

Electronic Supplementary Information

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

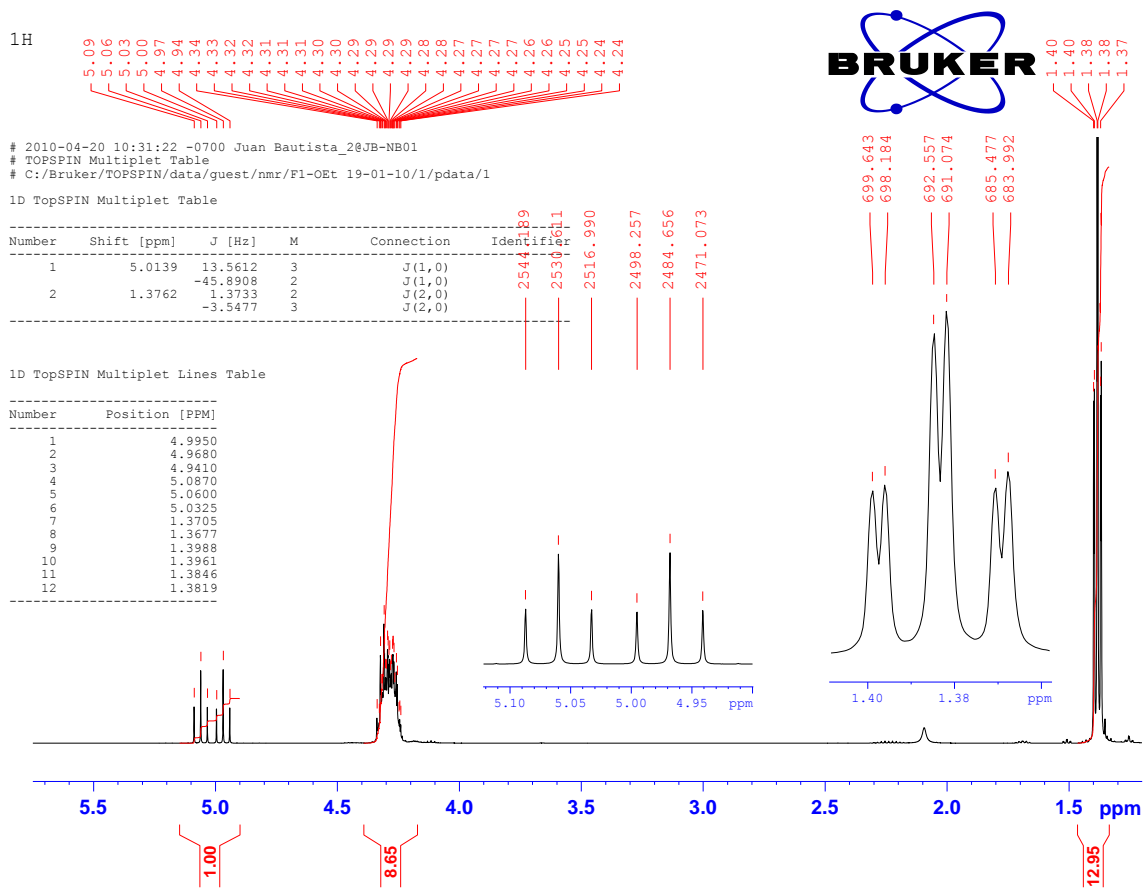
Sergio H. Szajnman,^a Valeria S. Rosso,^{a,b} Leena Malayil,^b Alyssa Smith,^b Silvia N. J. Moreno,^b Roberto Docampo,^b and Juan B. Rodriguez^{a,*}

^a*Departamento de Química Orgánica and UMYMFOR (CONICET-FCEyN), Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Pabellón 2, Ciudad Universitaria, C1428EHA, Buenos Aires, Argentina,* ^b*Center for Tropical and Emerging Global Diseases and Department of Cellular Biology, University of Georgia, Athens, Georgia, 30602, USA*

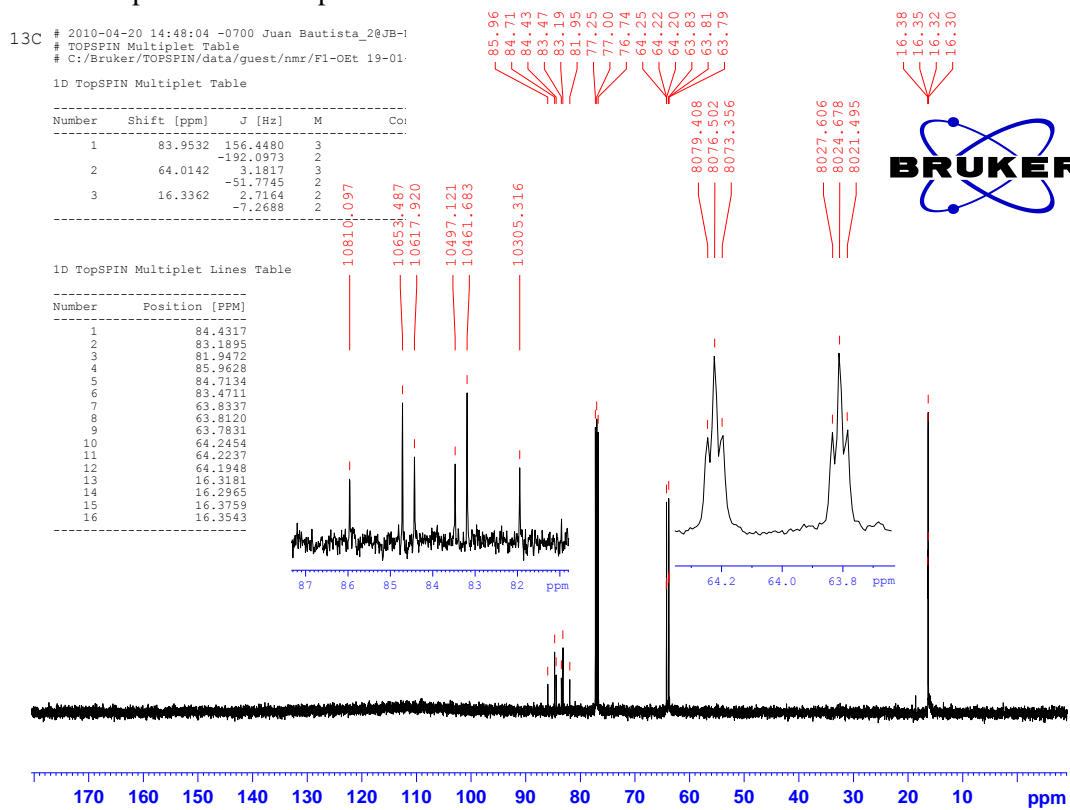
List of Contents

¹ H NMR spectrum of compound 14	Page 3
¹³ C NMR spectrum of compound 14	Page 3
³¹ P NMR spectrum of compound 14	Page 4
¹ H NMR spectrum of compound 35	Page 4
¹³ C NMR spectrum of compound 35	Page 5
³¹ P NMR spectrum of compound 35	Page 5
¹ H NMR spectrum of compound 26	Page 6
¹³ C NMR spectrum of compound 26	Page 6
³¹ P NMR spectrum of compound 26	Page 7
¹ H NMR spectrum of compound 36	Page 7
¹³ C NMR spectrum of compound 36	Page 8
³¹ P NMR spectrum of compound 36	Page 8
¹ H NMR spectrum of compound 27	Page 9
¹³ C NMR spectrum of compound 27	Page 9
³¹ P NMR spectrum of compound 27	Page 10
¹ H NMR spectrum of compound 37	Page 10
¹³ C NMR spectrum of compound 37	Page 11
³¹ P NMR spectrum of compound 37	Page 11
¹ H NMR spectrum of compound 28	Page 12
¹³ C NMR spectrum of compound 28	Page 12
³¹ P NMR spectrum of compound 28	Page 13
¹ H NMR spectrum of compound 38	Page 13
¹³ C NMR spectrum of compound 38	Page 14
³¹ P NMR spectrum of compound 38	Page 14
¹ H NMR spectrum of compound 29	Page 15
¹³ C NMR spectrum of compound 29	Page 15
³¹ P NMR spectrum of compound 29	Page 16
¹ H NMR spectrum of compound 39	Page 16
¹³ C NMR spectrum of compound 39	Page 17
¹ H NMR spectrum of compound 30	Page 17

