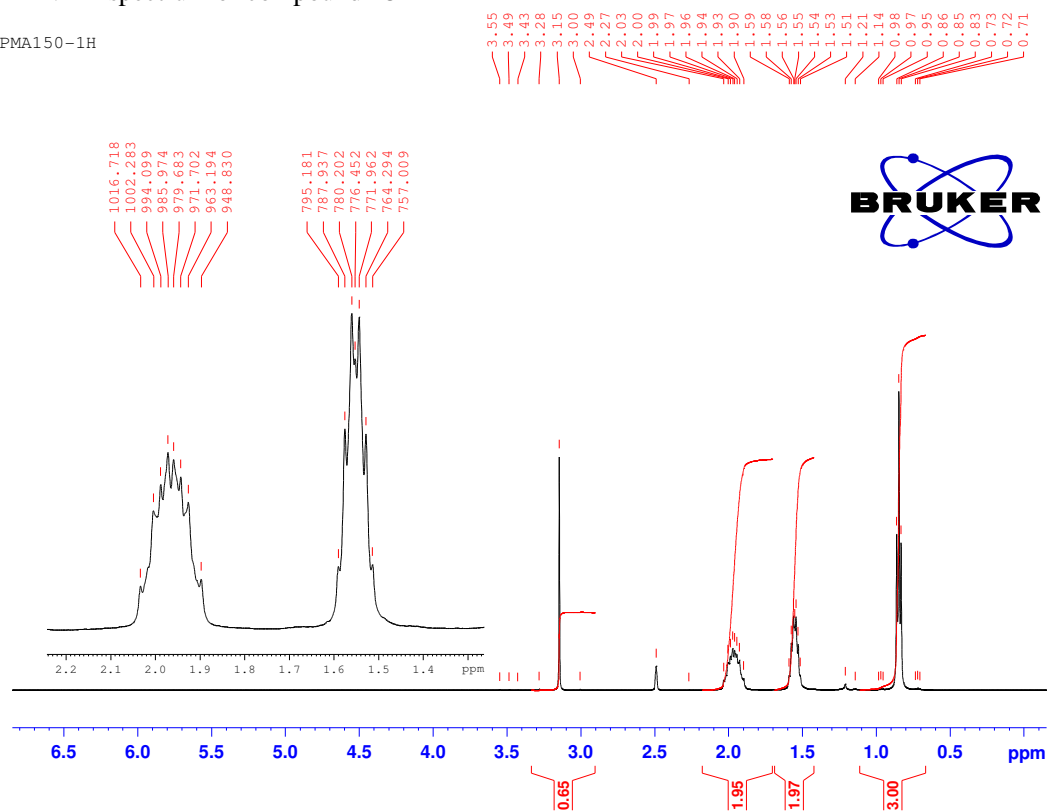
F4-OEt # //CDCl3//, 13C* 8/10/10.