¹³ C NMR spectrum of compound 30	Page 18
³¹ P NMR spectrum of compound 30	Page 18
¹ H NMR spectrum of compound 40	Page 19
¹³ C NMR spectrum of compound 40	Page 19
¹ H NMR spectrum of compound 31	Page 20
¹³ C NMR spectrum of compound 31	Page 20
³¹ P NMR spectrum of compound 31	Page 21
¹ H NMR spectrum of compound 41	Page 21
¹³ C NMR spectrum of compound 41	Page 22
³¹ P NMR spectrum of compound 41	Page 22
¹ H NMR spectrum of compound 32	Page 23
¹³ C NMR spectrum of compound 32	Page 23
³¹ P NMR spectrum of compound 32	Page 24
¹ H NMR spectrum of compound 42	Page 24
¹³ C NMR spectrum of compound 42	Page 25
³¹ P NMR spectrum of compound 42	Page 25
¹ H NMR spectrum of compound 33	Page 26
¹³ C NMR spectrum of compound 33	Page 26
³¹ P NMR spectrum of compound 33	Page 27
¹ H NMR spectrum of compound 43	Page 27
¹³ C NMR spectrum of compound 43	Page 28
³¹ P NMR spectrum of compound 43	Page 28
¹ H NMR spectrum of compound 34	Page 29
¹³ C NMR spectrum of compound 34	Page 29
³¹ P NMR spectrum of compound 34	Page 30
¹ H NMR spectrum of compound 44	Page 30
¹³ C NMR spectrum of compound 44	Page 31
³¹ P NMR spectrum of compound 44	Page 31
¹ H NMR spectrum of compound 16	Page 32
¹³ C NMR spectrum of compound 16	Page 32
³¹ P NMR spectrum of compound 16	Page 33
¹ H NMR spectrum of compound 17	Page 33
¹³ C NMR spectrum of compound 17	Page 34
³¹ P NMR spectrum of compound 17	Page 34
¹ H NMR spectrum of compound 18	Page 35
¹³ C NMR spectrum of compound 18	Page 35
¹ H NMR spectrum of compound 19	Page 36
¹³ C NMR spectrum of compound 19	Page 36
¹ H NMR spectrum of compound 20	Page 37
¹³ C NMR spectrum of compound 20	Page 37
³¹ P NMR spectrum of compound 20	Page 38
¹ H NMR spectrum of compound 21	Page 38
¹³ C NMR spectrum of compound 21	Page 39
¹ H NMR spectrum of compound 22	Page 39
¹³ C NMR spectrum of compound 22	Page 40
³¹ P NMR spectrum of compound 22	Page 40
¹ H NMR spectrum of compound 23	Page 41
¹³ C NMR spectrum of compound 23	Page 41
¹ H NMR spectrum of compound 24	Page 42
¹³ C NMR spectrum of compound 24	Page 42
Copy of the Elemental Analysis for compound 21	Page 43
Copy of the Elemental Analysis for compound 22	Page 43
Copy of the Elemental Analysis for compound 23	Page 43



¹H NMR spectrum of compound 14



¹³C NMR spectrum of compound 14

³¹P F1-(OEt)3



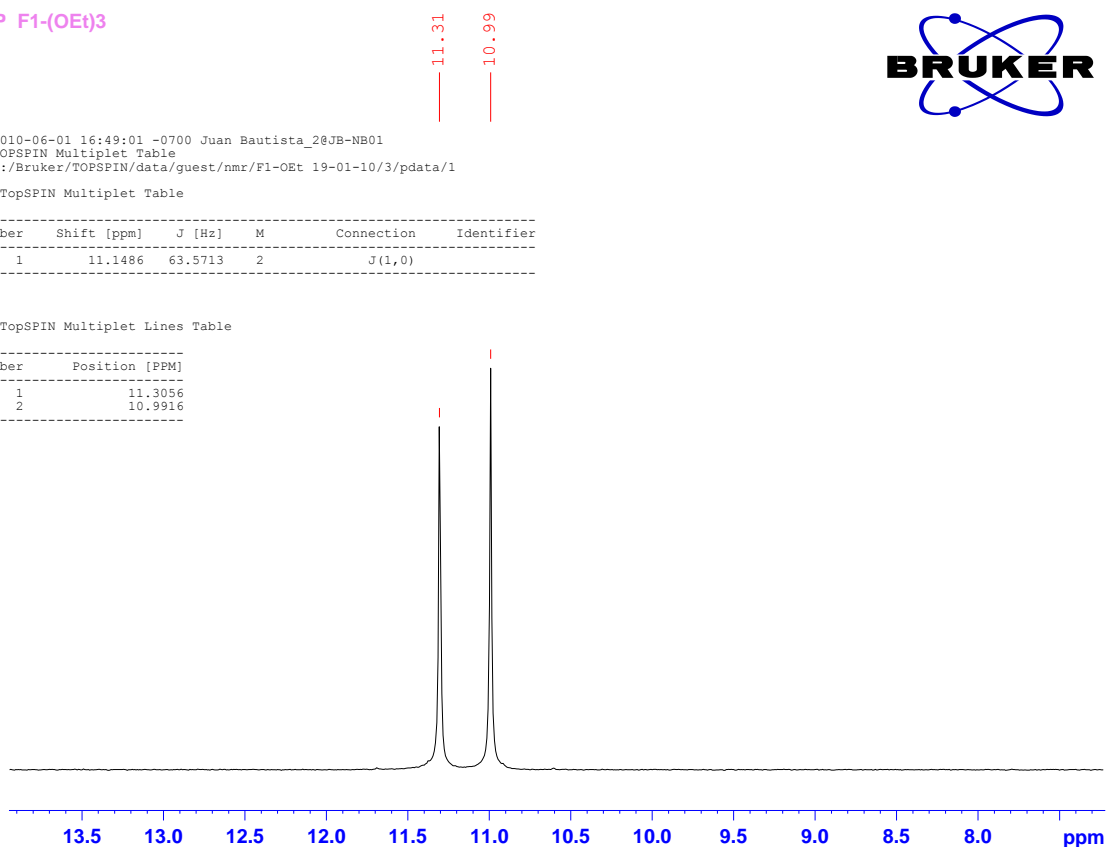
2010-06-01 16:49:01 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/F1-OEt 19-01-10/3/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	11.1486	63.5713	2	J(1,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	11.3056
2	10.9916



³¹P NMR spectrum of compound 14

PMA120-1H

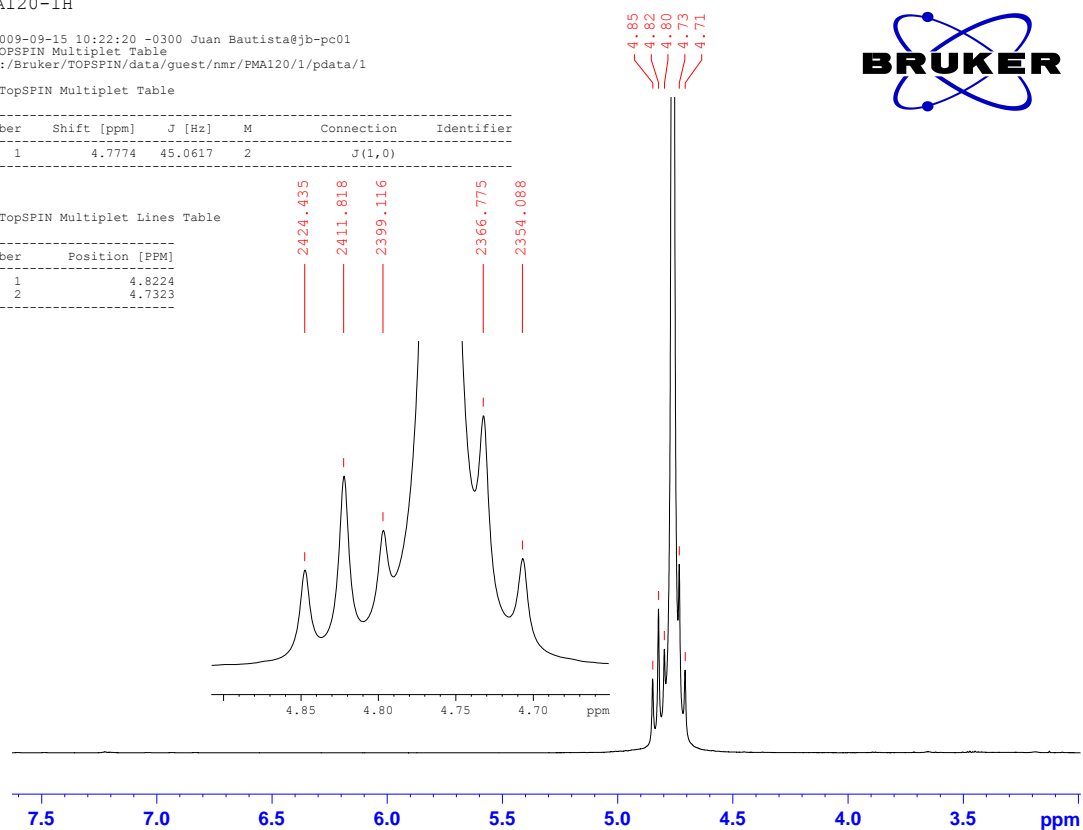
2009-09-15 10:22:20 -0300 Juan Bautista@jb-pc01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/PMA120/1/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	4.7774	45.0617	2	J(1,0)	

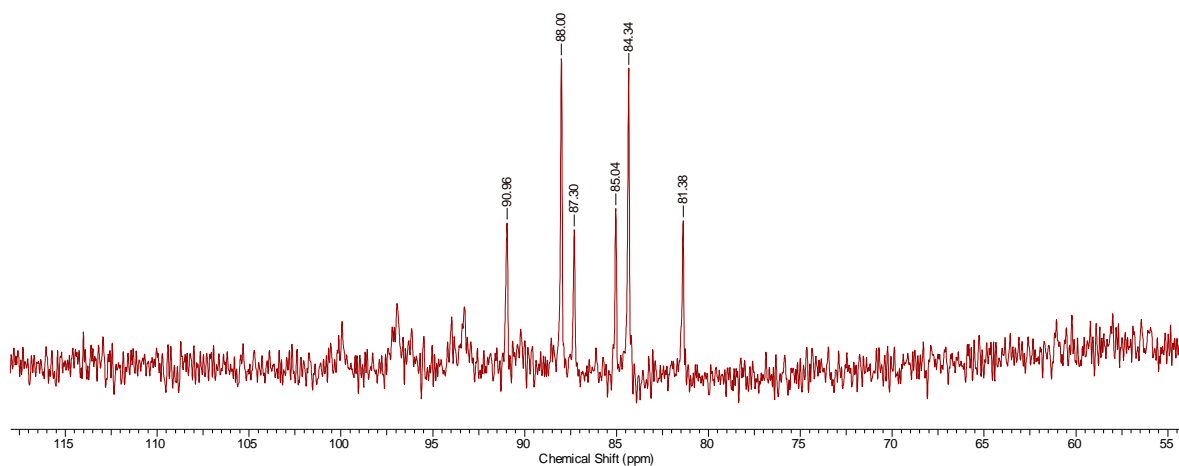
1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	4.8224
2	4.7323



¹H NMR spectrum of compound 35

Acquisition Time (sec)	0.7447	Date	02 Jun 2010 14:54:00	File Name	C:\Documents\RMNI\PMA120C(dmsd).int				
Frequency (MHz)	50.33	Nucleus	¹³ C	Number of Transients	16960	Original Points Count	8192	Points Count	32768
Solvent	Cl ₃ CD	Sweep Width (Hz)	11000.00						



No.	(ppm)	(Hz)	Height
1	81.38	4095.5	0.0116
2	84.34	4244.6	0.0240
3	85.04	4279.8	0.0126
4	87.30	4393.6	0.0108
5	88.00	4428.9	0.0248
6	90.96	4577.9	0.0114

¹³C NMR spectrum of compound 35

PMA120-P31

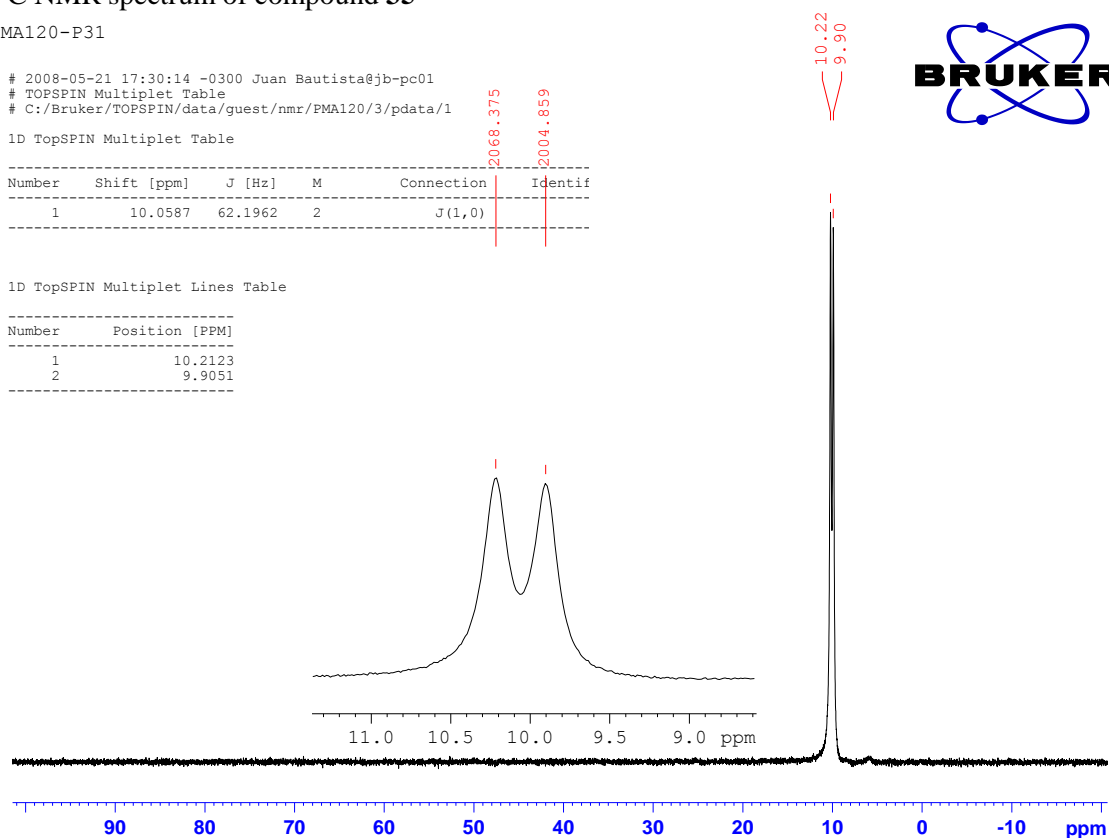
2008-05-21 17:30:14 -0300 Juan Bautista@jb-pc01
 # TOPSPIN Multiplet Table
 # C:/Bruker/TOPSPIN/data/guest/nmr/PMA120/3/pdata/1