¹³C NMR spectrum of compound 28

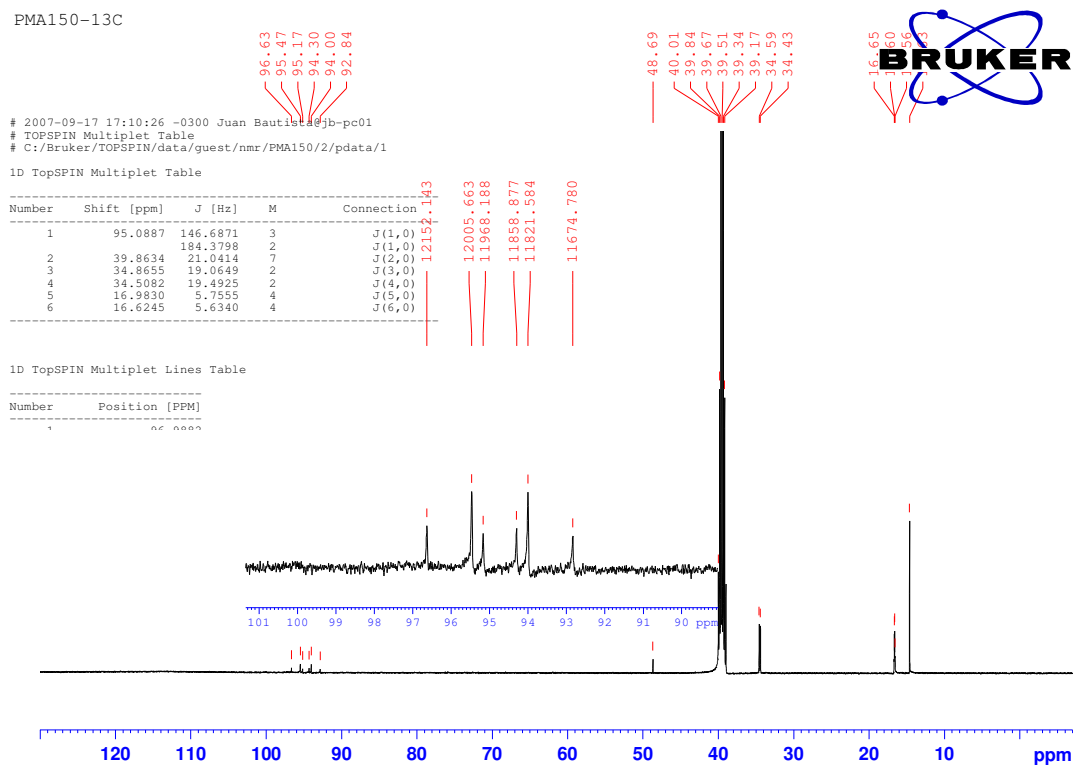
F4 OEt 31P NMR CCCI3

³¹P NMR spectrum of compound 28

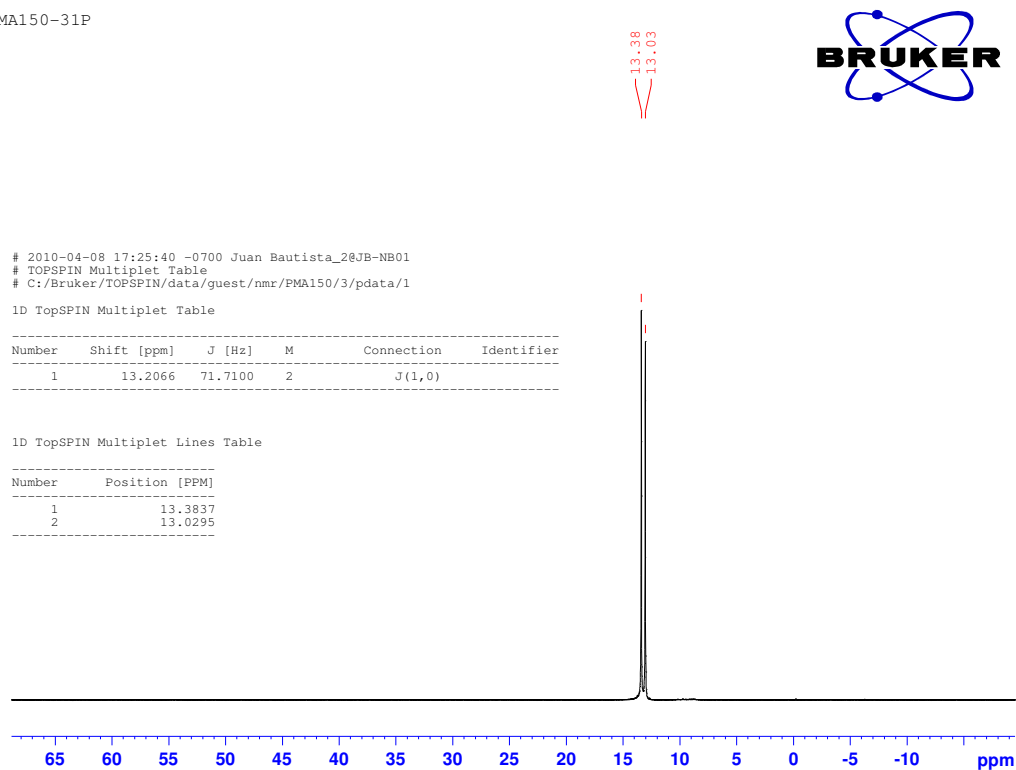
PMA150-1H

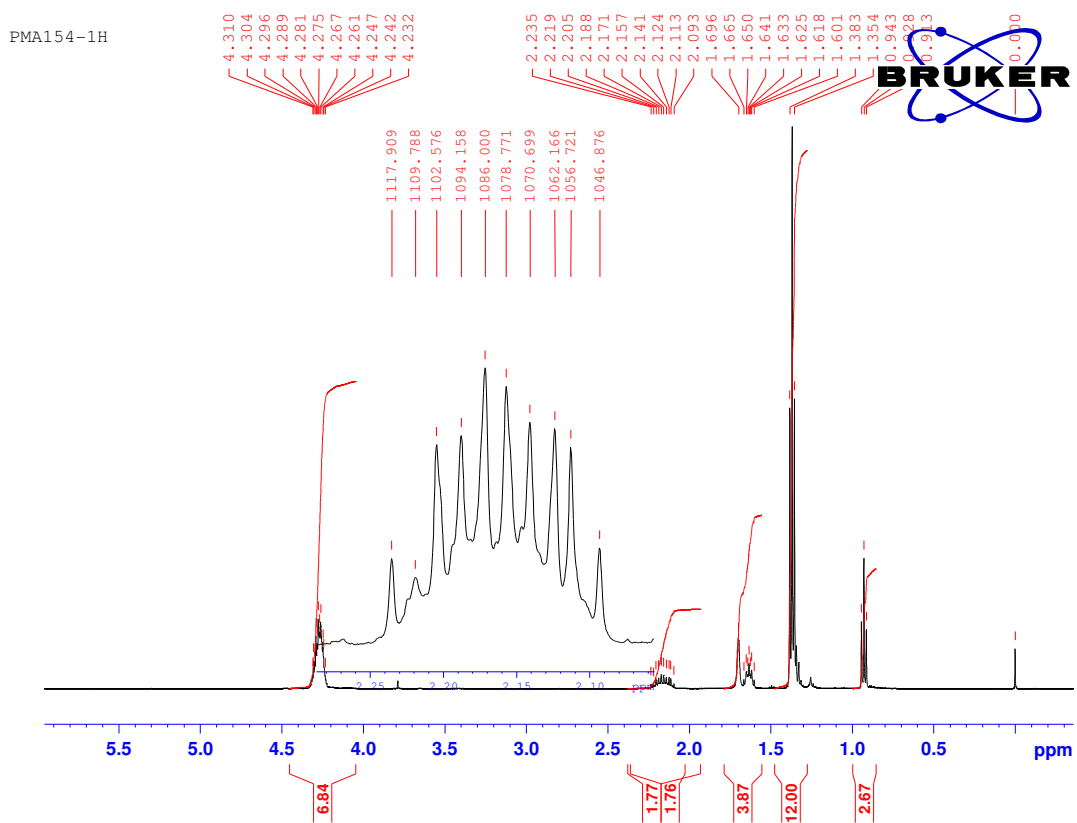
¹H NMR spectrum of compound 38

PMA150-13C

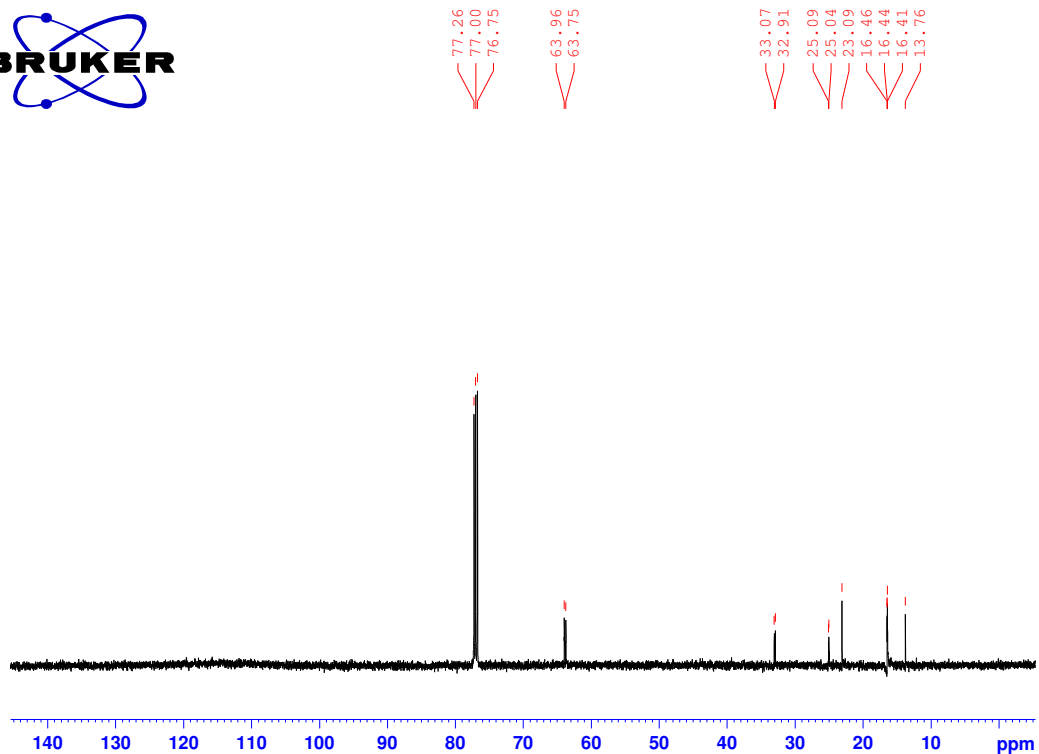
¹³C NMR spectrum of compound 38

PMA150-31P

³¹P NMR spectrum of compound 38

¹H NMR spectrum of compound **29**

PMA154-13C

¹³C NMR spectrum of compound **29**

PMA154-31P



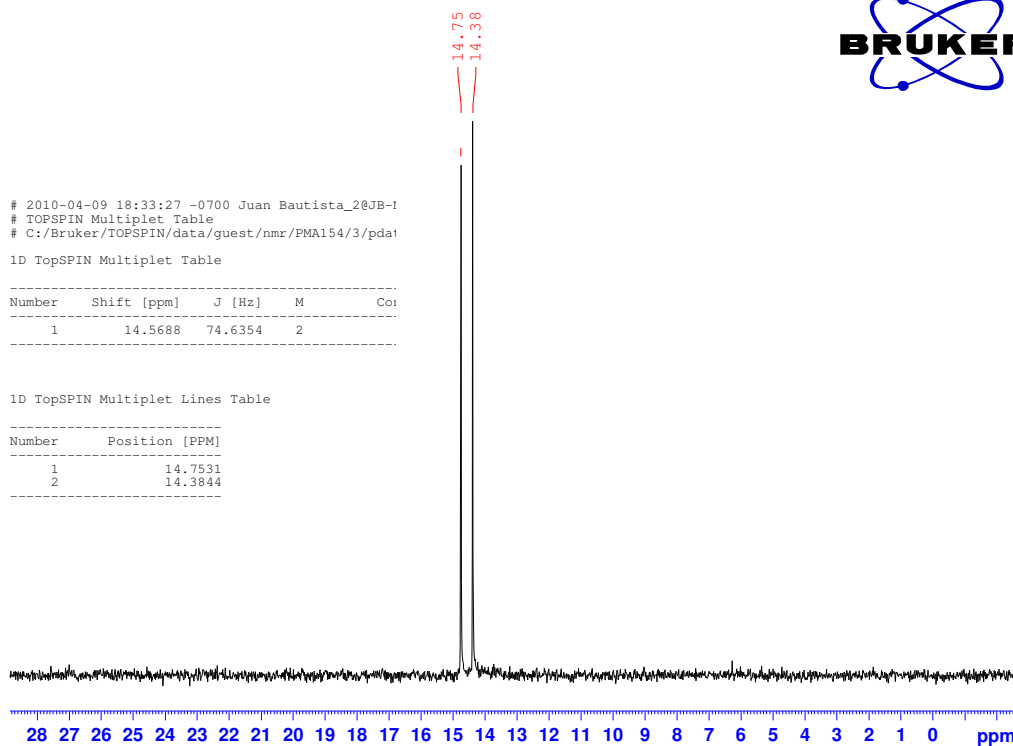
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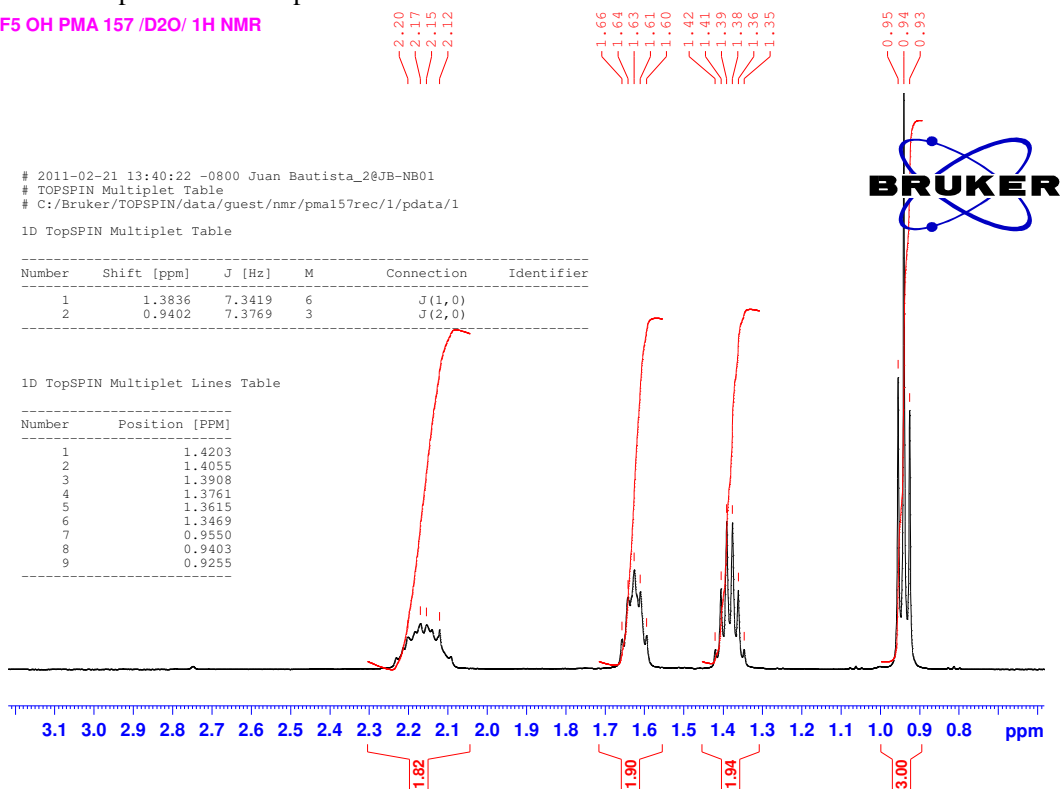
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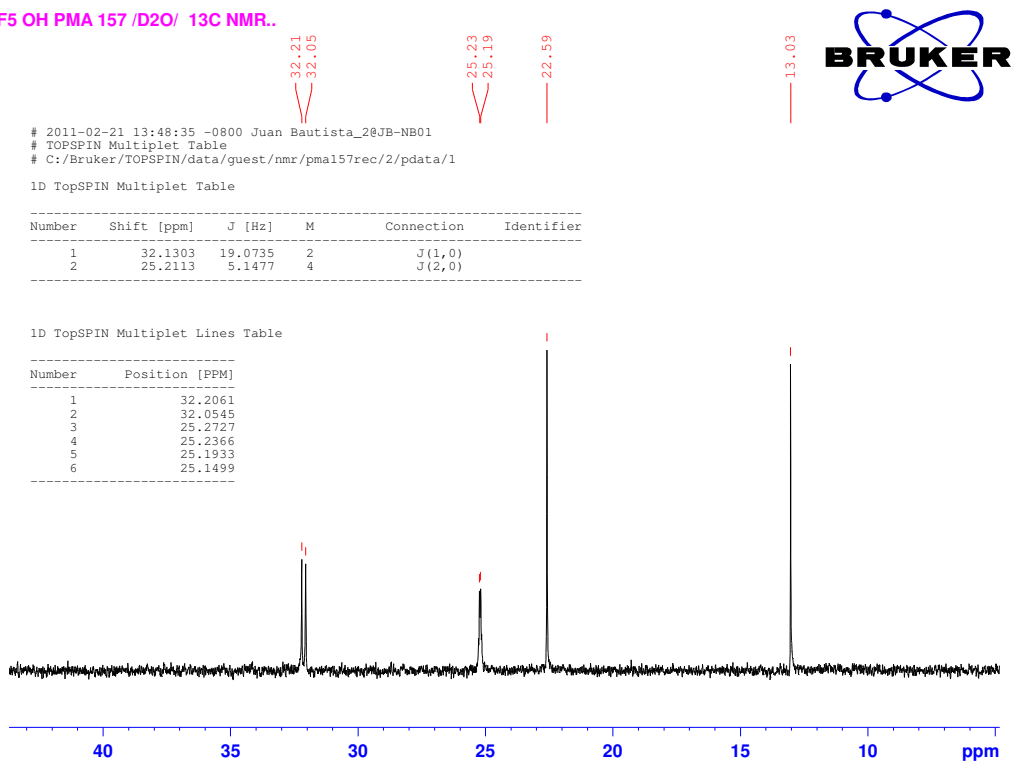
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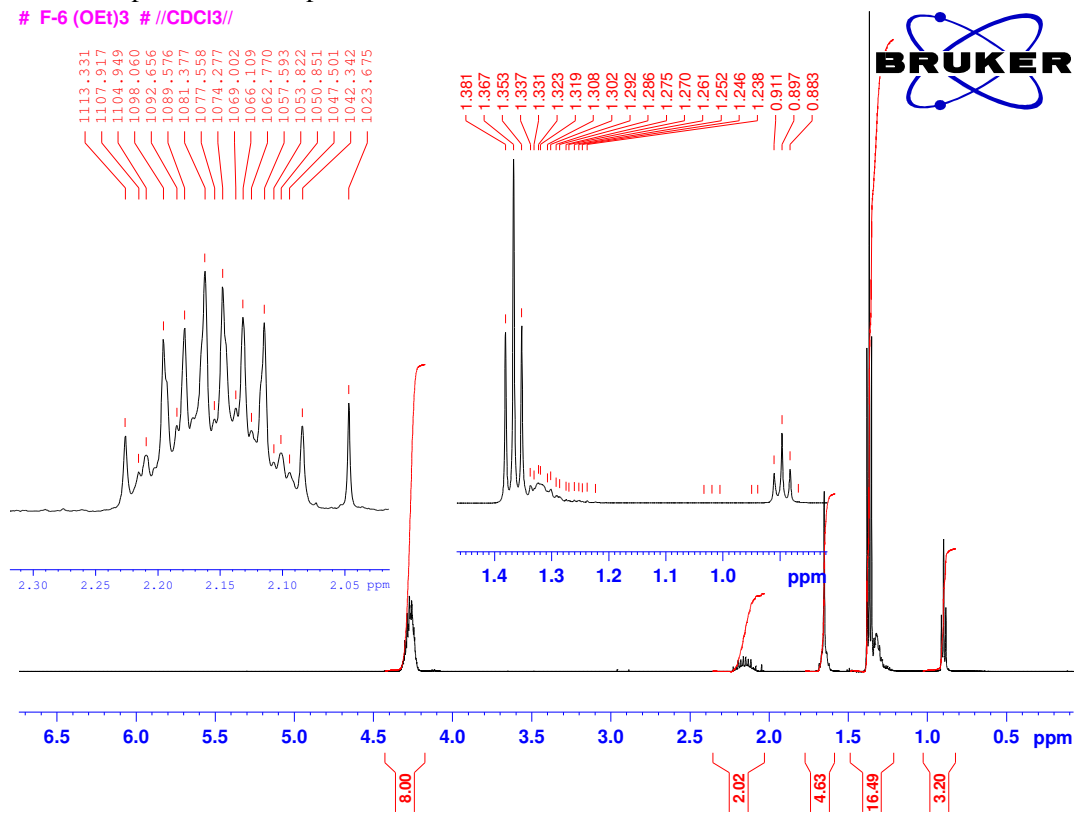
³¹P NMR spectrum of compound 29

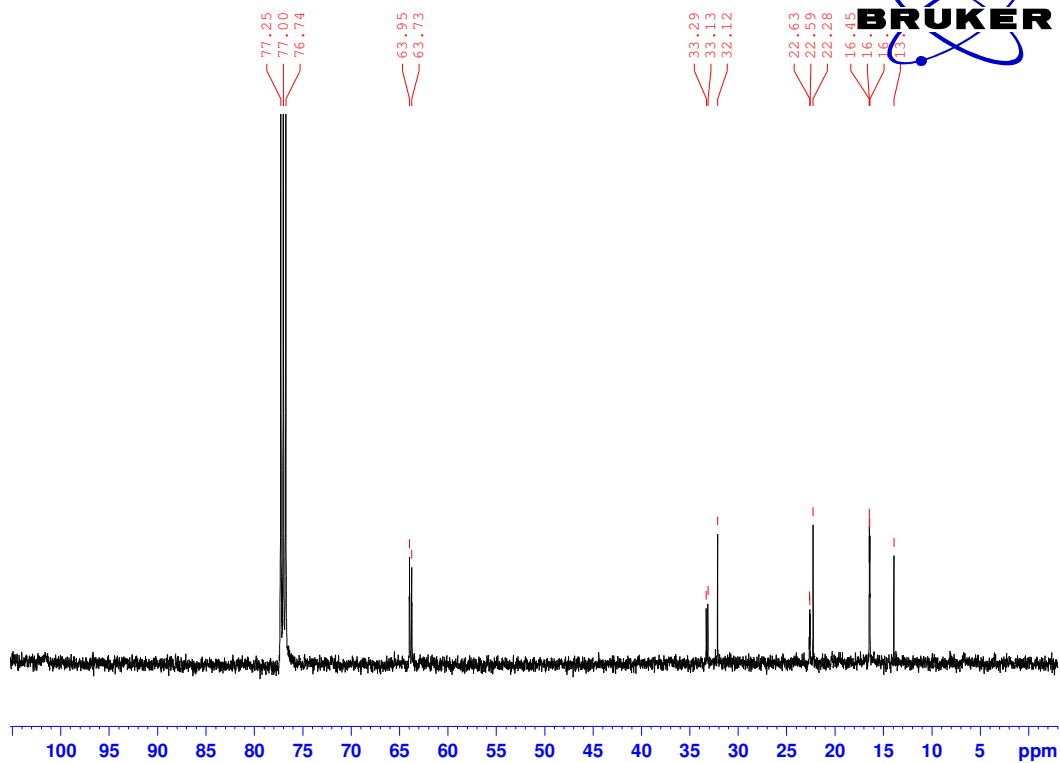
F5 OH PMA 157 /D2O/ 1H NMR

¹H NMR spectrum of compound 39

F5 OH PMA 157 /D2O/ ¹³C NMR..¹³C NMR spectrum of compound 39

F-6 (OE)3 # //CDCl3//

¹H NMR spectrum of compound 30

PMA-156 - #1 # //CDCI3//, ¹³C NMR*¹³C NMR spectrum of compound **30**# PMA-156 - #1 # //CDCI3//, ³¹P NMR

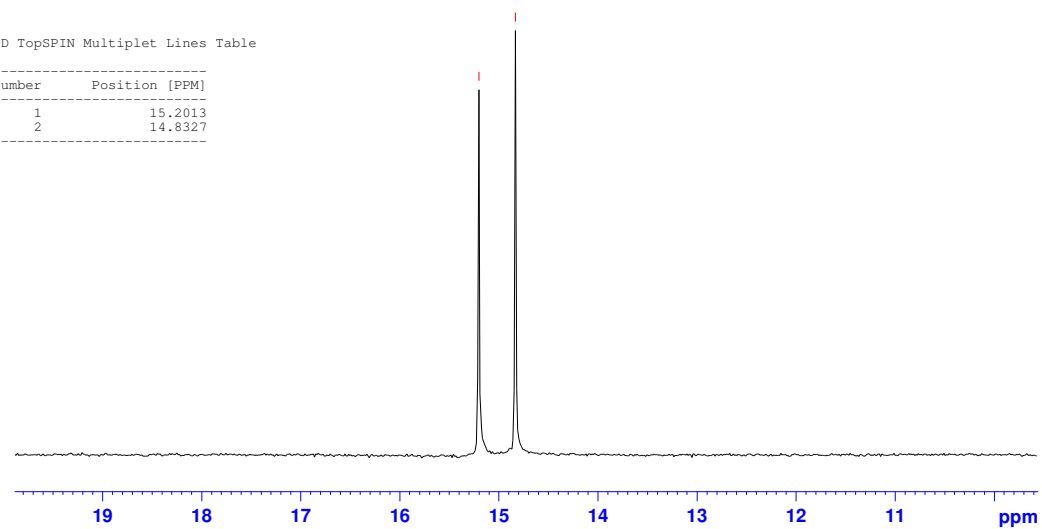
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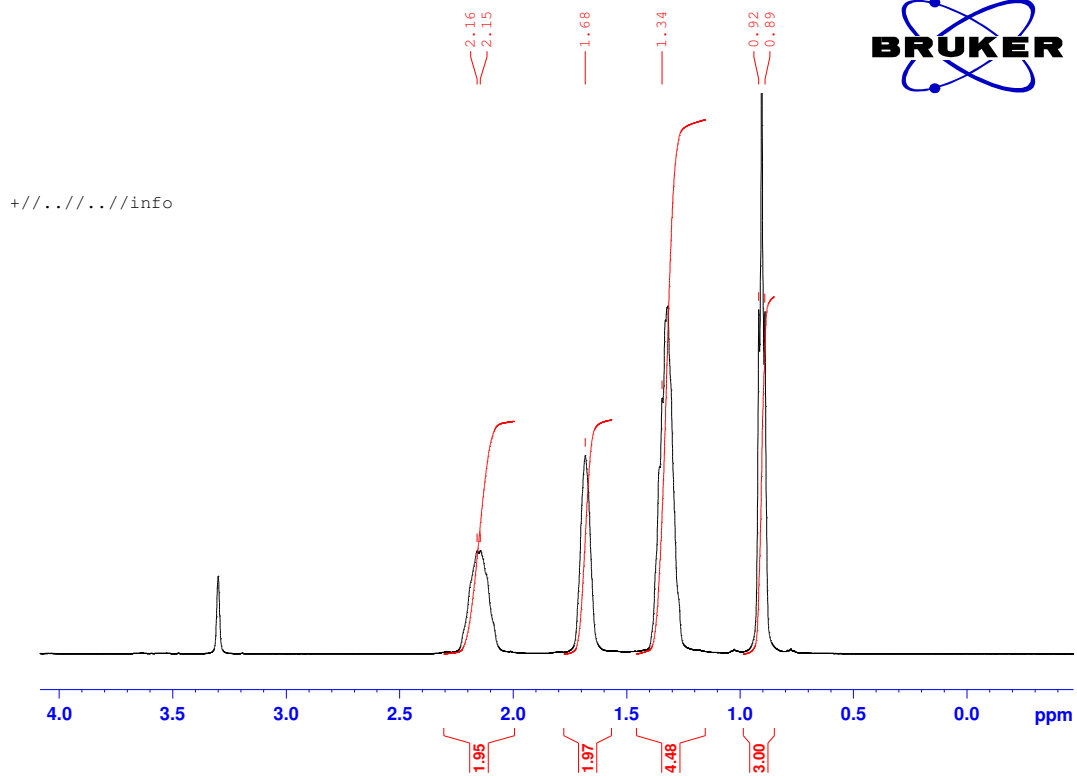
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1D TopSPIN Multiplet Lines Table

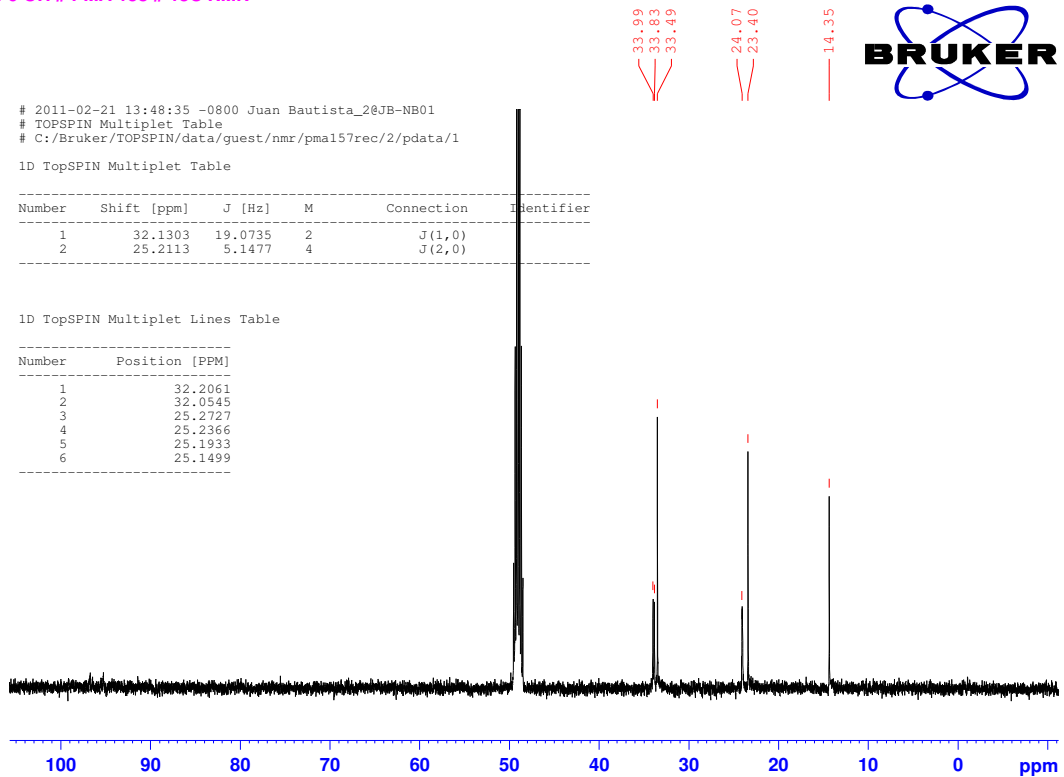
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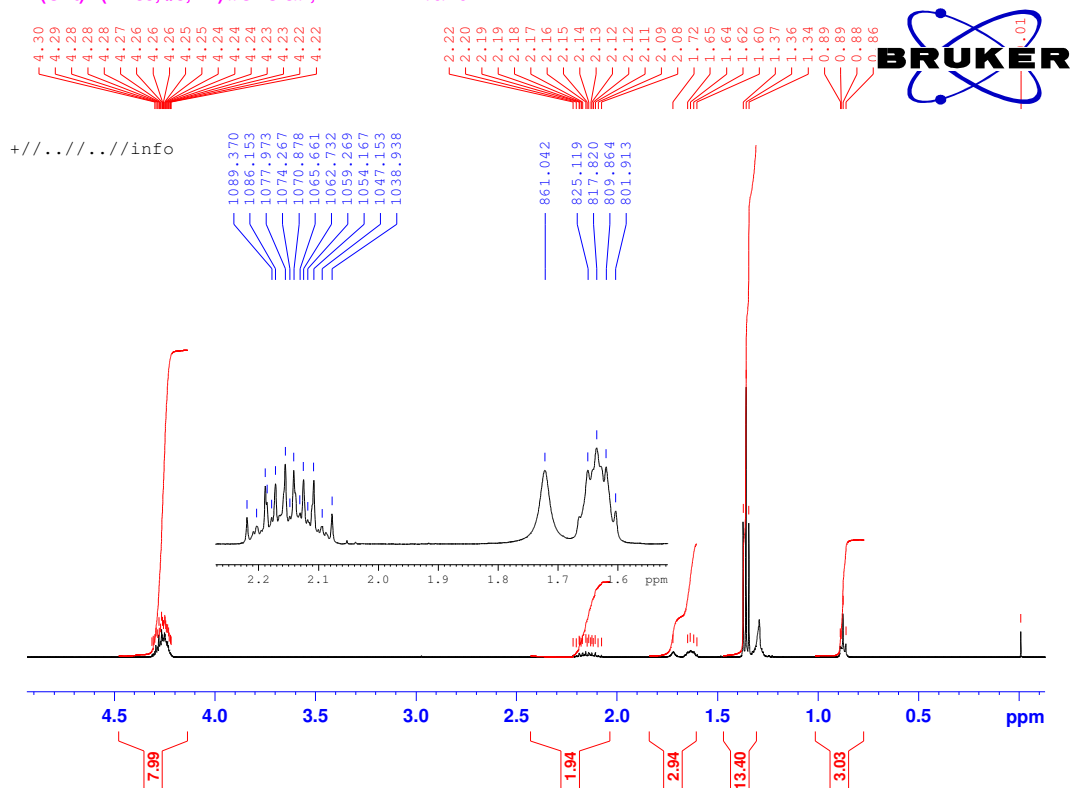
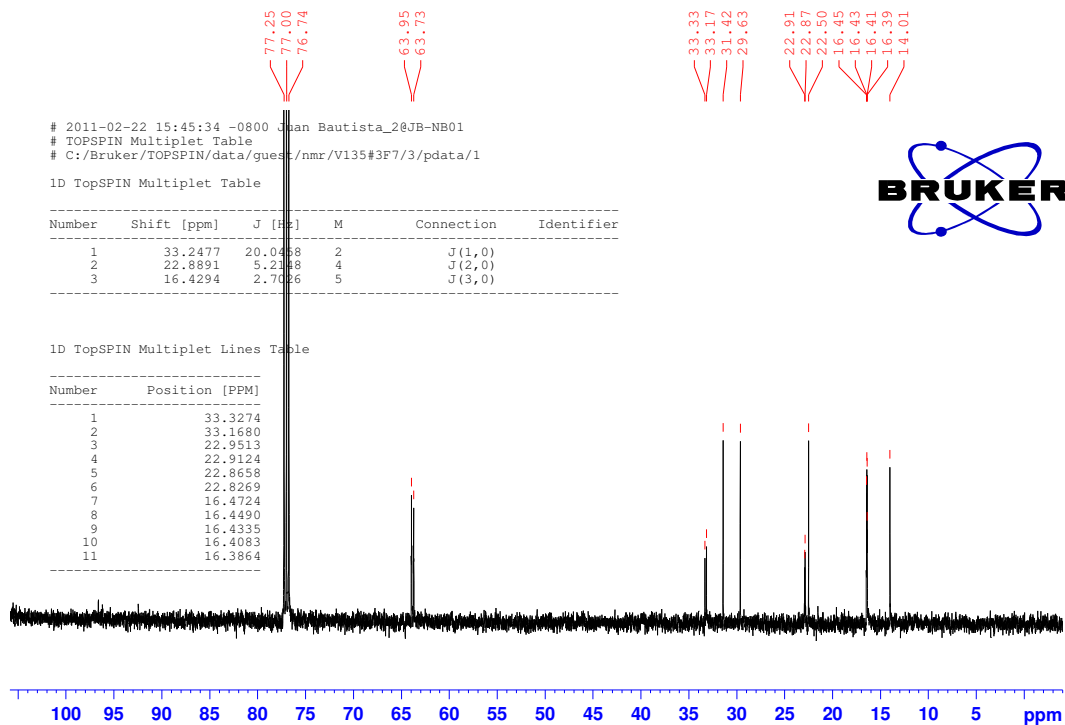
³¹P NMR spectrum of compound **30**

F6 OH PMA-158 # 1H NMR

¹H NMR spectrum of compound **40**

F6 OH # PMA-158 # 13C NMR

¹³C NMR spectrum of compound **40**

F7 (OE)2 (V 135, #3, F7) //CDCl3//, ¹H NMR 2/6/10.¹H NMR spectrum of compound 31F7 (OE)2 (V 135, #3, F7) # //CDCl3//, ¹³C NMR 2/6/10.¹³C NMR spectrum of compound 31

F7 (OEt)2 # (V 135, #3, F7) # //CDCI3//, ³¹P NMR 2/6/10.

14.77
14.40



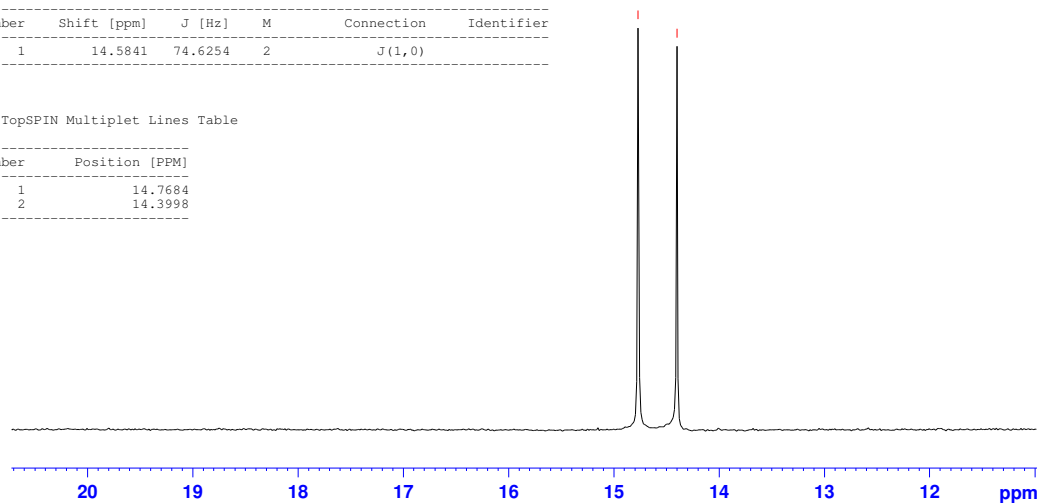
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1D TopSPIN Multiplet Table

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1	14.5841	74.6254	2	J(1,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	14.7684
2	14.3998



³¹P NMR spectrum of compound 31

V 135 Hid. # //D2O//, ¹H 2/6/10.

2.06
2.04
2.03
2.01
1.99
1.98
1.53
1.51
1.50
1.48
1.26
1.24
1.22
1.21
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0.77
0.76

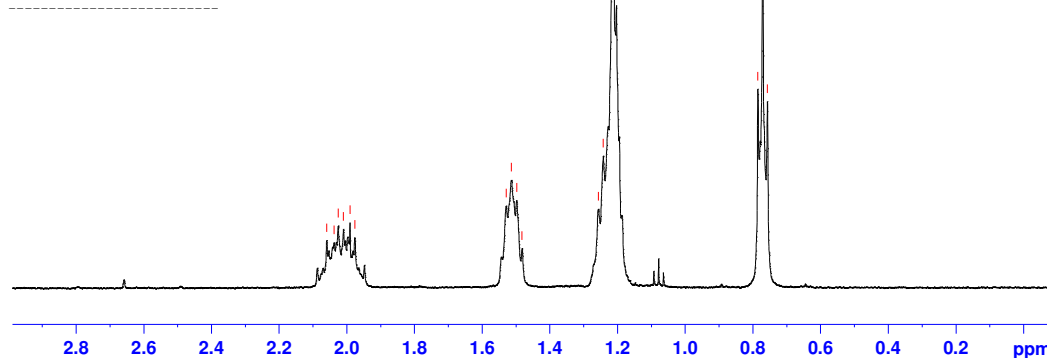


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1D TopSPIN Multiplet Lines Table



¹H NMR spectrum of compound 41

V 135 Hid. # //D2O// , 13C* 9/6/10.

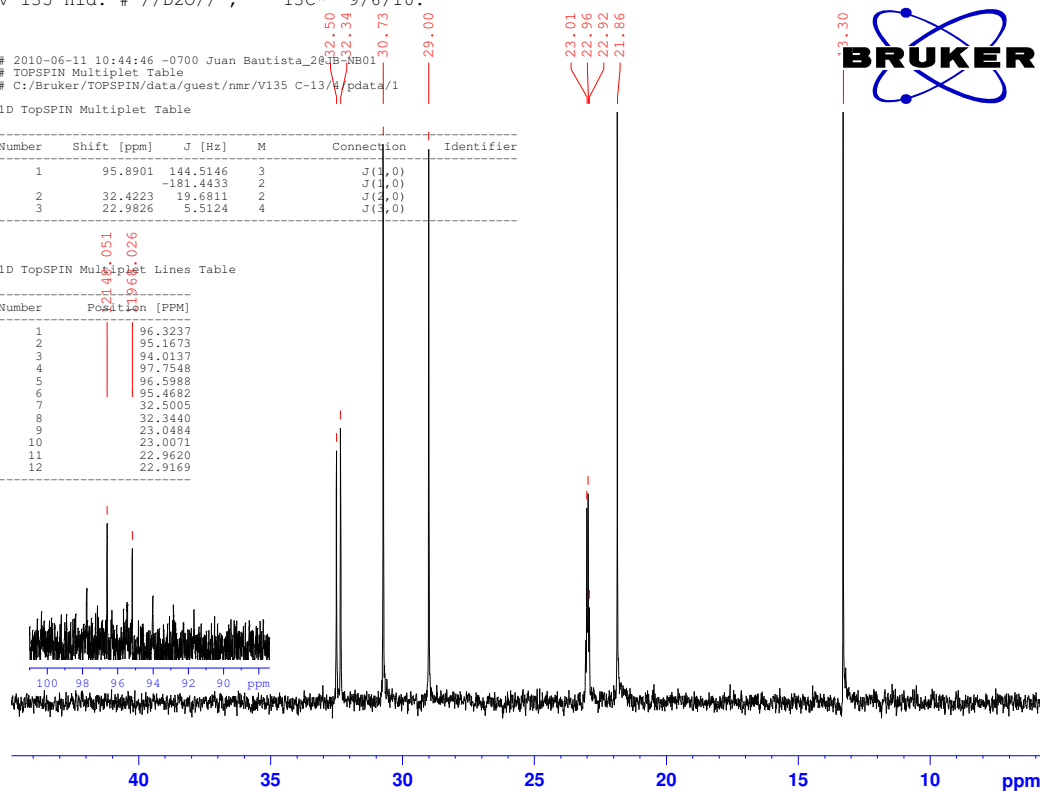
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1D TopSPIN Multiplet Lines Table

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4	97.7548
5	96.5988
6	95.4682
7	32.5005
8	32.3440
9	23.0484
10	23.0071
11	22.9620
12	22.9169

¹³C NMR spectrum of compound 41

V 135 hid. # //D2O// , 31P* 2/6/10.

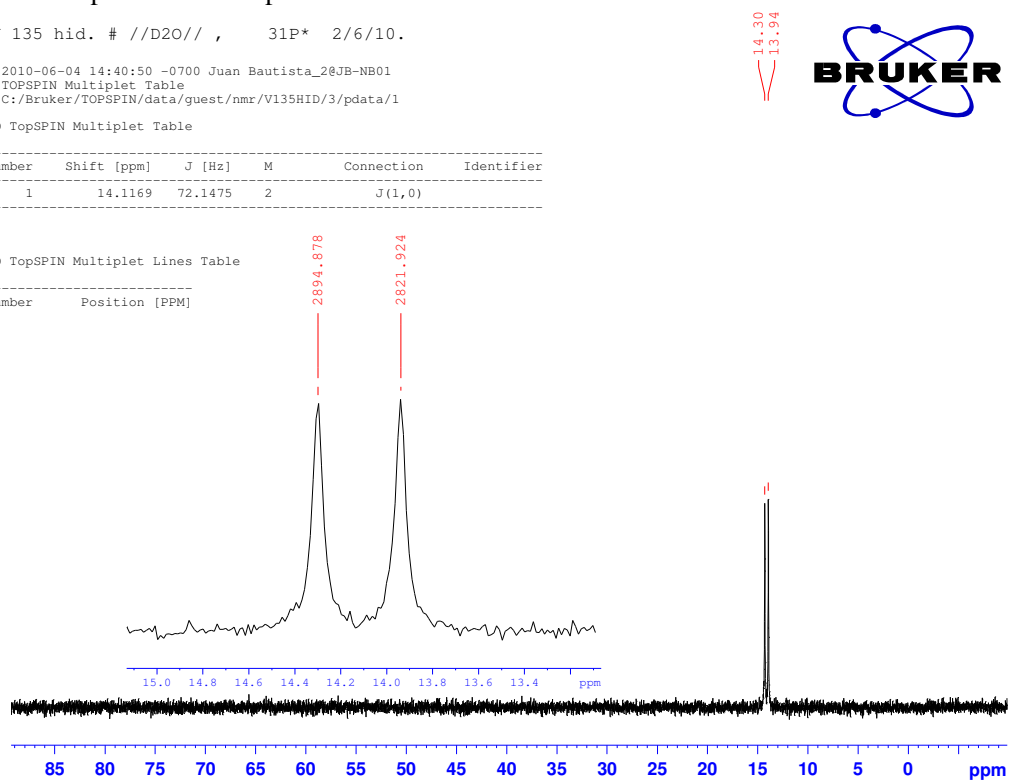
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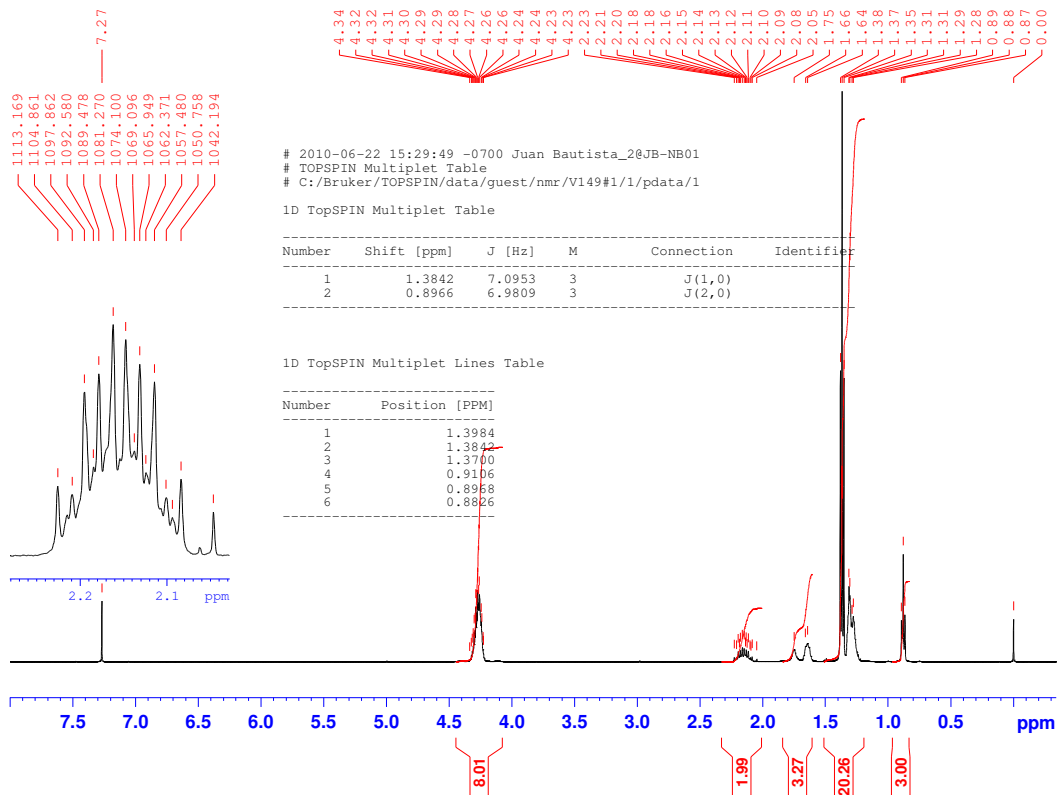
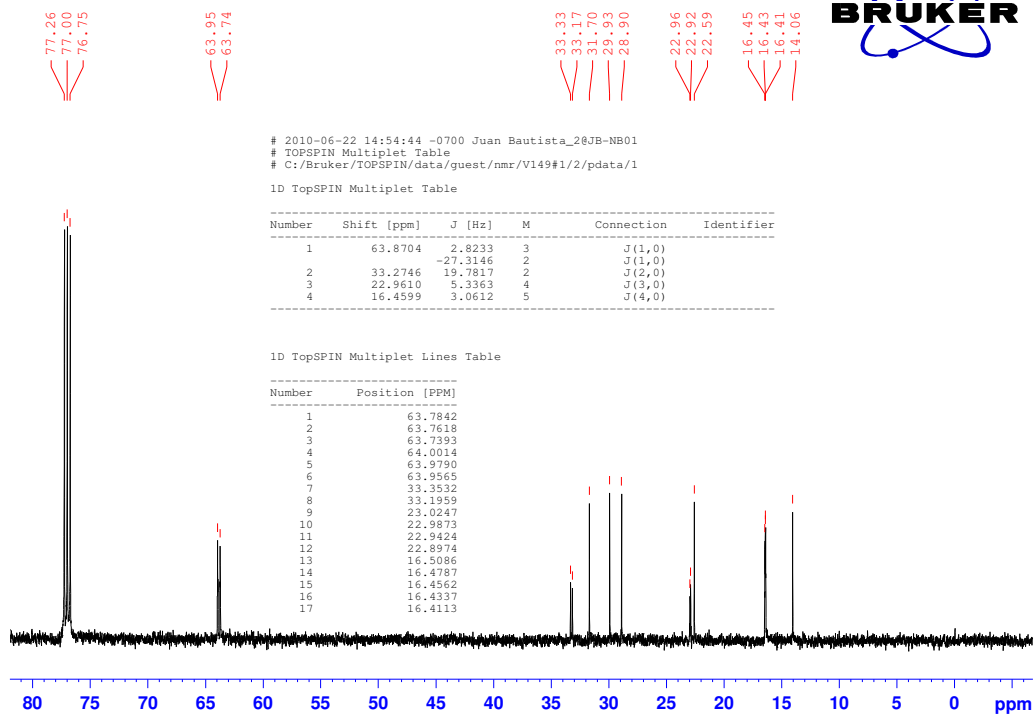
1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	14.1169	72.1475	2	J(1,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	2894.878
2	2821.924

³¹P NMR spectrum of compound 41

V149 /CDCl₃/ ¹H NMR F8 (OE) 18/6/10.¹H NMR spectrum of compound 32V149 # 1 /CDCl₃/ ¹³C NMR F8 OE 18/6/10.¹³C NMR spectrum of compound 32

V149 # 1 /CDCl₃/ ³¹P NMR F8 OEI 18/6/10.