1D TopSPIN Multiplet Table

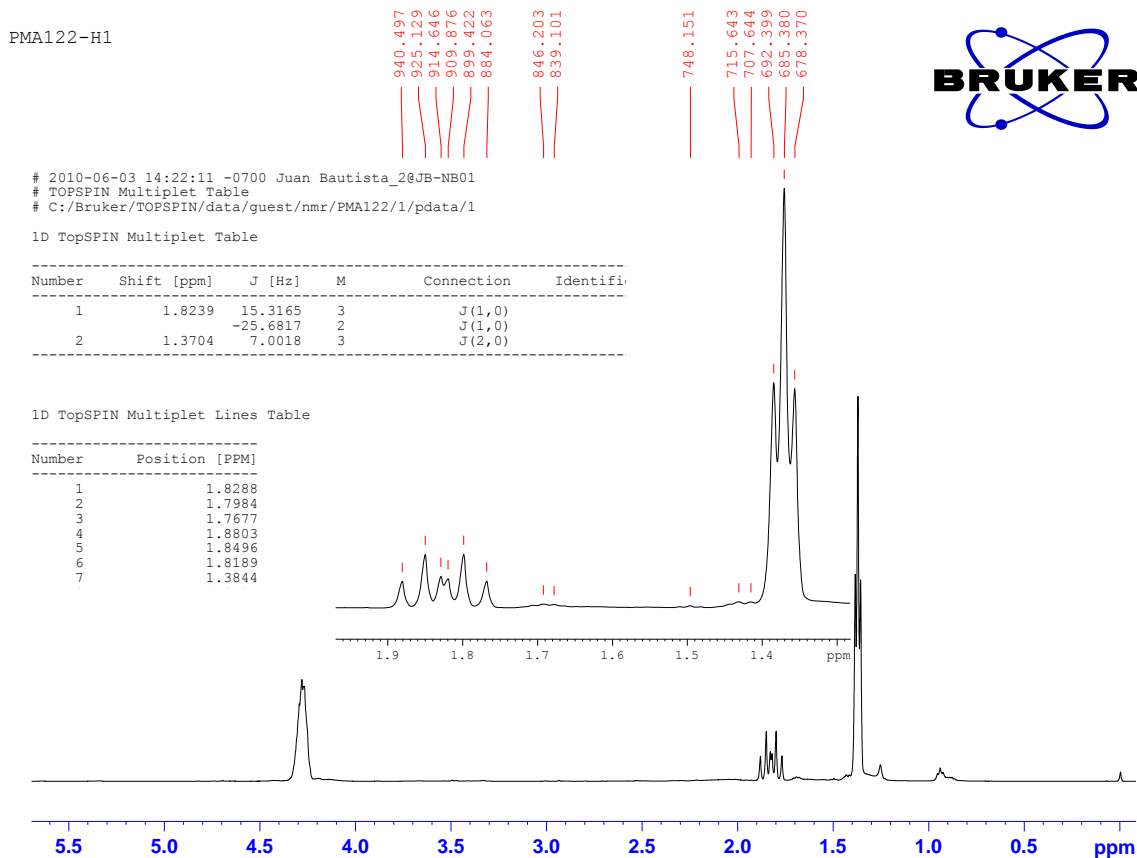
Number	Shift [ppm]	J [Hz]	M	Connection	Identif
1	10.0587	62.1962	2	J(1,0)	

1D TopSPIN Multiplet Lines Table

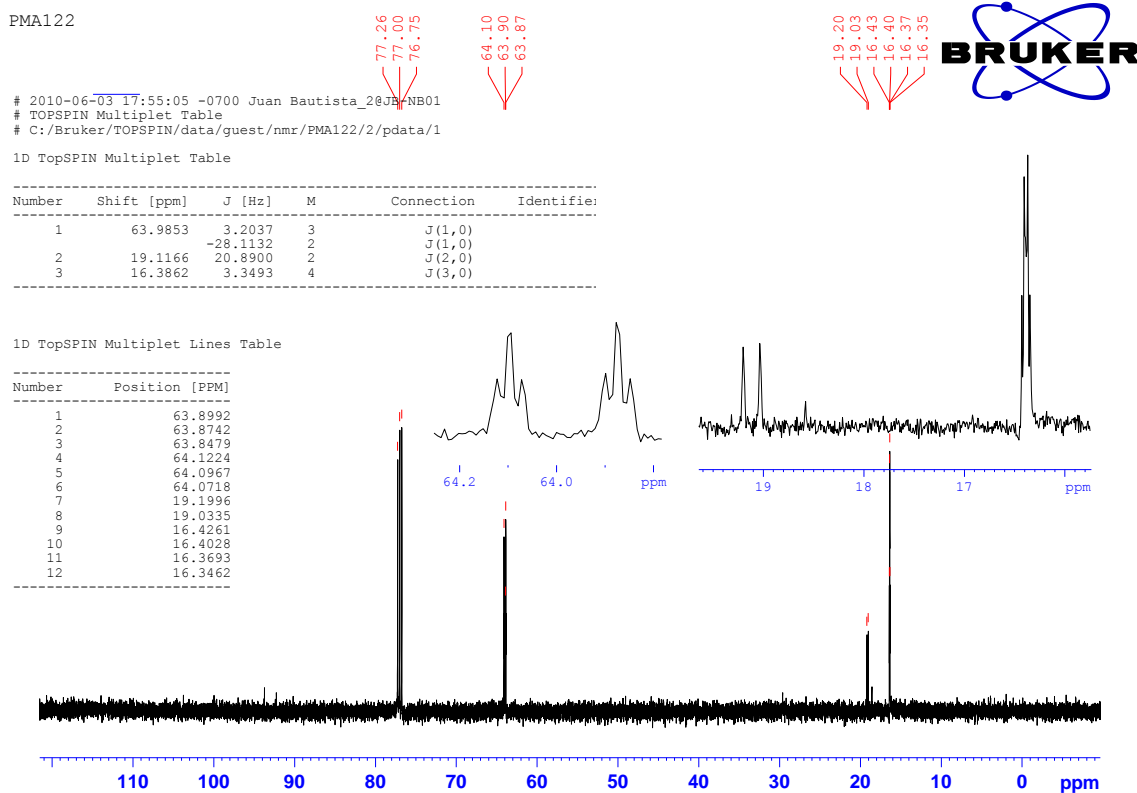
Number	Position [PPM]
1	10.2123
2	9.9051



³¹P NMR spectrum of compound 35



¹H NMR spectrum of compound **26**



¹³C NMR spectrum of compound **26**

PMA122-31P



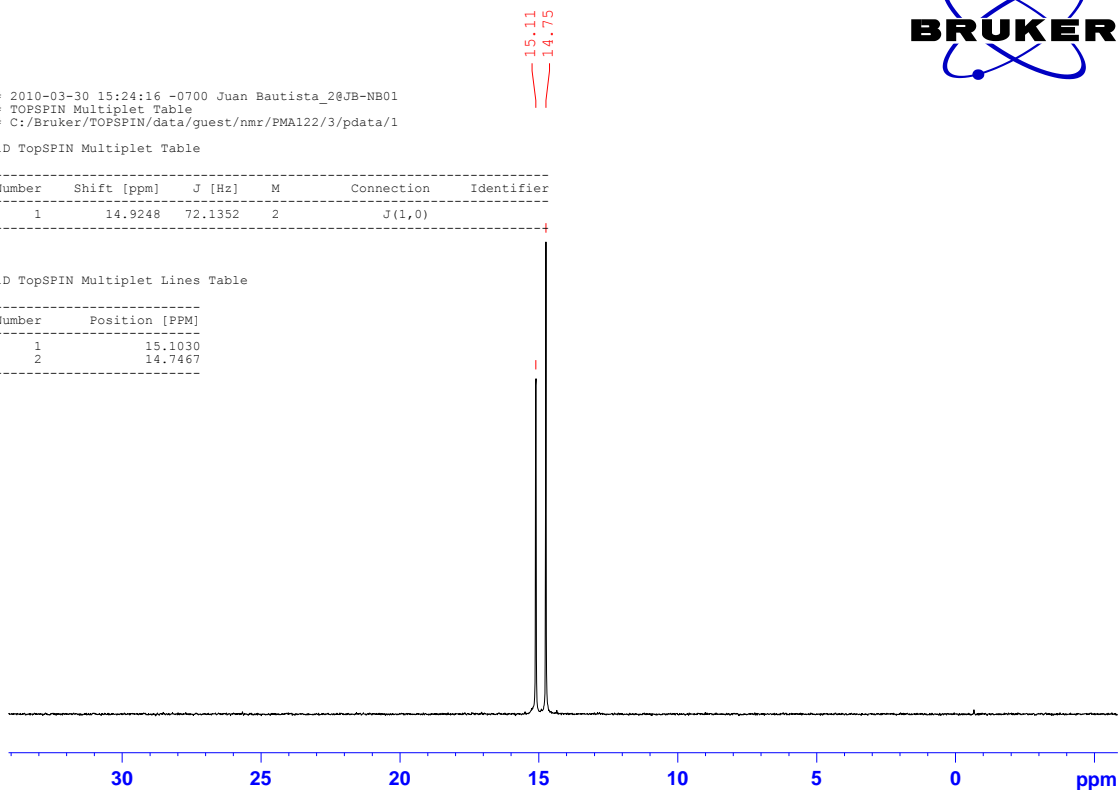
2010-03-30 15:24:16 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/PMA122/3/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	14.9248	72.1352	2	J(1,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	15.1030
2	14.7467