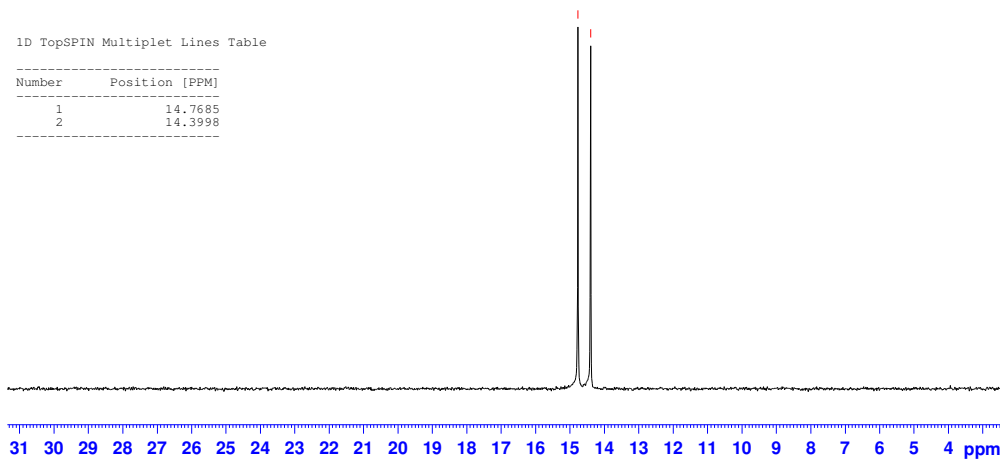
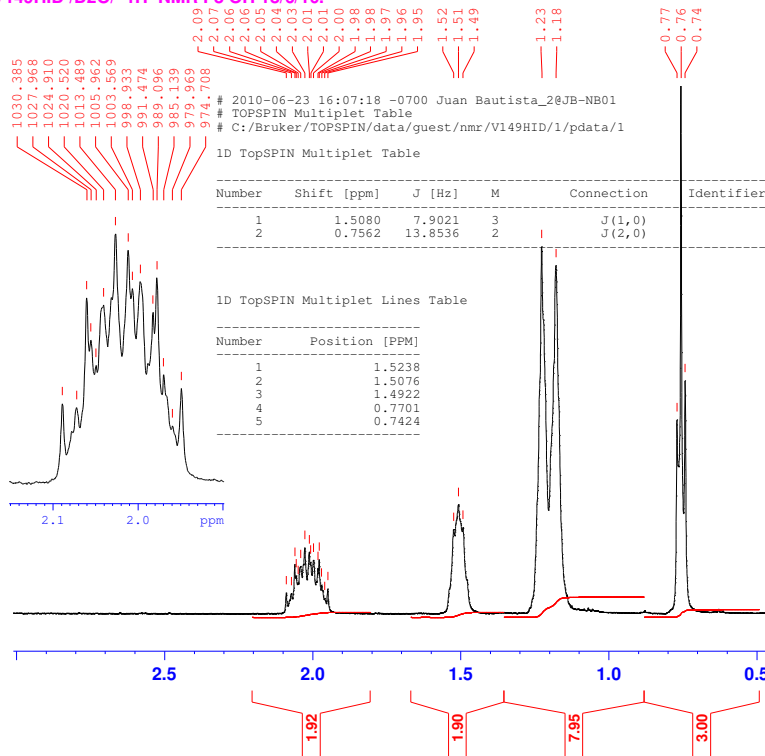
2010-06-22 14:27:58 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/V149#1/3/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	14.5841	74.6354	2	J(1,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	14.7685
2	14.3998

³¹P NMR spectrum of compound 32V149HID /D₂O/ ¹H NMR F8 OH 18/6/10.¹H NMR spectrum of compound 42

V149HID /D2O/ ¹³C NMR F8 OH 18/6/10.

32.50
32.35
31.00
29.32
28.13

23.10
23.05
21.95

13.35



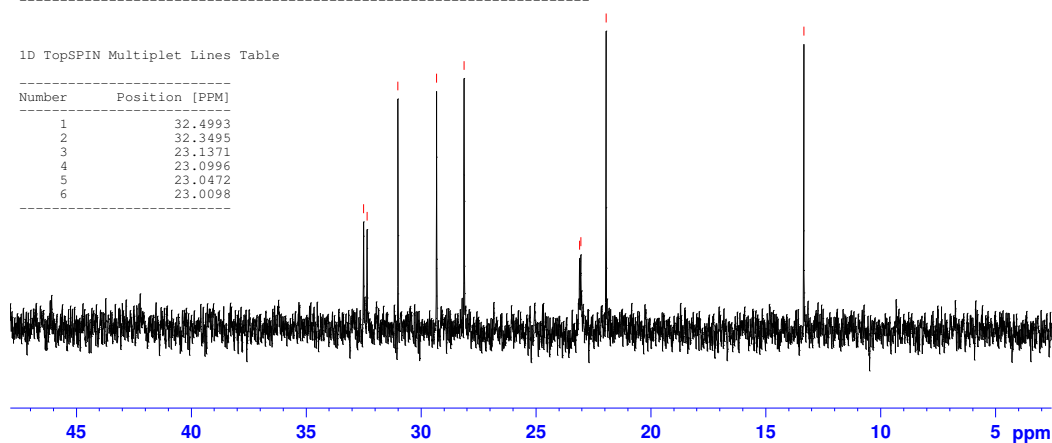
2010-06-23 16:53:09 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/V149HID/2/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	32.4244	18.8380	2	J(1,0)	
2	23.0734	5.3363	4	J(2,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	32.4993
2	32.3495
3	23.1371
4	23.0996
5	23.0472
6	23.0098

¹³C NMR spectrum of compound 42V149HID /D2O/ F8 OH ³¹P NMR 18/6/10.

2918.221
2844.574

14.41
14.05



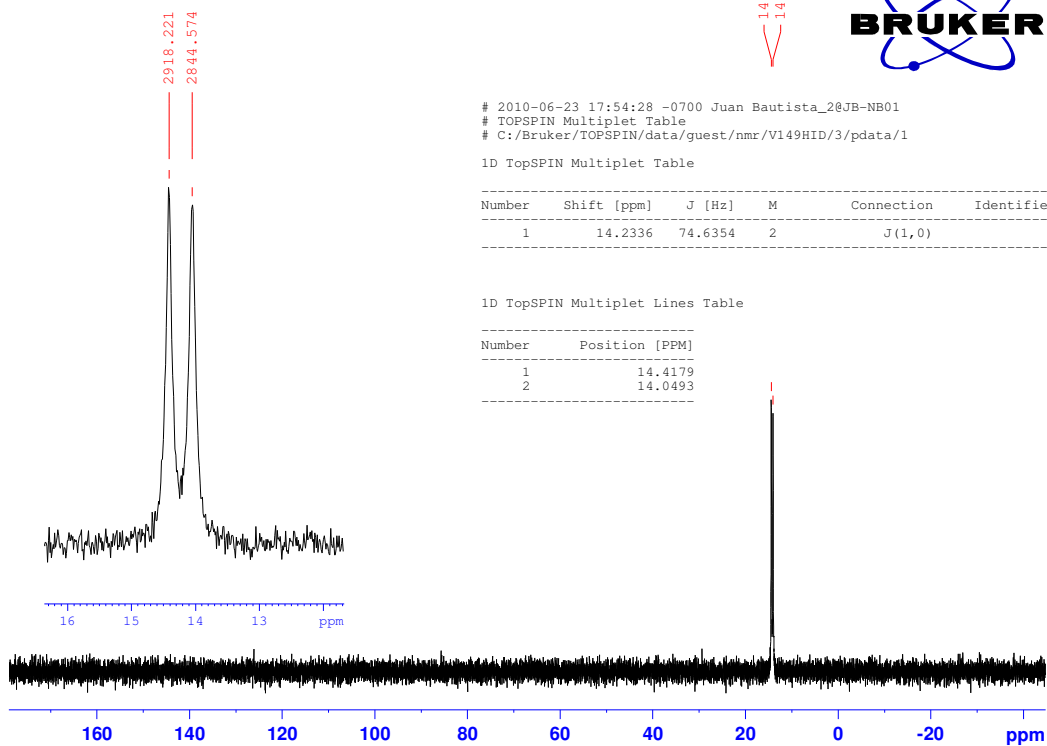
2010-06-23 17:54:28 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
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1D TopSPIN Multiplet Table

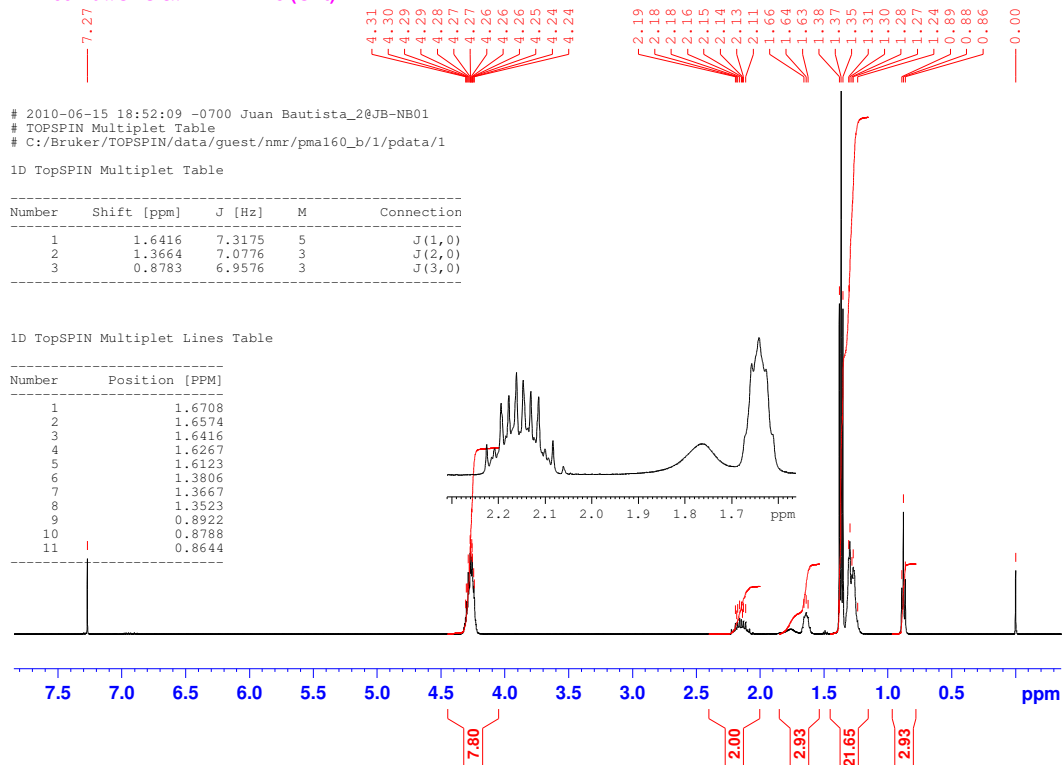
Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	14.2336	74.6354	2	J(1,0)	

1D TopSPIN Multiplet Lines Table

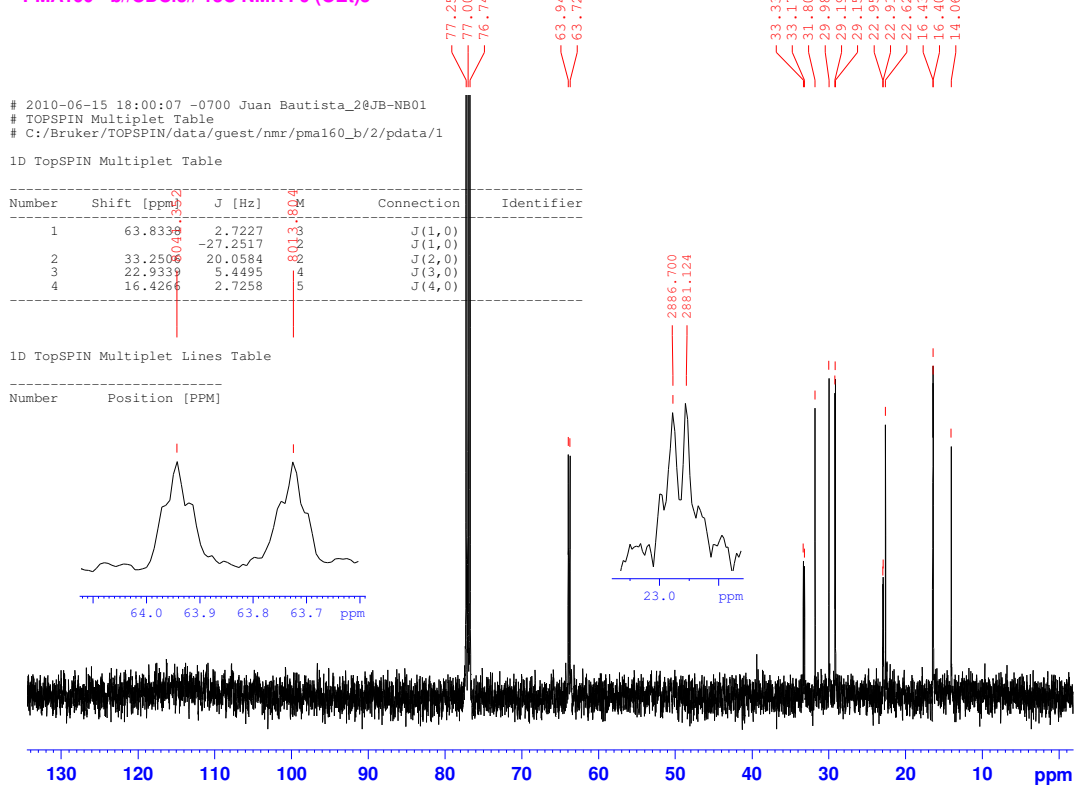
Number	Position [PPM]
1	14.4179
2	14.0493

³¹P NMR spectrum of compound 42

PMA 160 - b //CDCI3// 1H NMR F9 (OEt)

¹H NMR spectrum of compound 33

PMA160 - b//CDCI3// 13C NMR F9 (OEt)3

¹³C NMR spectrum of compound 33

PMA160 - b //CDCl₃// 31P NMR

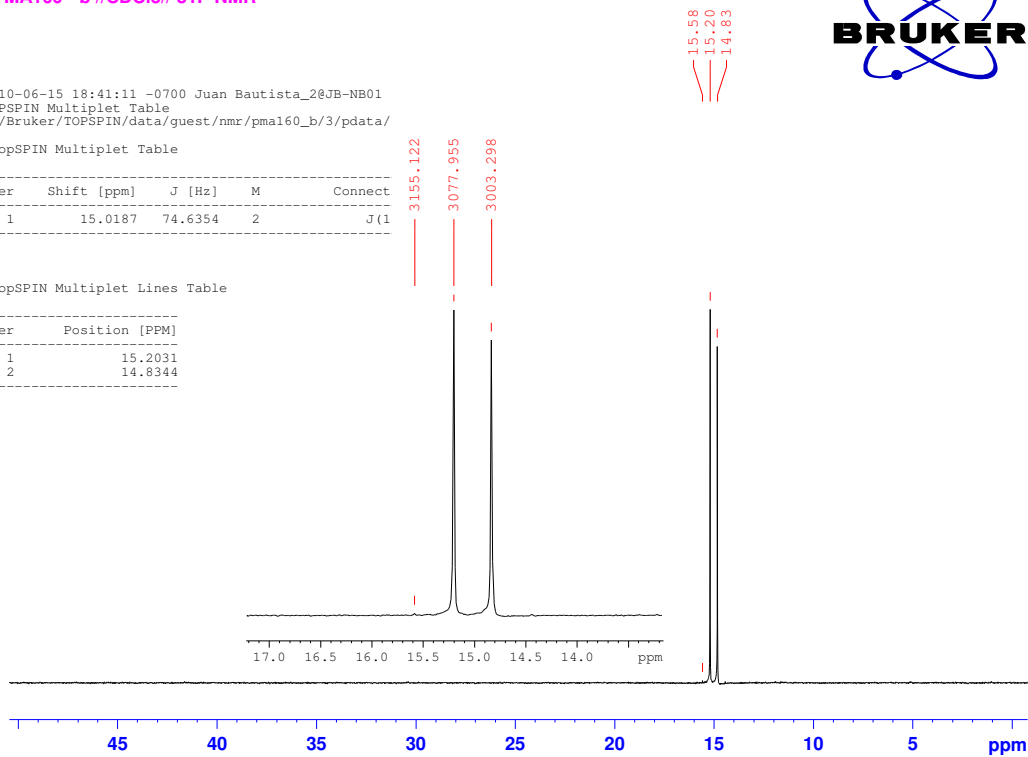
2010-06-15 18:41:11 -0700 Juan Bautista_20JB-NB01
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1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connect
1	15.0187	74.6354	2	J(1)

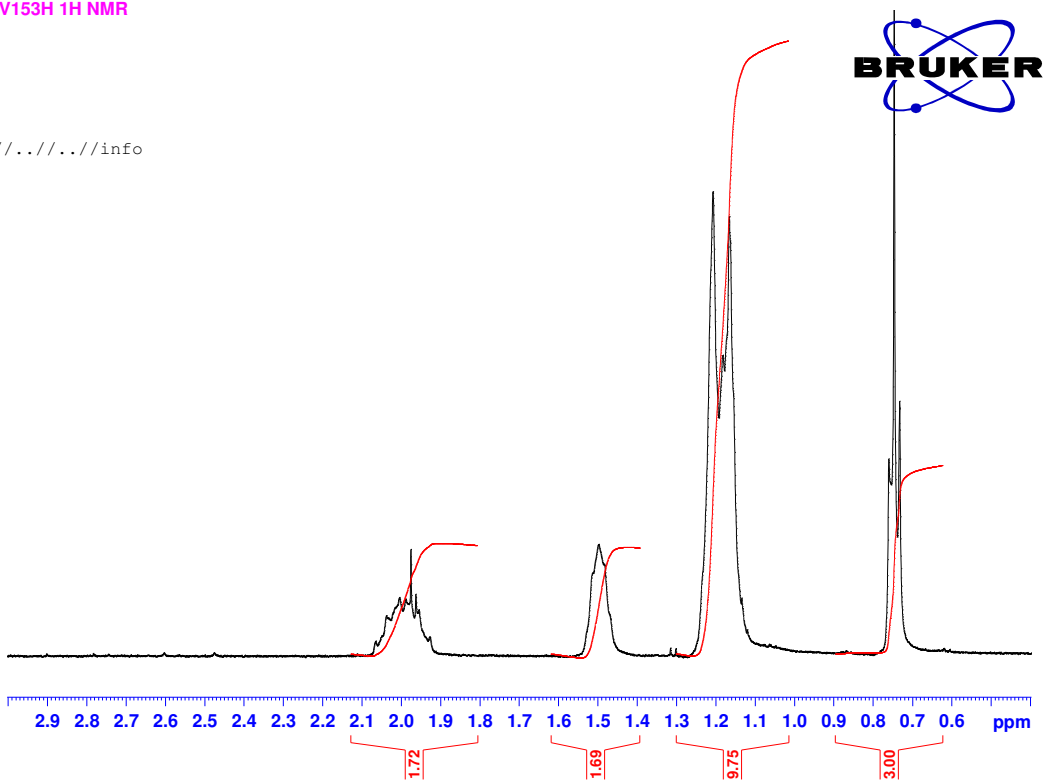
1D TopSPIN Multiplet Lines Table

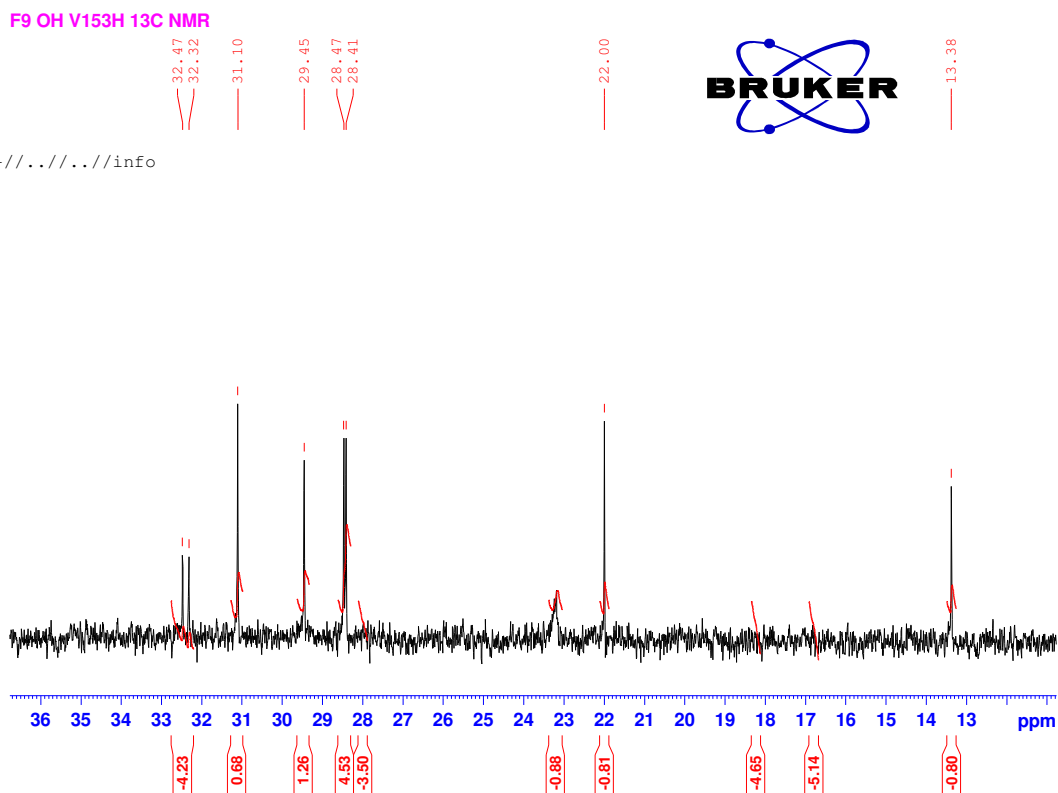
Number	Position [PPM]
1	15.2031
2	14.8344

³¹P NMR spectrum of compound 33

V153H 1H NMR

+//...//info

¹H NMR spectrum of compound 43

**¹³C NMR spectrum of compound 43**

F9 hid. # //D2O//, 31P* 20/7/10,

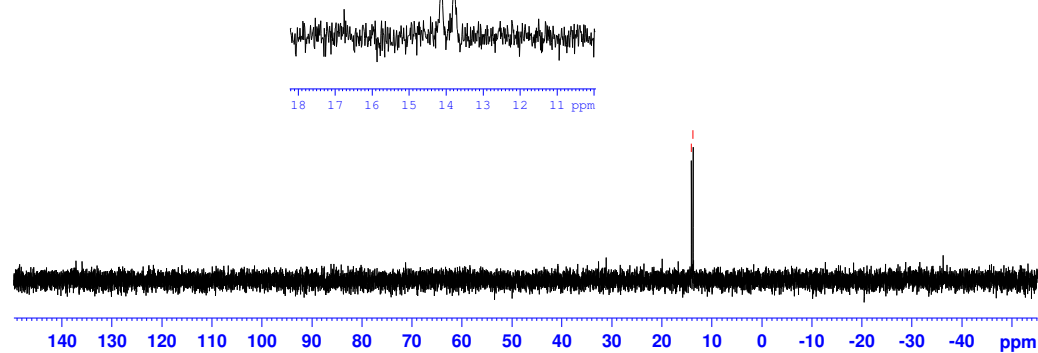
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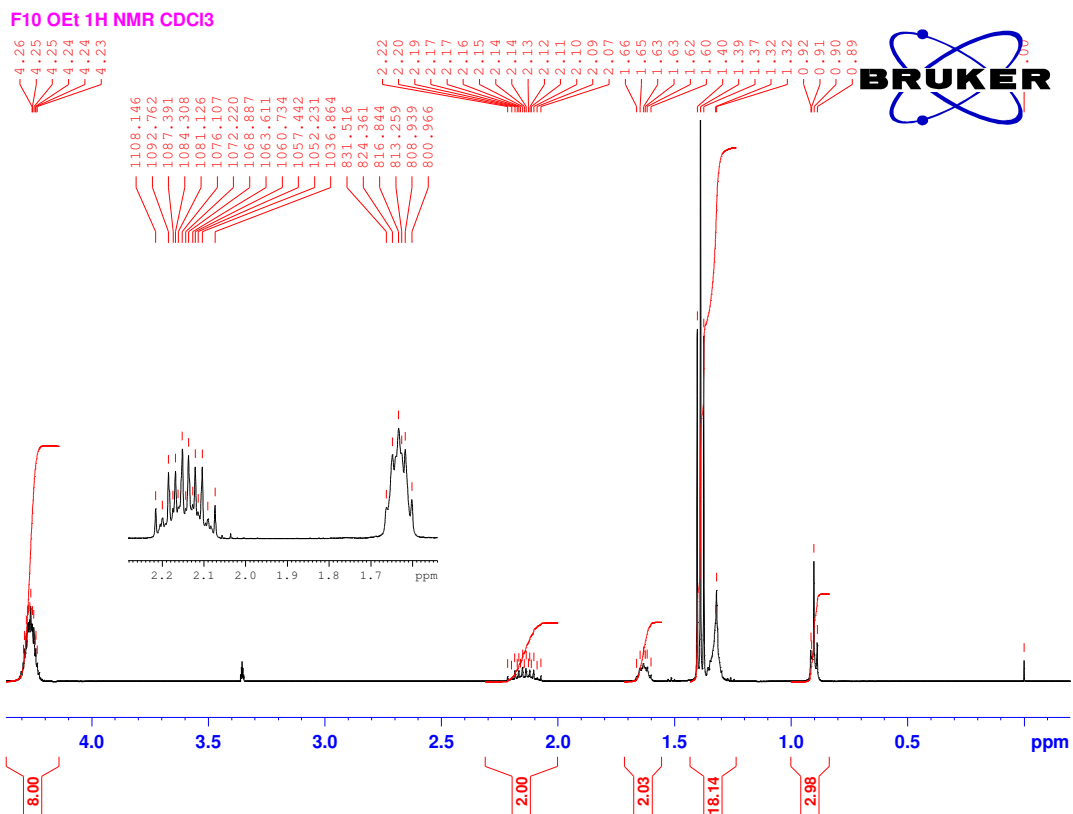
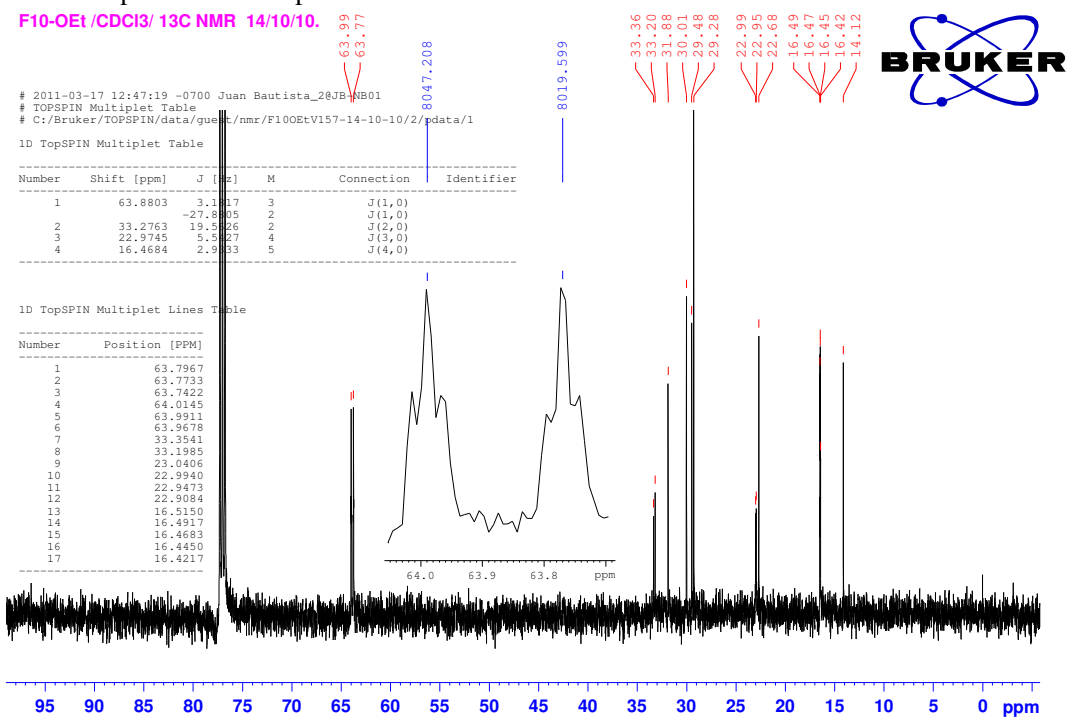
1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	13.9540	69.7462	2	J(1,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	14.1263
2	13.7818

**³¹P NMR spectrum of compound 43**

¹H NMR spectrum of compound 34¹³C NMR spectrum of compound 34

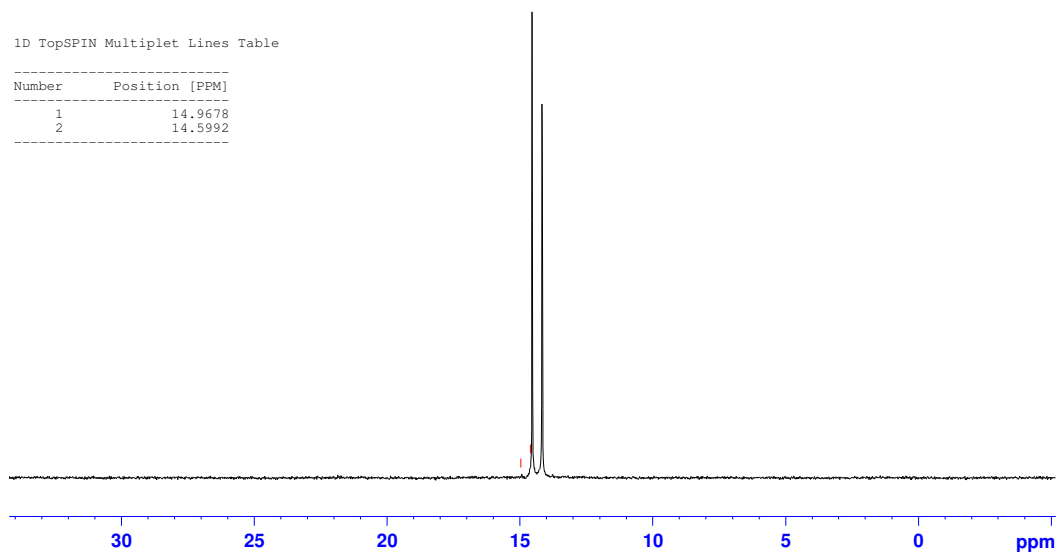
³¹P F10 (OEt) CDCl₃

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	14.7835	74.6354	2	J(1,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	14.9678
2	14.5992

**³¹P NMR spectrum of compound 34****F10 OH D2O 1H NMR**

2.00
1.97
1.96
1.93

1.46

1.17
1.14
1.13
1.12

0.72
0.70
0.69



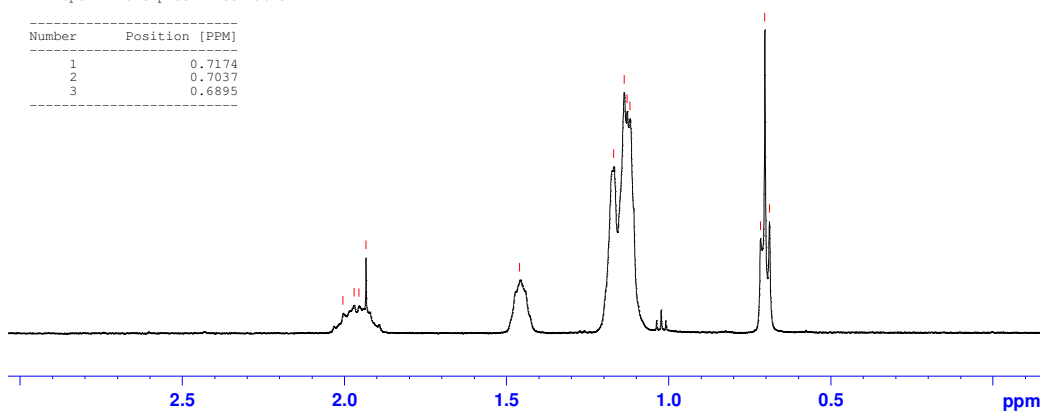
2010-09-29 17:33:20 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/V157HID/1/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	0.7034	6.9809	3	J(1,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	0.7174
2	0.7037
3	0.6895

**¹H NMR spectrum of compound 44**

F10 OH D2O 13C NMR



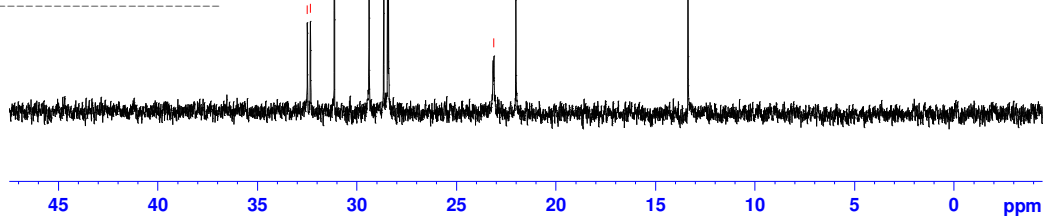
2010-09-29 17:47:42 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/V157HID/3/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	32.4184	19.9817	2	J(1,0)	
2	23.1378	5.4495	4	J(2,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	32.4979
2	32.3390
3	23.2028
4	23.1667
5	23.1161
6	23.0728

¹³C NMR spectrum of compound 44

F10 OH D2O 31P NMR decoupled with 1H "POWGATE"



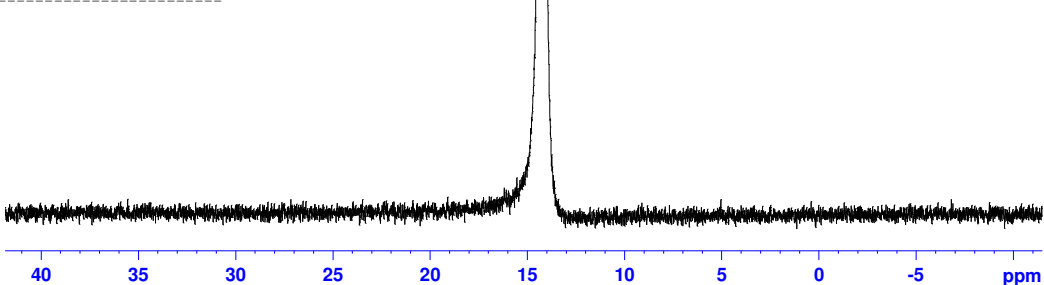
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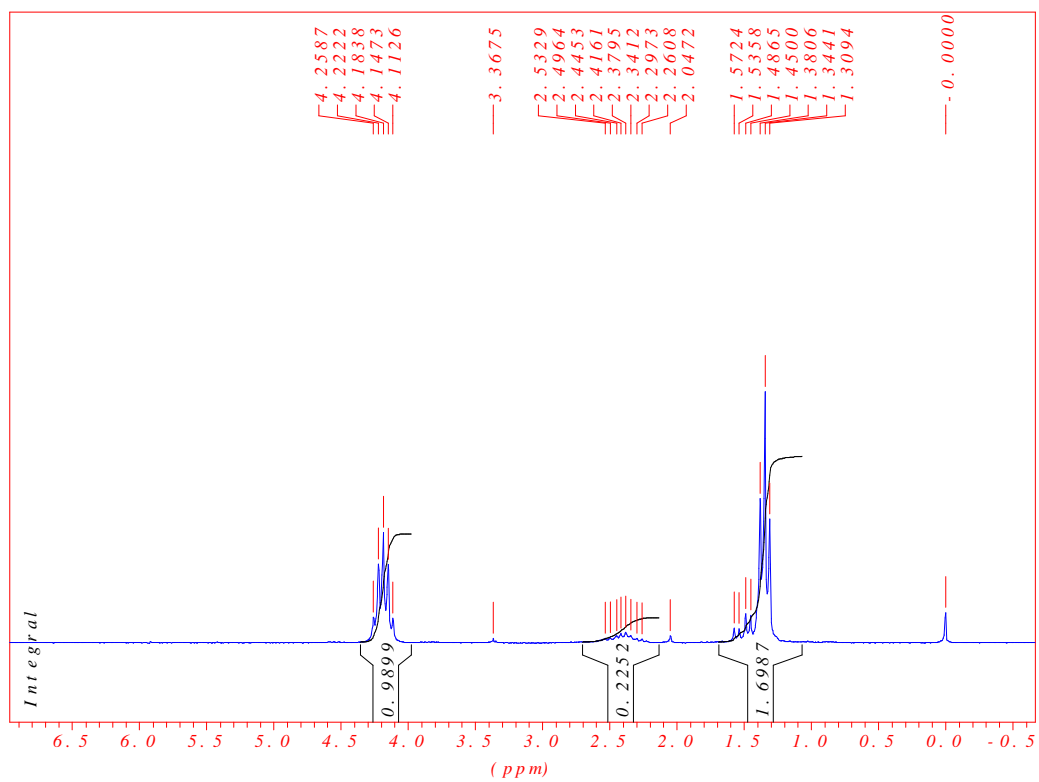
1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	14.2268	71.6229	2	J(1,0)	

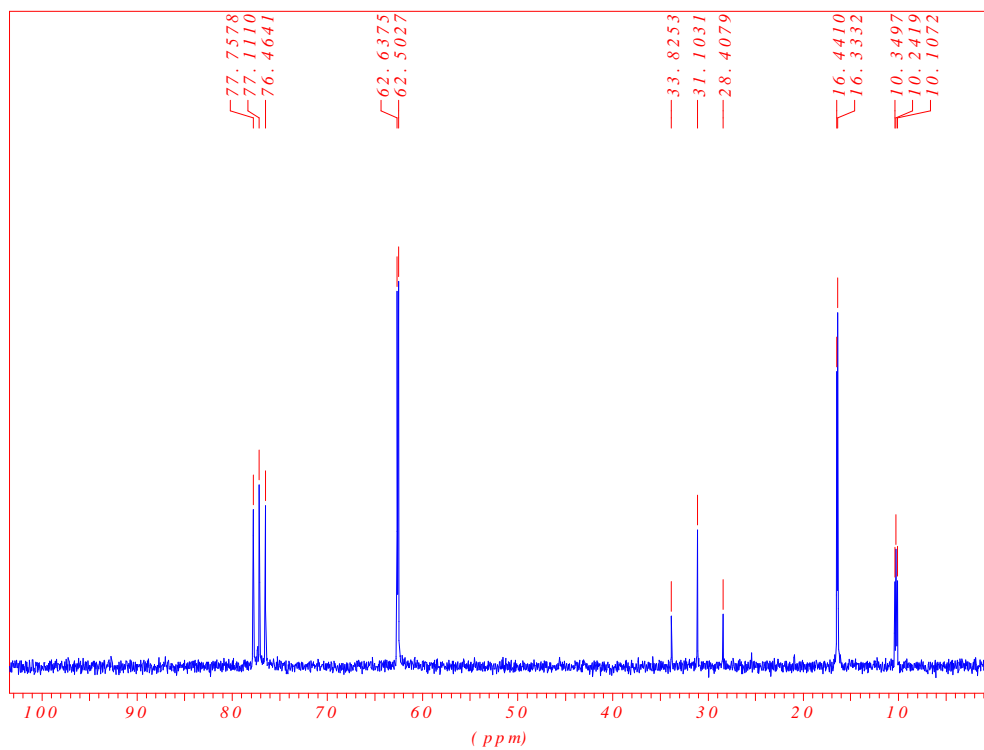
1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	14.4037
2	14.0500