³¹P NMR spectrum of compound **26**

¹H

1.71
1.68
1.66
1.63
1.60



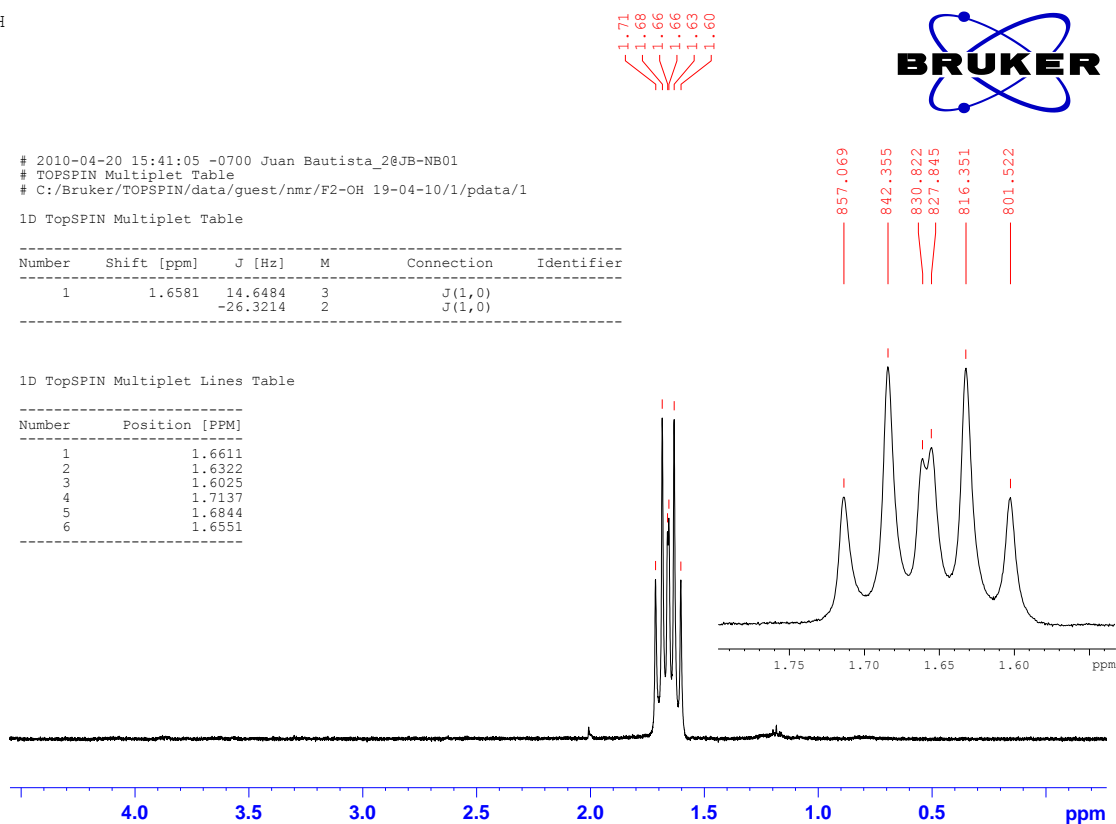
2010-04-20 15:41:05 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/F2-OH 19-04-10/1/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	1.6581	14.6484	3	J(1,0)	
		-26.3214	2	J(1,0)	

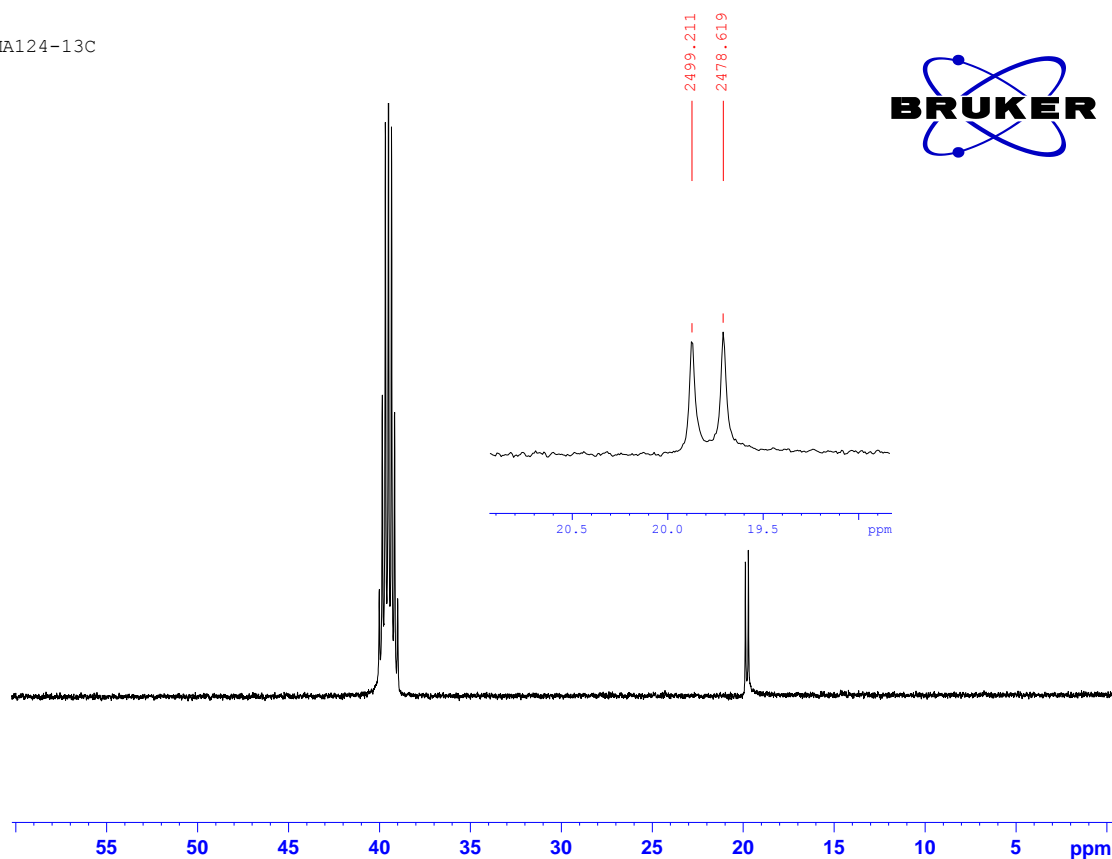
1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	1.6611
2	1.6322
3	1.6025
4	1.7137
5	1.6844
6	1.6551



¹H NMR spectrum of compound **36**

PMA124-13C



¹³C NMR spectrum of compound 36

PMA124-31P

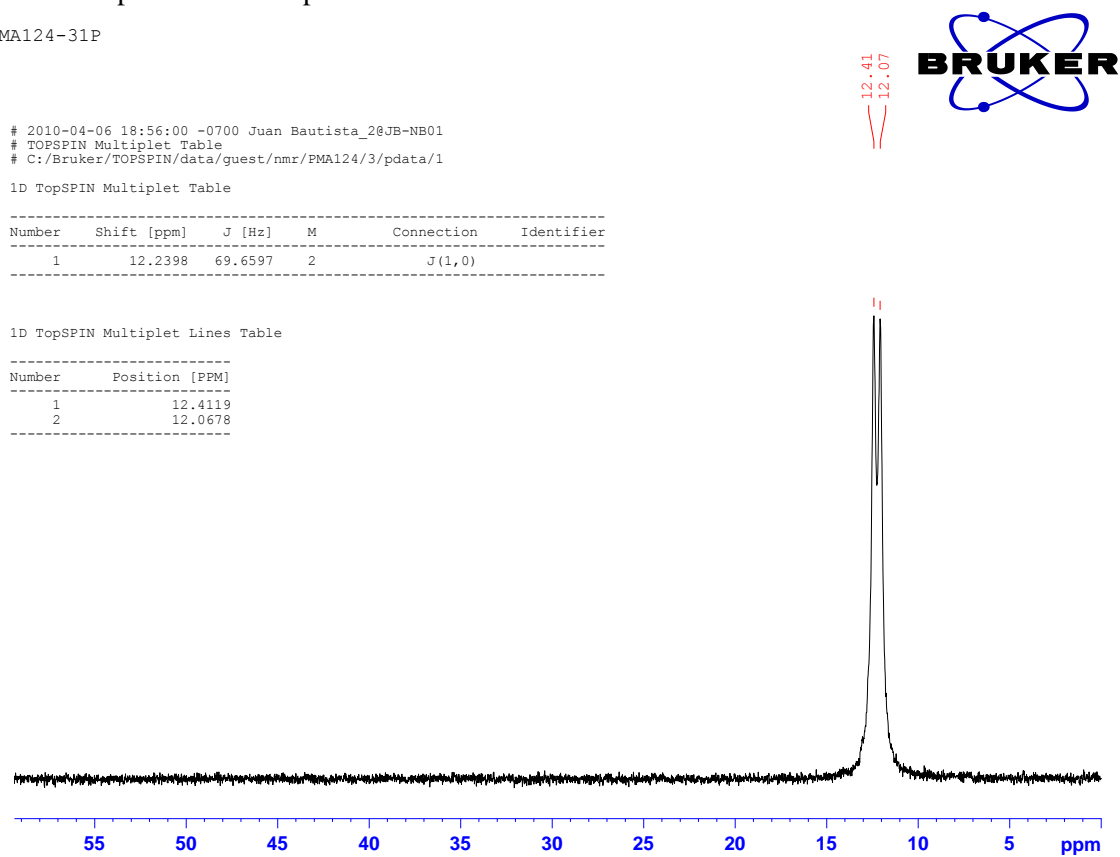
2010-04-06 18:56:00 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/PMA124/3/pdata/1

1D TopSPIN Multiplet Table

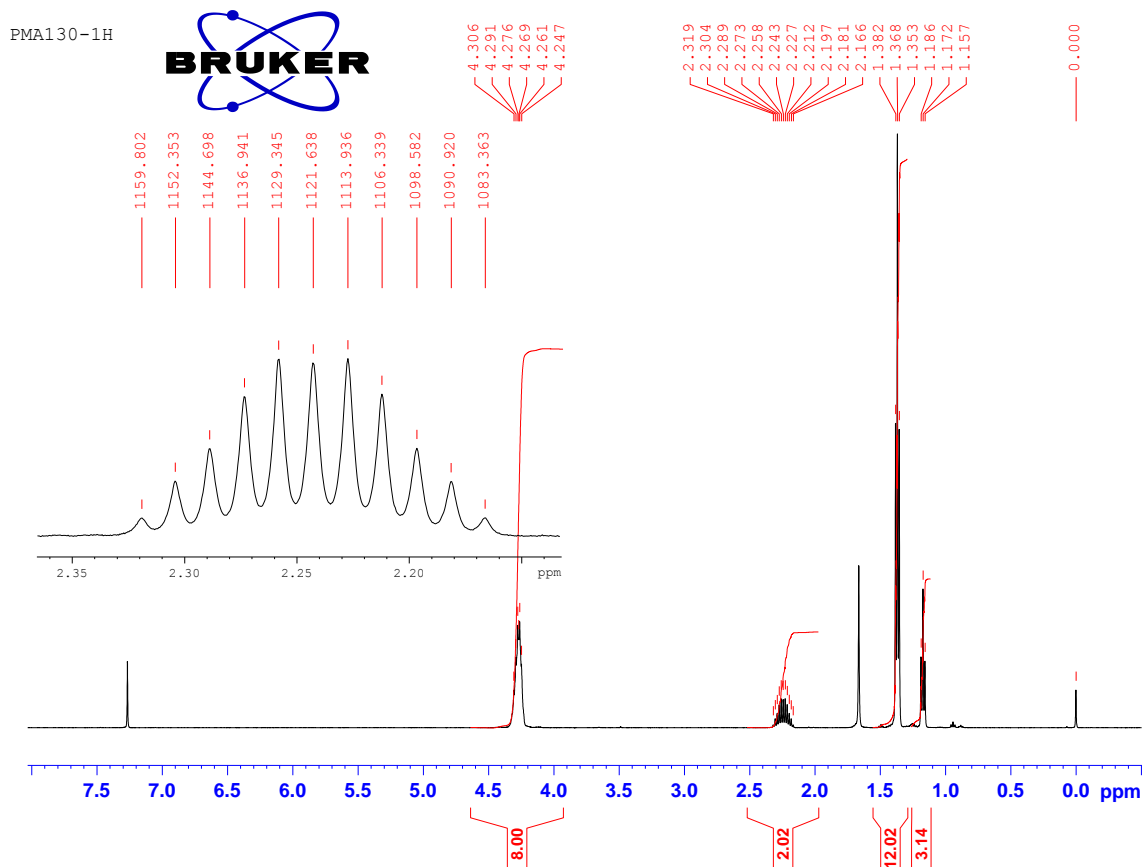
Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	12.2398	69.6597	2	J(1,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	12.4119
2	12.0678