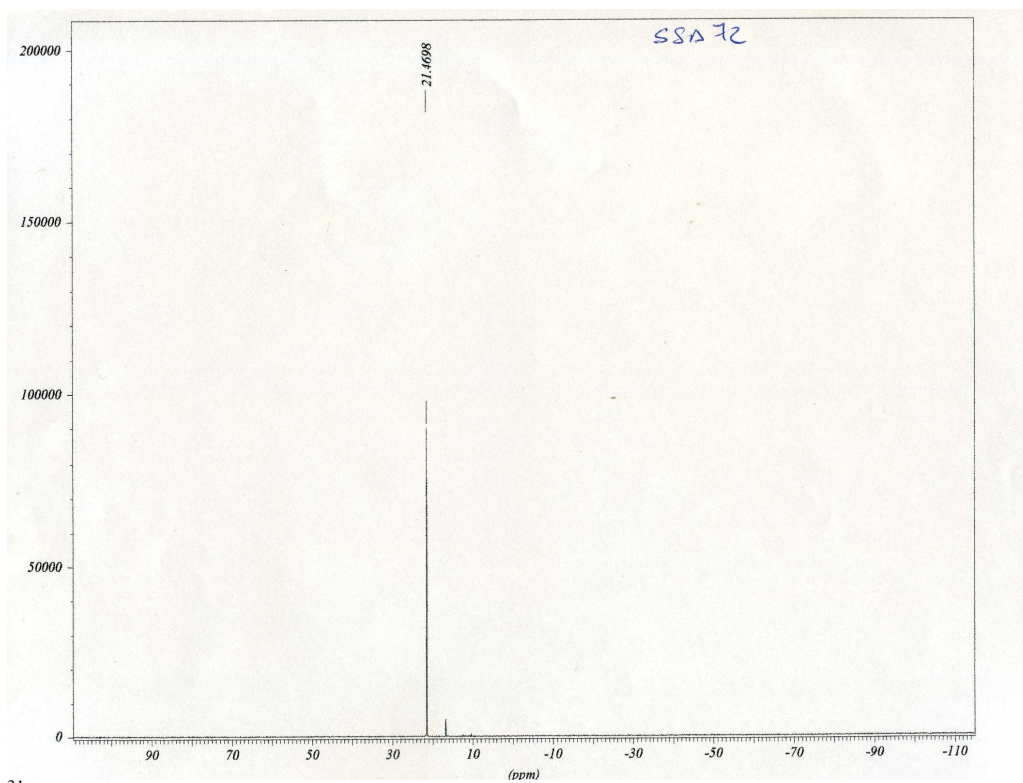
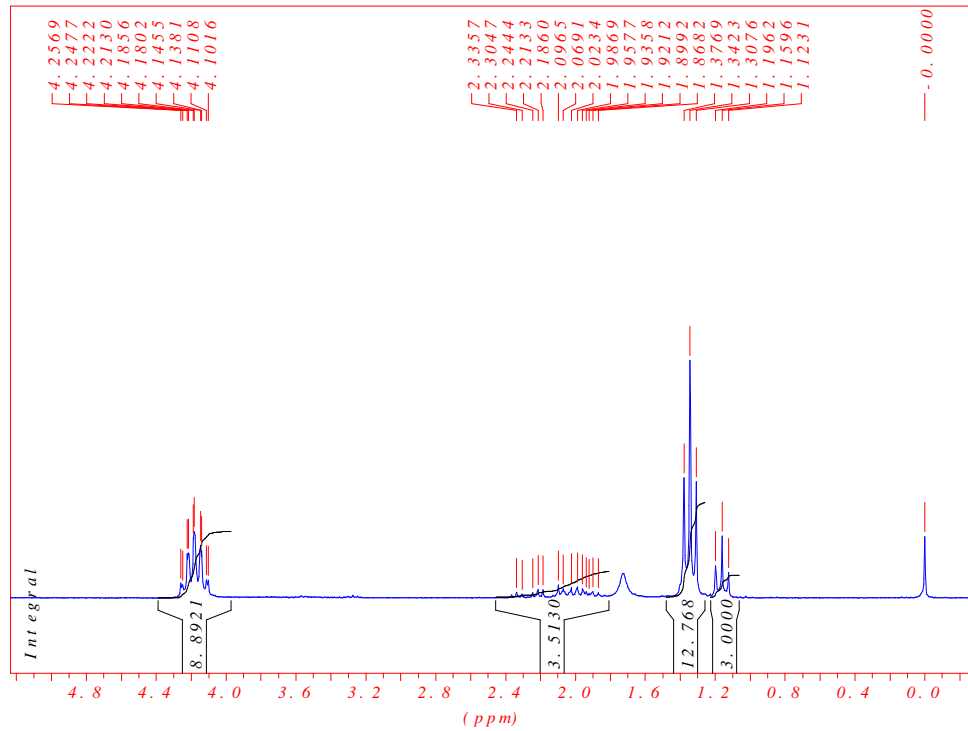
³¹P NMR spectrum of compound 44

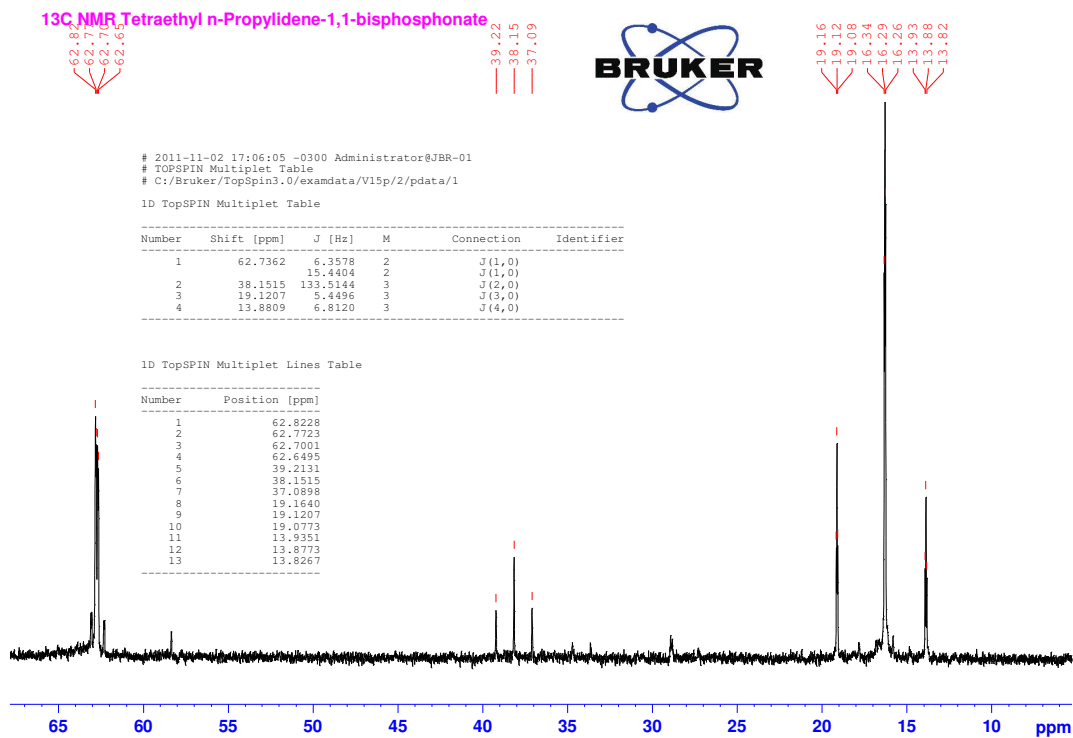


¹H NMR Spectrum of compound **16**



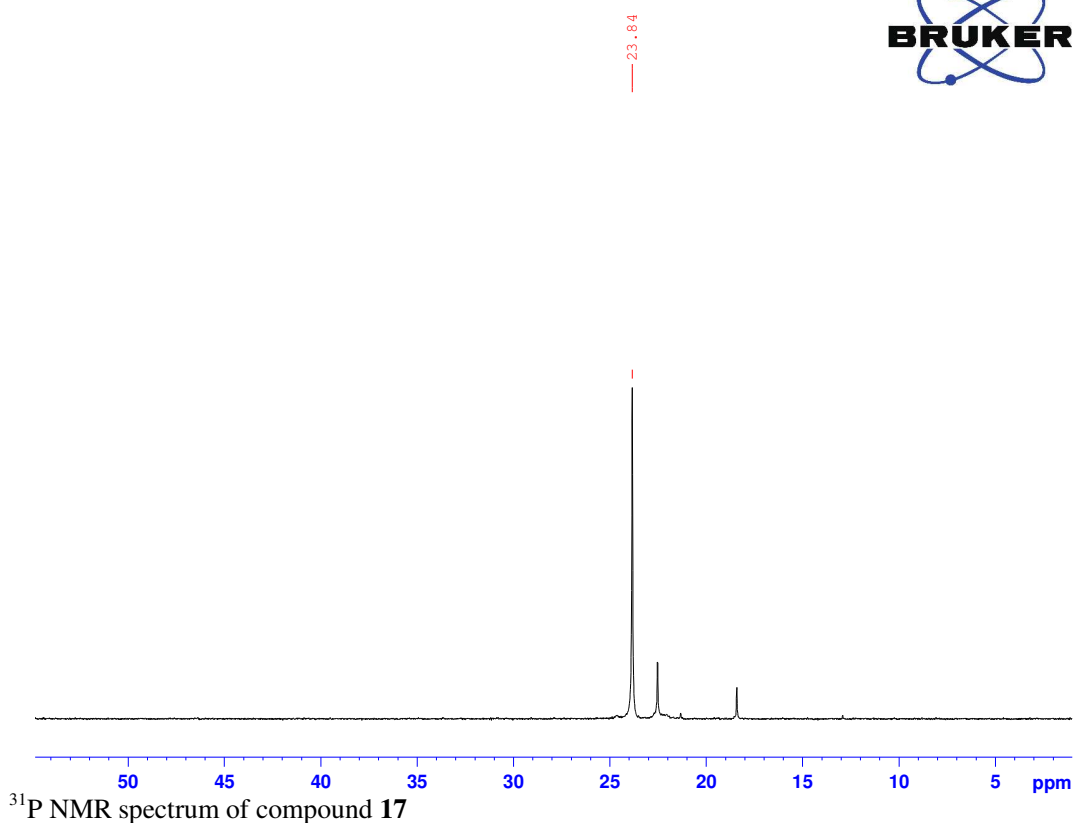
¹³C NMR Spectrum of compound **16**

 ^{31}P NMR spectrum of compound **16** ^1H NMR Spectrum of compound **17**

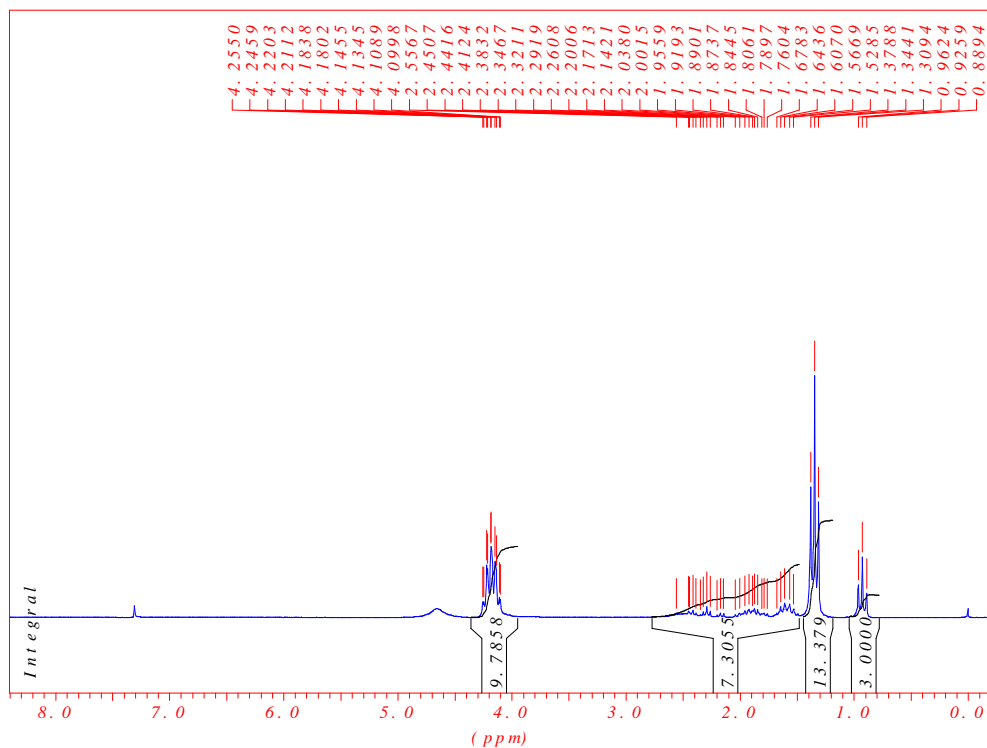
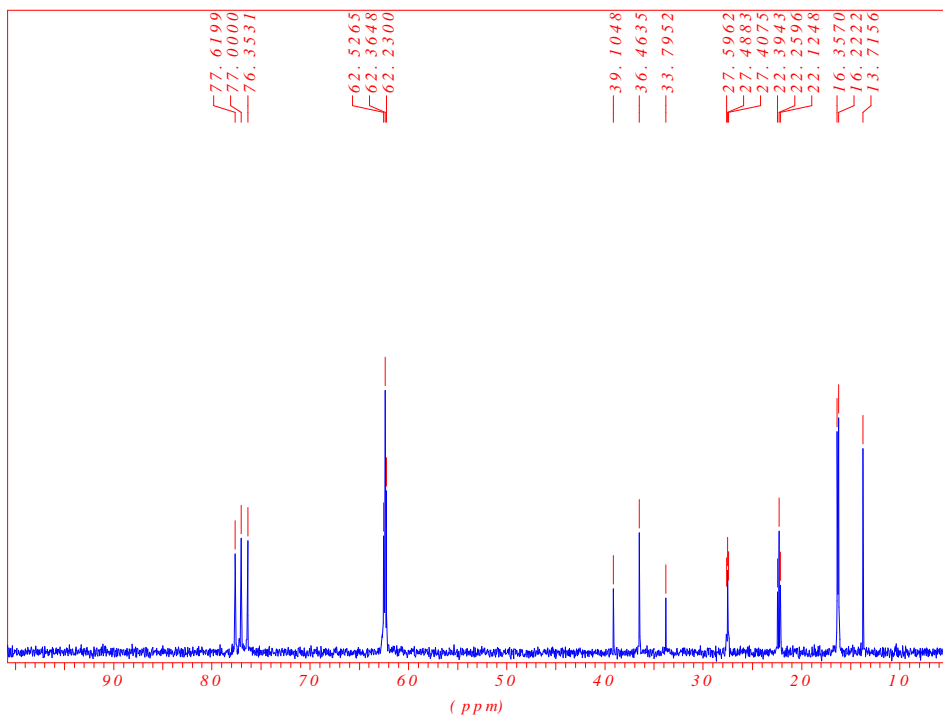