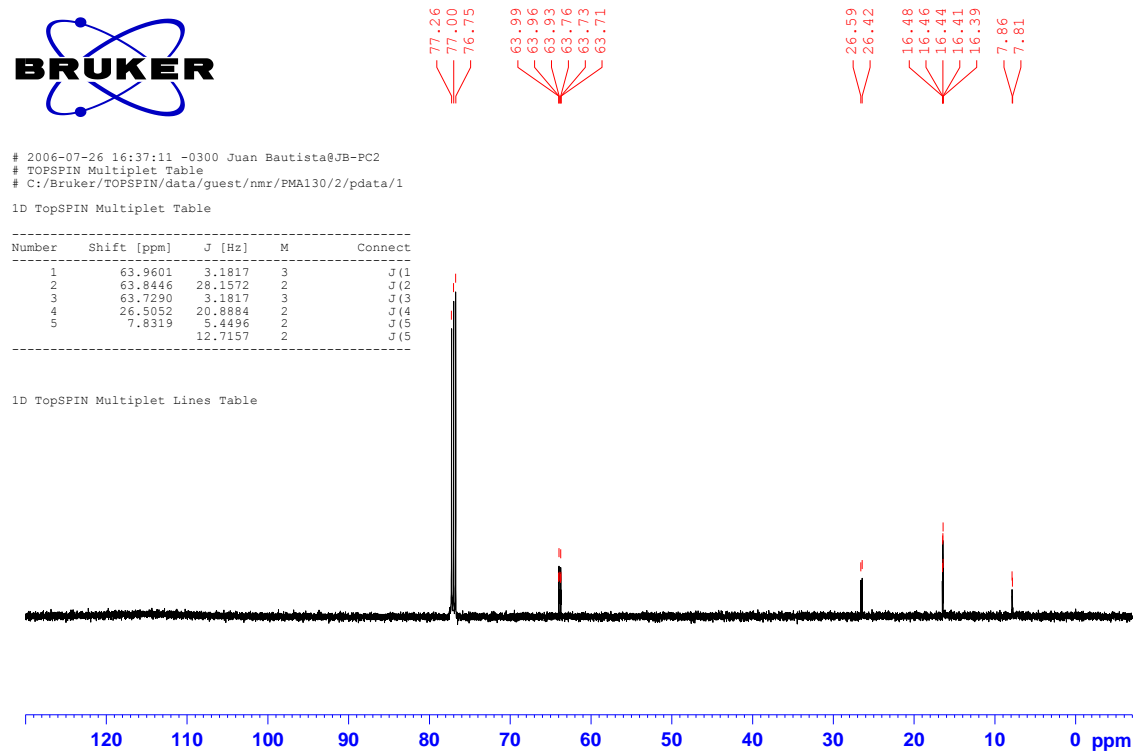


³¹P NMR spectrum of compound 36



¹H NMR spectrum of compound **27**

PMA130-13C



¹³C NMR spectrum of compound **27**

PMA130-31P

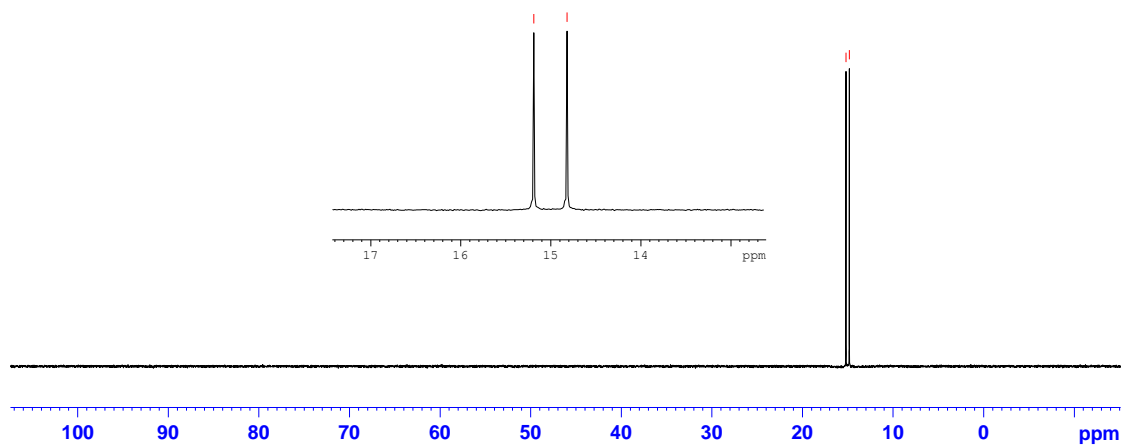
2010-04-08 13:28:59 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/PMA130/3/pdata/1

1D TopSPIN Multiplet Table

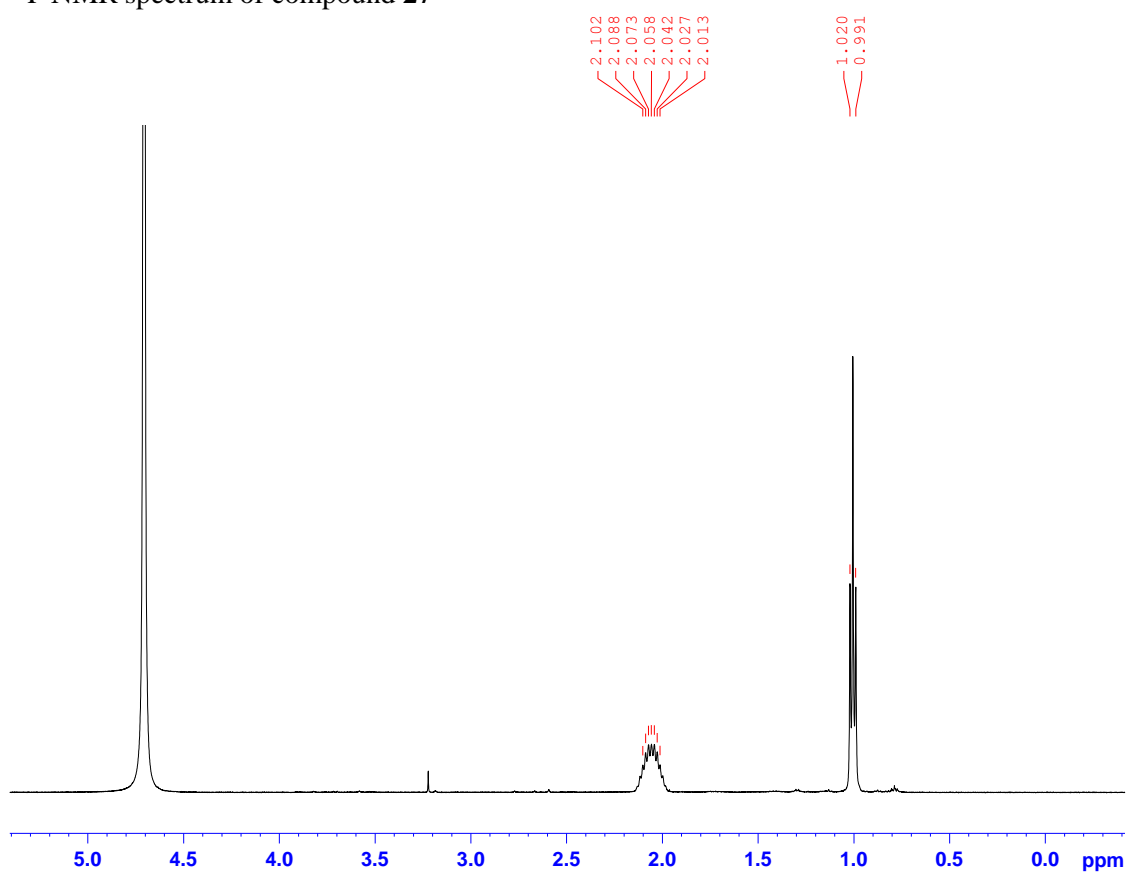
Number	Shift [ppm]	J [Hz]	M	Connection	Ic
1	15.0047	74.6354	2	J(1,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	15.1890
2	14.8204



³¹P NMR spectrum of compound **27**



¹H NMR spectrum of compound **37**

F3 OH V 145 Hid. # //D2O// , 13C* 9/6/10.