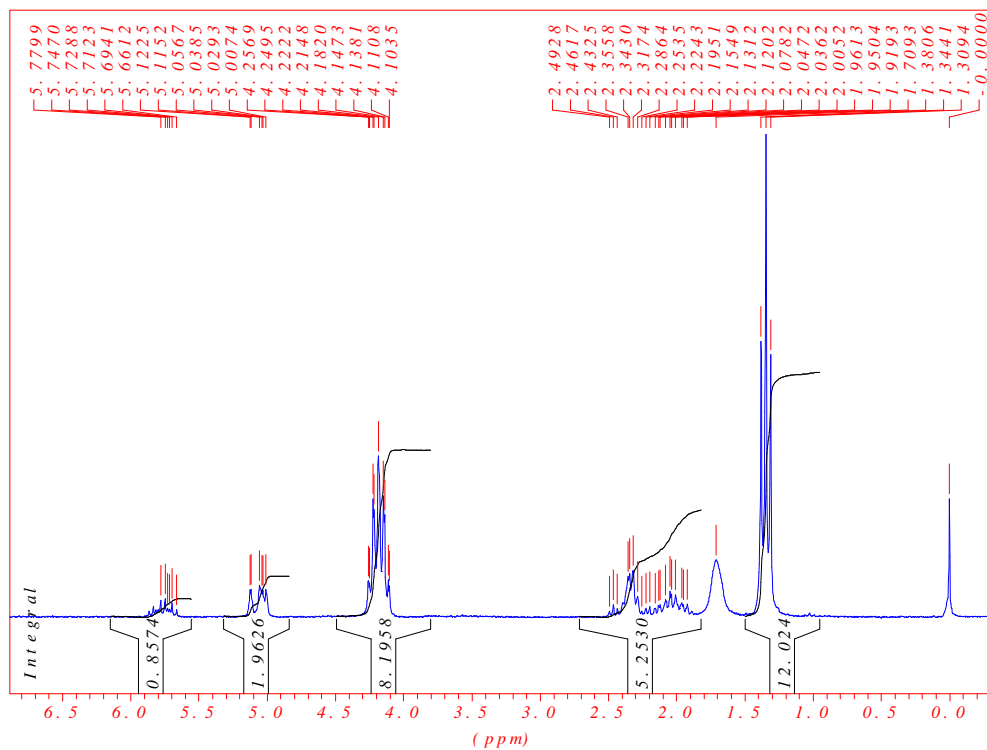
¹³C NMR Spectrum of compound 17

³¹P NMR Tetraethyl n-Propylidene-1,1-bisphosphonate

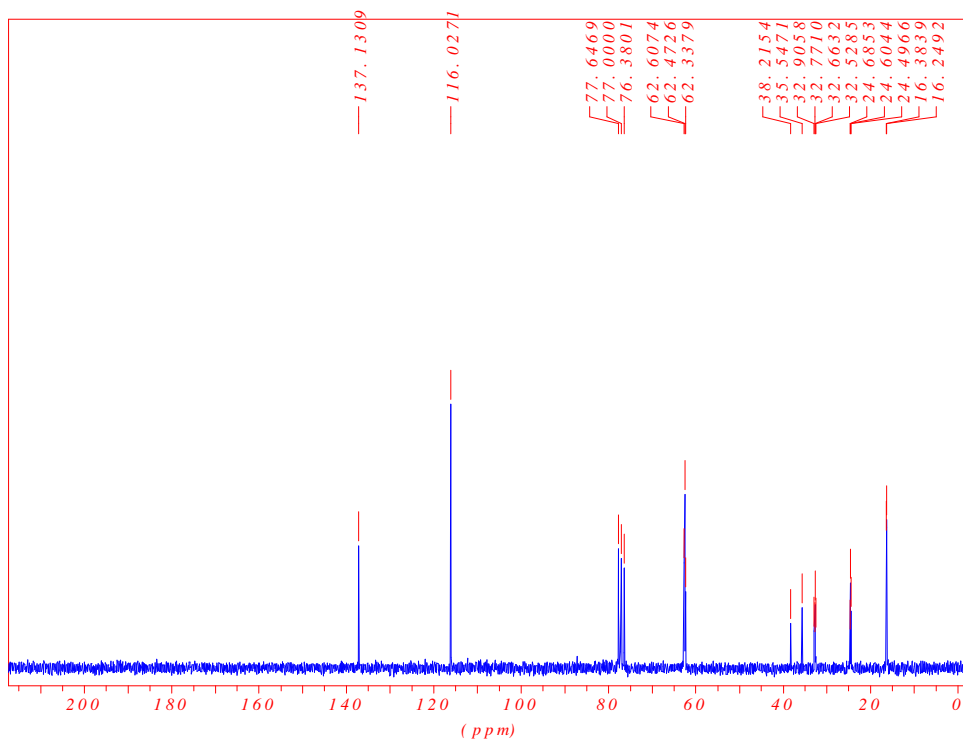


³¹P NMR spectrum of compound 17

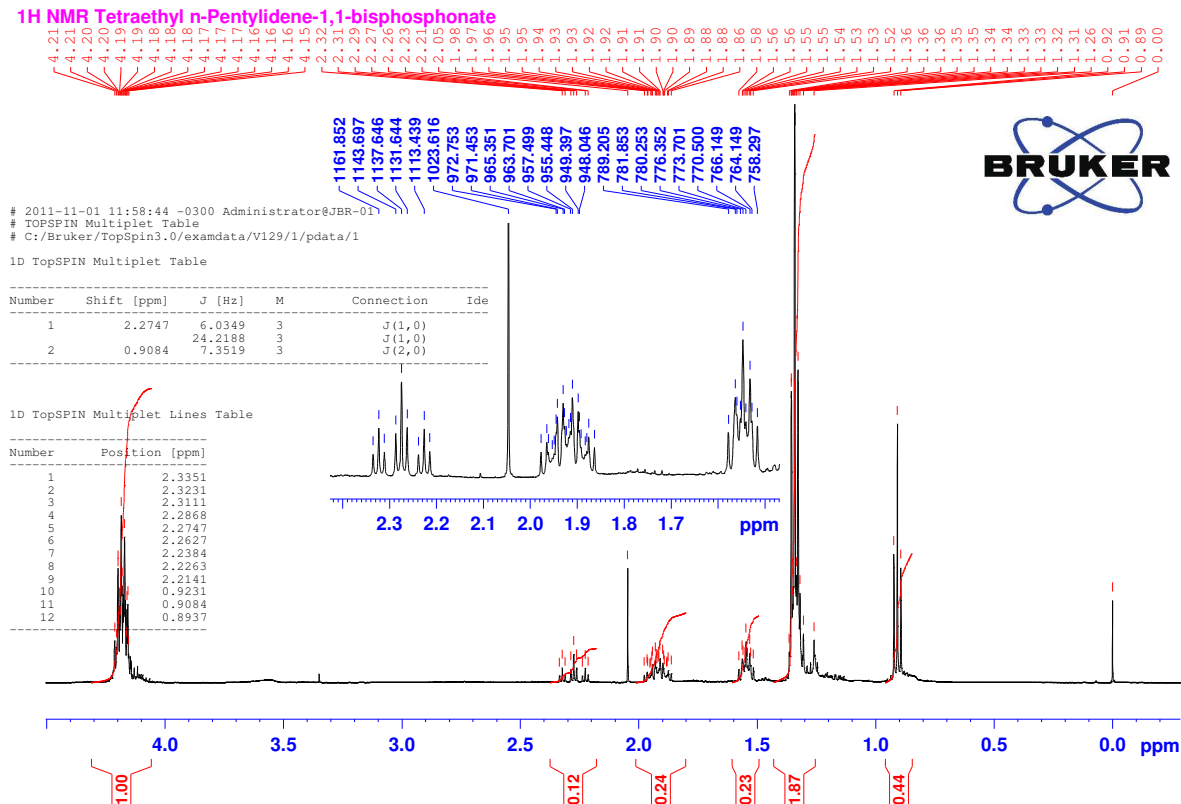
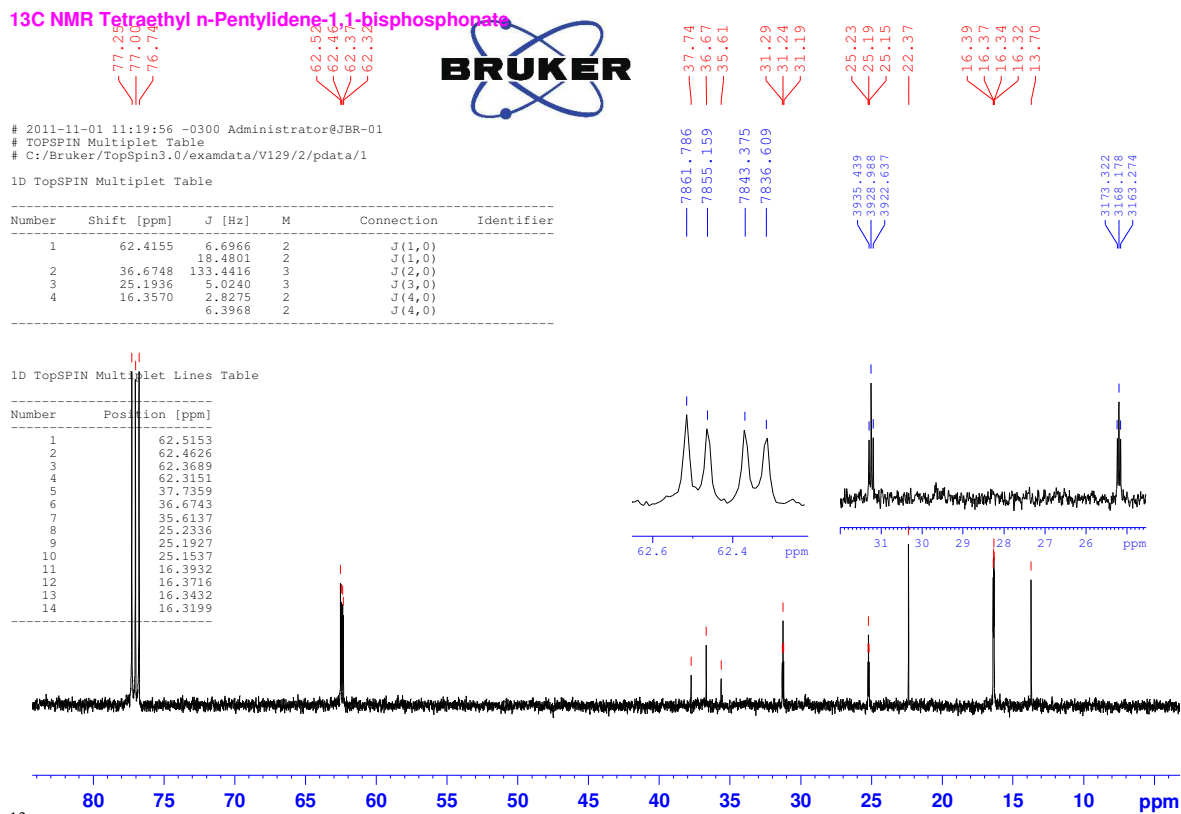
¹H NMR Spectrum of compound **18**¹³C NMR Spectrum of compound **18**

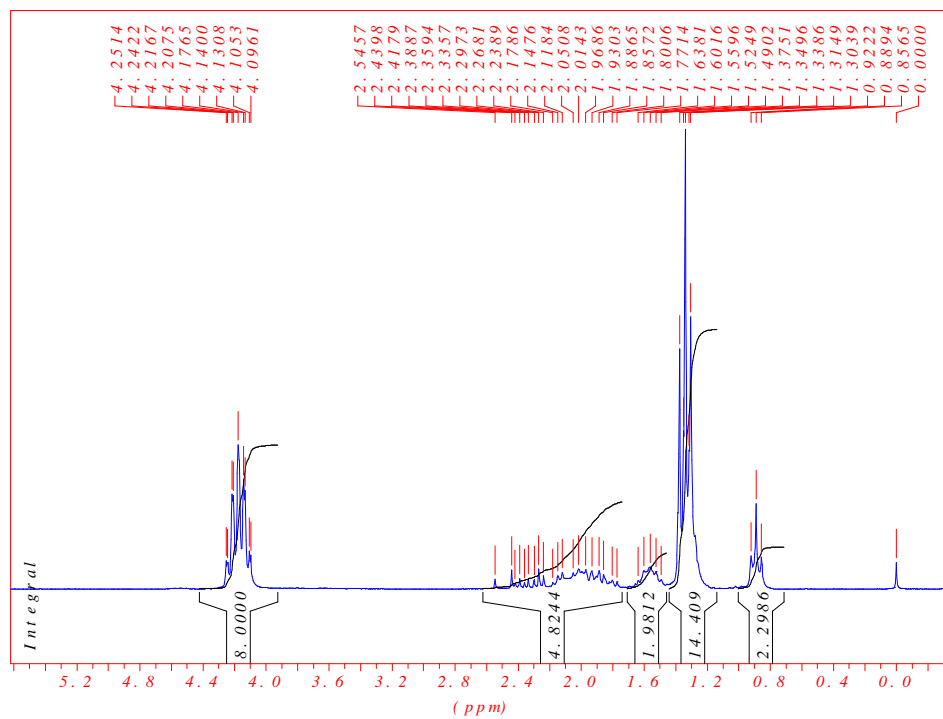
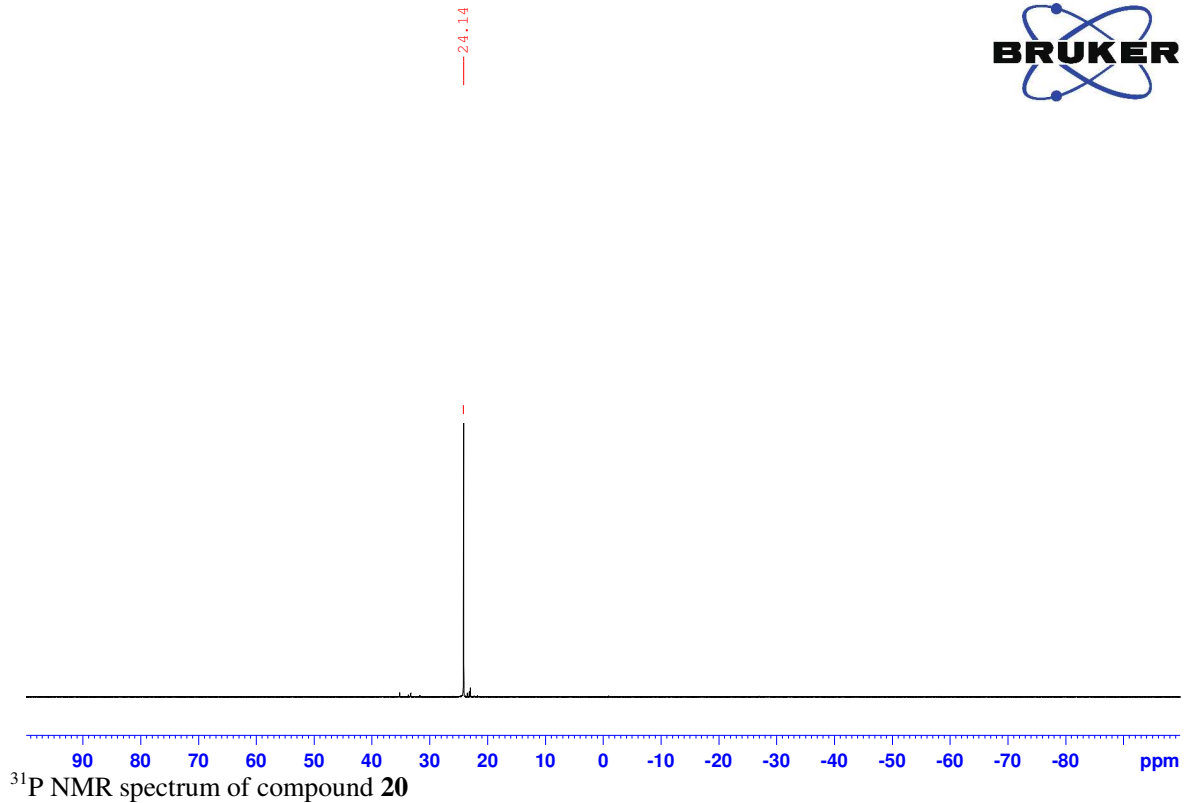


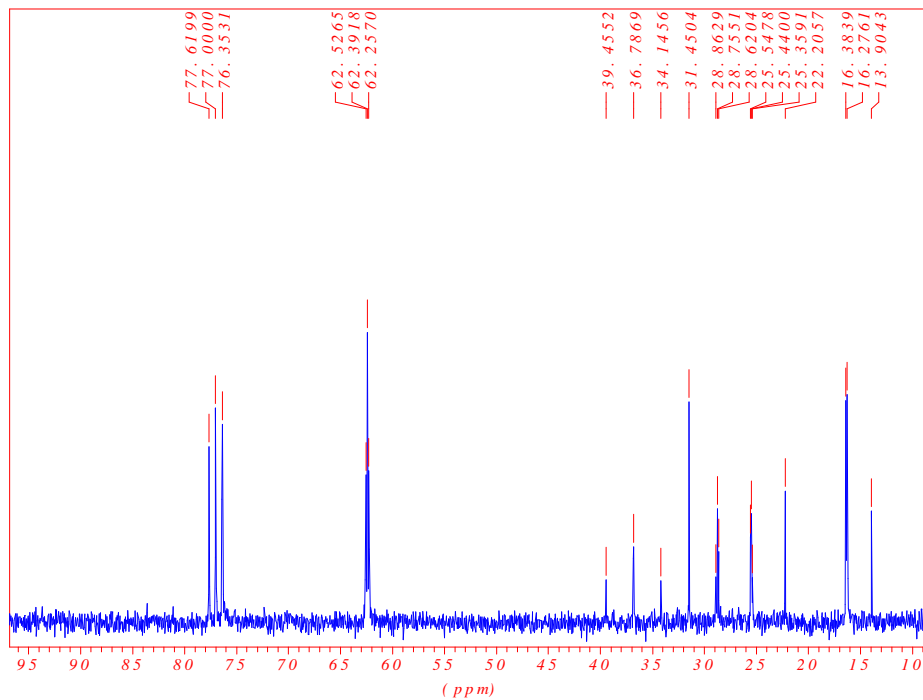
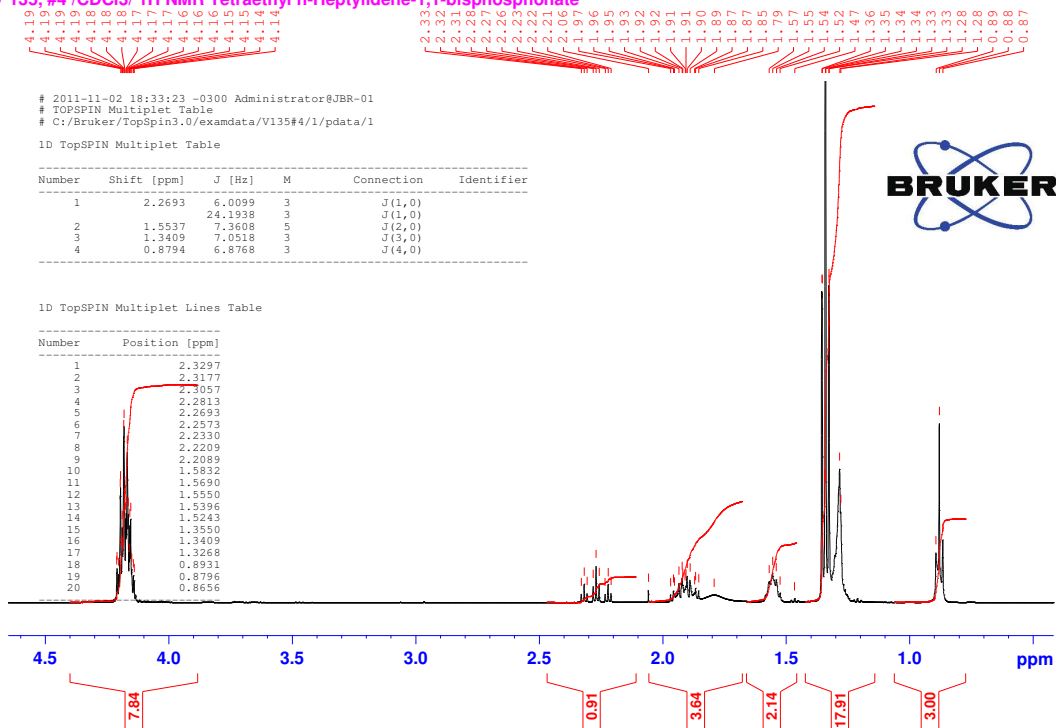
¹H NMR Spectrum of compound **19**

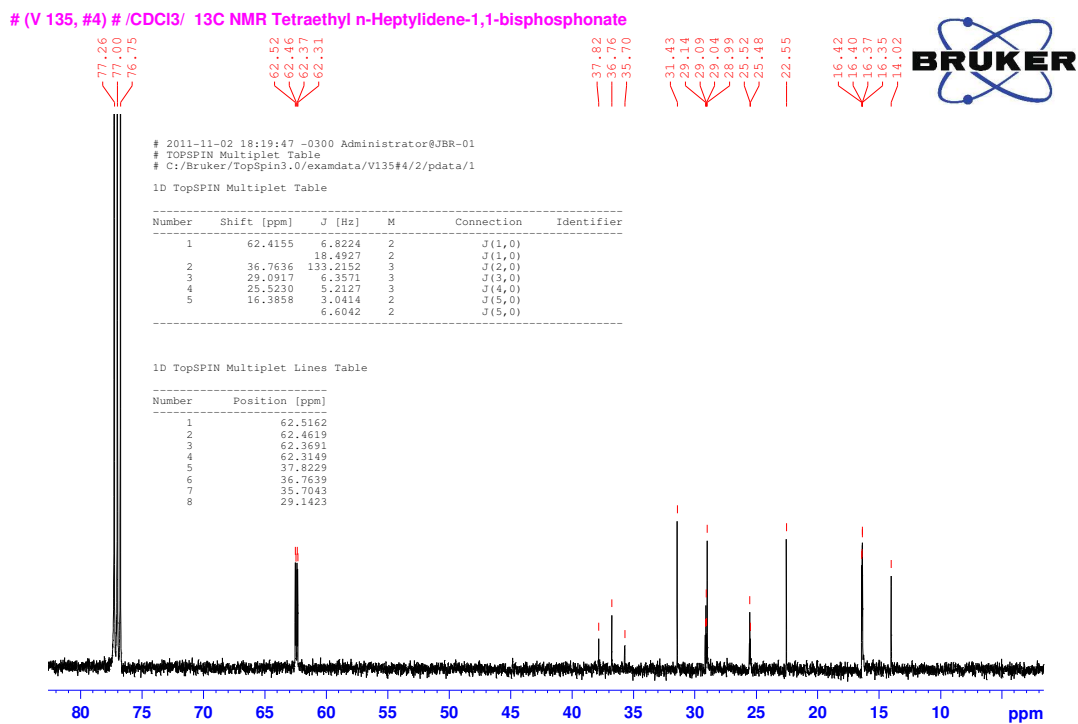
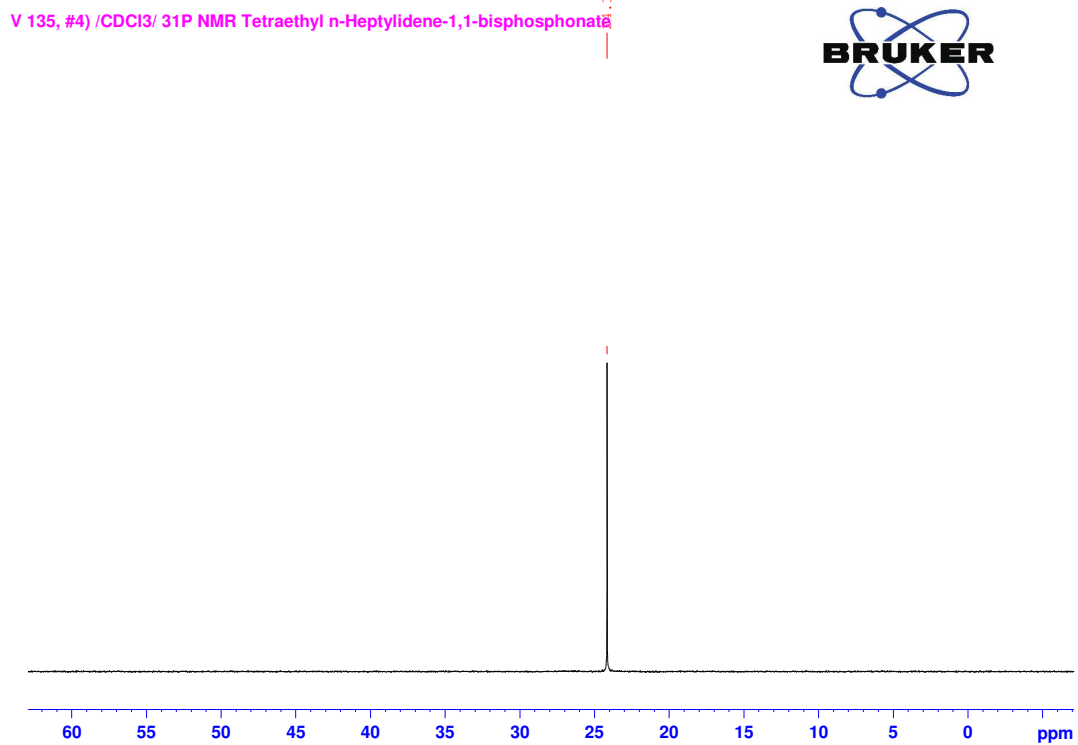


¹³C NMR Spectrum of compound **19**

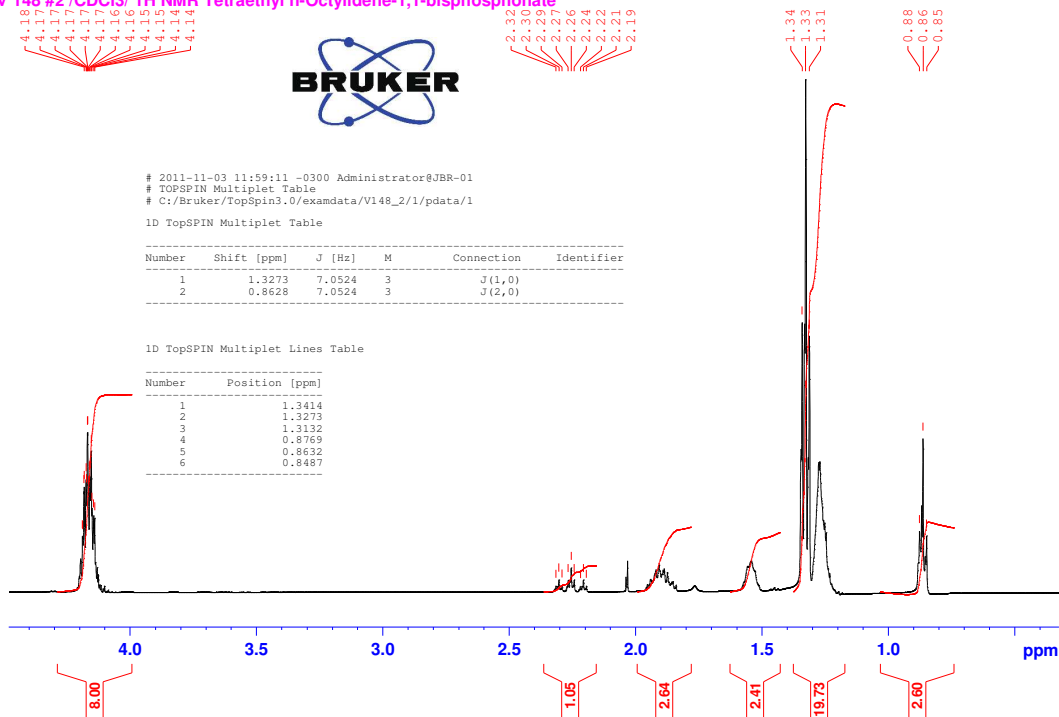
¹H NMR Tetraethyl n-Pentylidene-1,1-bisphosphonate¹H NMR spectrum of compound 20**¹³C NMR Tetraethyl n-Pentylidene-1,1-bisphosphonate**¹³C NMR spectrum of compound 20

³¹P NMR Tetraethyl n-Pentylidene-1,1-bisphosphonate**¹H NMR Spectrum of compound 21**

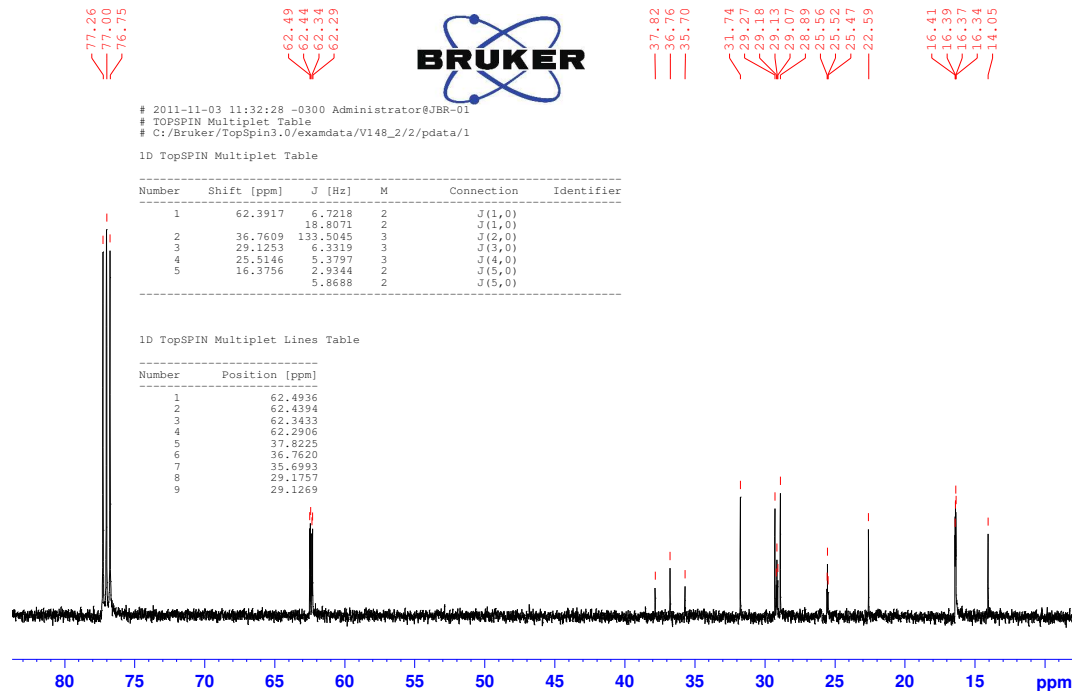
¹³C NMR Spectrum of compound 21V 135, #4 /CDCl₃/ ¹H NMR Tetraethyl n-Heptylidene-1,1-bisphosphonate¹H NMR spectrum of compound 22

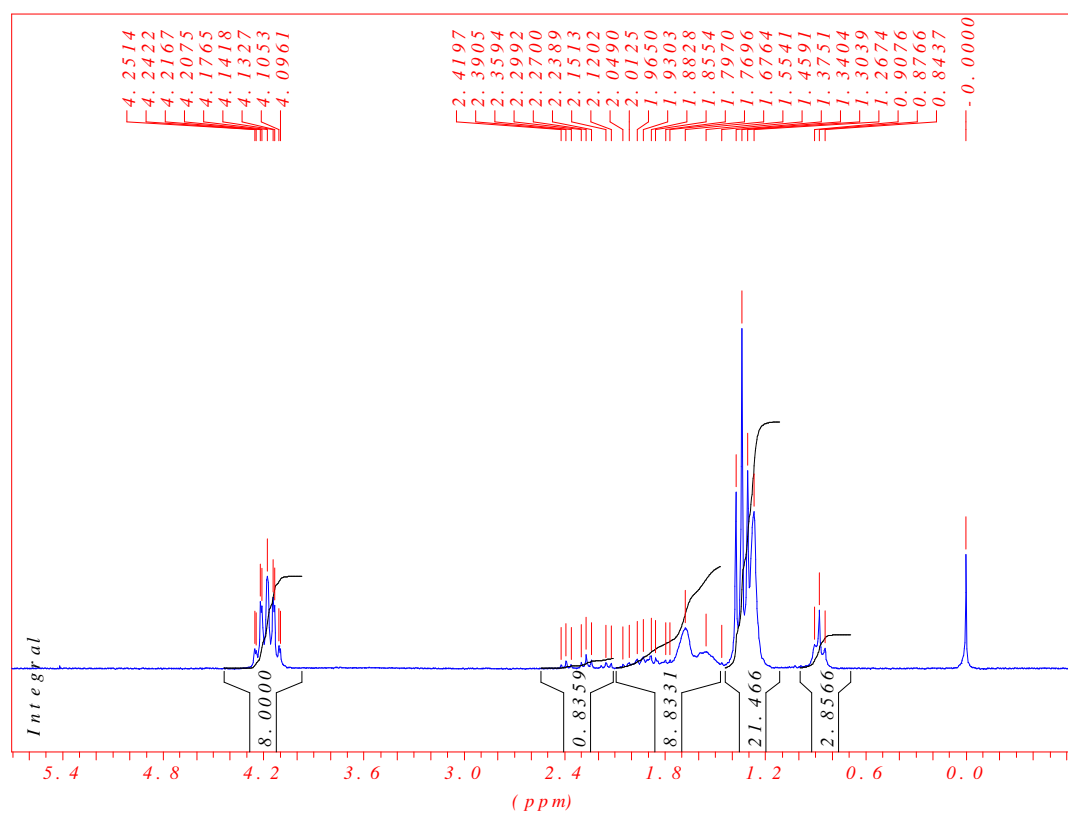
¹³C NMR spectrum of compound 22³¹P NMR spectrum of compound 22

V 148 #2 /CDCI3/ 1H NMR Tetraethyl n-Octylidene-1,1-bisphosphonate

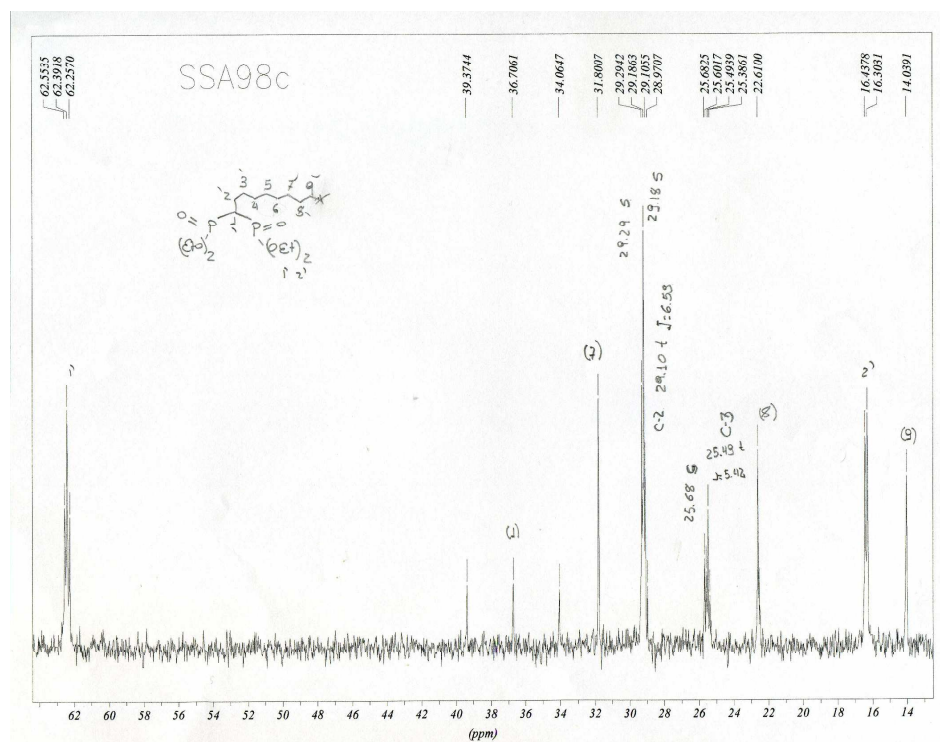


V 148 #2 /CDCI3/ 13C NMR Tetraethyl n-Octylidene-1,1-bisphosphonate





¹H NMR Spectrum of compound 24



¹³C NMR spectrum of compound 24

Sample No. 55A89 Company / School Dr. Juan B. Rodriguez SUBMITTER
 Address FACULTAD DE CIENCIAS EXACTAS Y NATURALES
DEPARTAMENTO DE QUIMICA ORGANICA
PABELLON 1, CIUDAD UNIVERSITARIA
1400 BUENOS AIRES ARGENTINA

P.O. Box 2288
 Norcross, Georgia 30091
 (770) 242-0082

NO CHARGE FOR DUPLICATES

PROFESSOR/SUPERVISOR: NAME SEP 24, 2001 DATE

Element	Theory	Found	
C	46.52	45.05	44.97
H	9.00	8.69	8.71
P	17.25	OUR LAB DOES NOT PERFORM PHOSPHORUS ANALYSIS.	

Single Duplicate
 Elements C, H, O, P
 Present: Analyze for C, H, P
 Hydroscopic Explosive
 M.P. B.P.
 To be dried: Yes No
 Temp. Vac. Time 3 h
 FAX Service 5411 4804-1692
 Fax Phone # 5411 4804-1692
 Rush Service (SEE CURRENT PRICE LIST)
 Phone Service (SEE CURRENT PRICE LIST)
 Phone No.

Date Received SEP 26 2001 Date Completed SEP 26 2001

Anal. Compd 21

Sample No. 55A87 Company / School Dr. Juan B. Rodriguez SUBMITTER
 Address FACULTAD DE CIENCIAS EXACTAS Y NATURALES
DEPARTAMENTO DE QUIMICA ORGANICA
PABELLON 1, CIUDAD UNIVERSITARIA
1400 BUENOS AIRES ARGENTINA

P.O. Box 2288
 Norcross, Georgia 30091
 (770) 242-0082

NO CHARGE FOR DUPLICATES

PROFESSOR/SUPERVISOR: NAME SEP 24, 2001 DATE

Element	Theory	Found	
C	48.38	47.41	47.49
H	9.20	9.13	9.27
P	16.64	OUR LAB DOES NOT PERFORM PHOSPHORUS ANALYSIS.	

Single Duplicate
 Elements C, H, O, P
 Present: Analyze for C, H, P
 Hydroscopic Explosive
 M.P. B.P.
 To be dried: Yes No
 Temp. Vac. Time 3 h
 FAX Service 5411 4804-1692
 Fax Phone # 5411 4804-1692
 Rush Service (SEE CURRENT PRICE LIST)
 Phone Service (SEE CURRENT PRICE LIST)
 Phone No.

Date Received SEP 26 2001 Date Completed SEP 26 2001

Anal. Compound 22.

Sample No. 55A86 Company / School Dr. Juan B. Rodriguez SUBMITTER
 Address FACULTAD DE CIENCIAS EXACTAS Y NATURALES
DEPARTAMENTO DE QUIMICA ORGANICA
PABELLON 1, CIUDAD UNIVERSITARIA
1400 BUENOS AIRES ARGENTINA

P.O. Box 2288
 Norcross, Georgia 30091
 (770) 242-0082

NO CHARGE FOR DUPLICATES

PROFESSOR/SUPERVISOR: NAME SEP 24, 2001 DATE

Element	Theory	Found	
C	49.73	49.26	49.21
H	9.39	9.68	9.61
P	16.03	NOTE: OUR LAB DOES NOT PERFORM PHOSPHORUS ANALYSIS.	

Single Duplicate
 Elements C, H, O, P
 Present: Analyze for C, H, P
 Hydroscopic Explosive
 M.P. B.P.
 To be dried: Yes No
 Temp. Vac. Time
 FAX Service 5411 4804-1692
 Fax Phone # 5411 4804-1692
 Rush Service (SEE CURRENT PRICE LIST)
 Phone Service (SEE CURRENT PRICE LIST)
 Phone No.

Date Received SEP 26 2001 Date Completed SEP 26 2001

Anal. Compound 23.