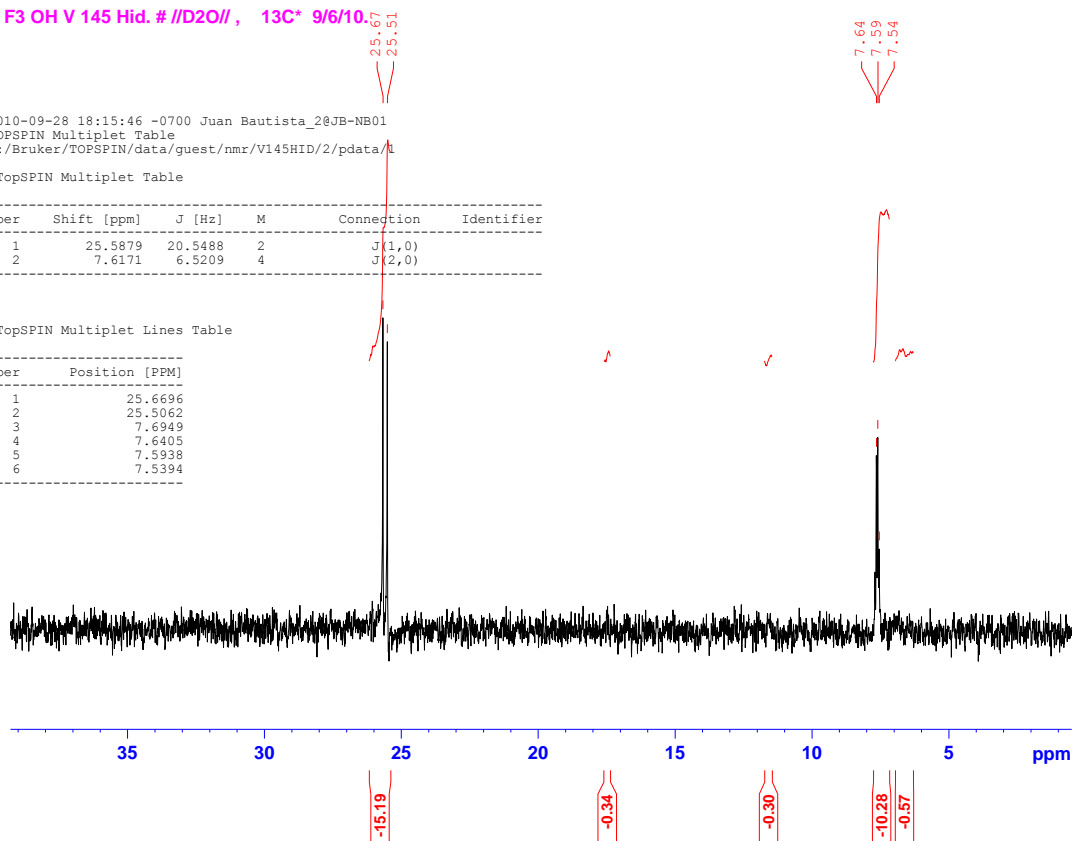
2010-09-28 18:15:46 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/V145HID/2/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	25.5879	20.5488	2	J(1,0)	
2	7.6171	6.5209	4	J(2,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	25.6696
2	25.5062
3	7.6949
4	7.6405
5	7.5938
6	7.5394



¹³C NMR spectrum of compound **37**

F3OH V 145 Hid. # //D2O// , 31P* 9/6/10.

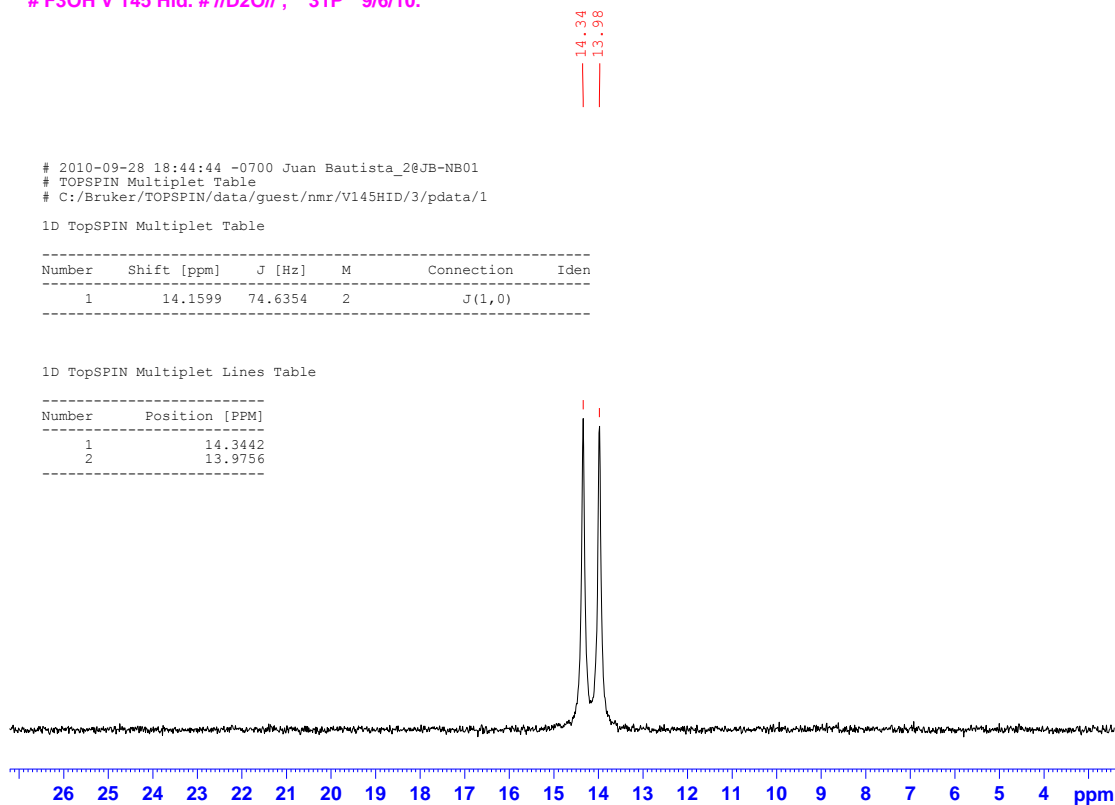
2010-09-28 18:44:44 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/V145HID/3/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Iden
1	14.1599	74.6354	2	J(1,0)	

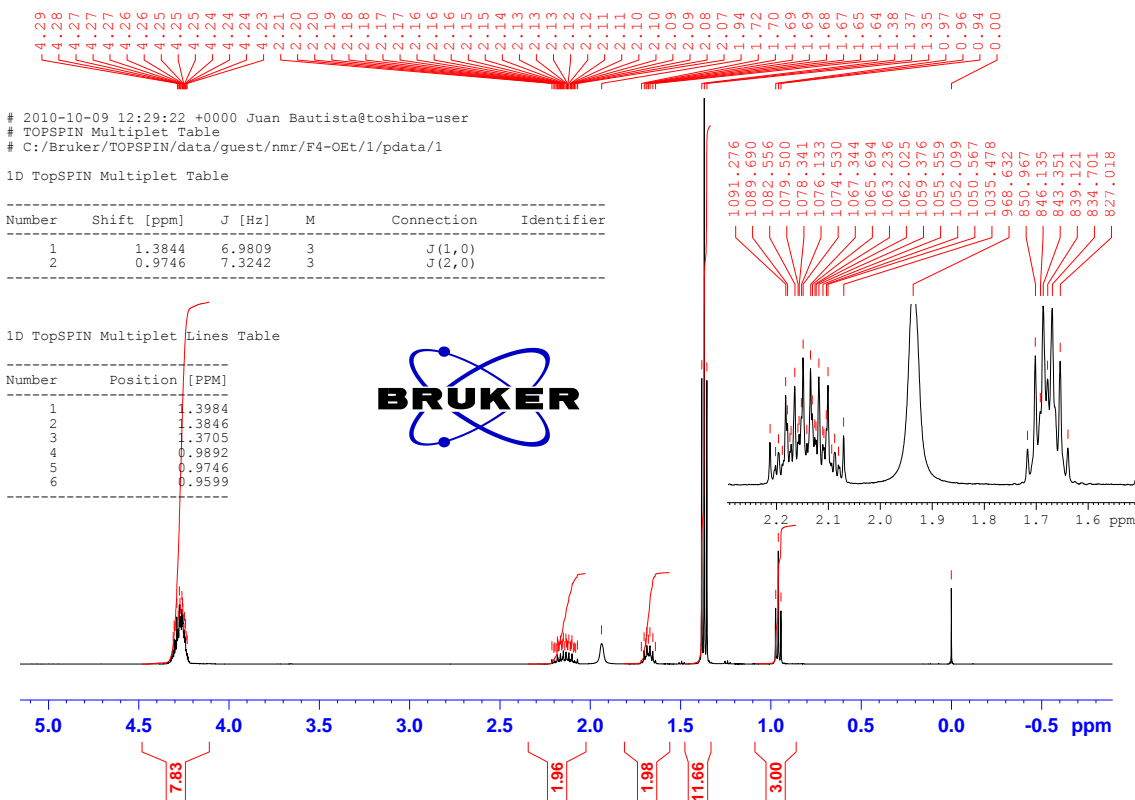
1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	14.3442
2	13.9756



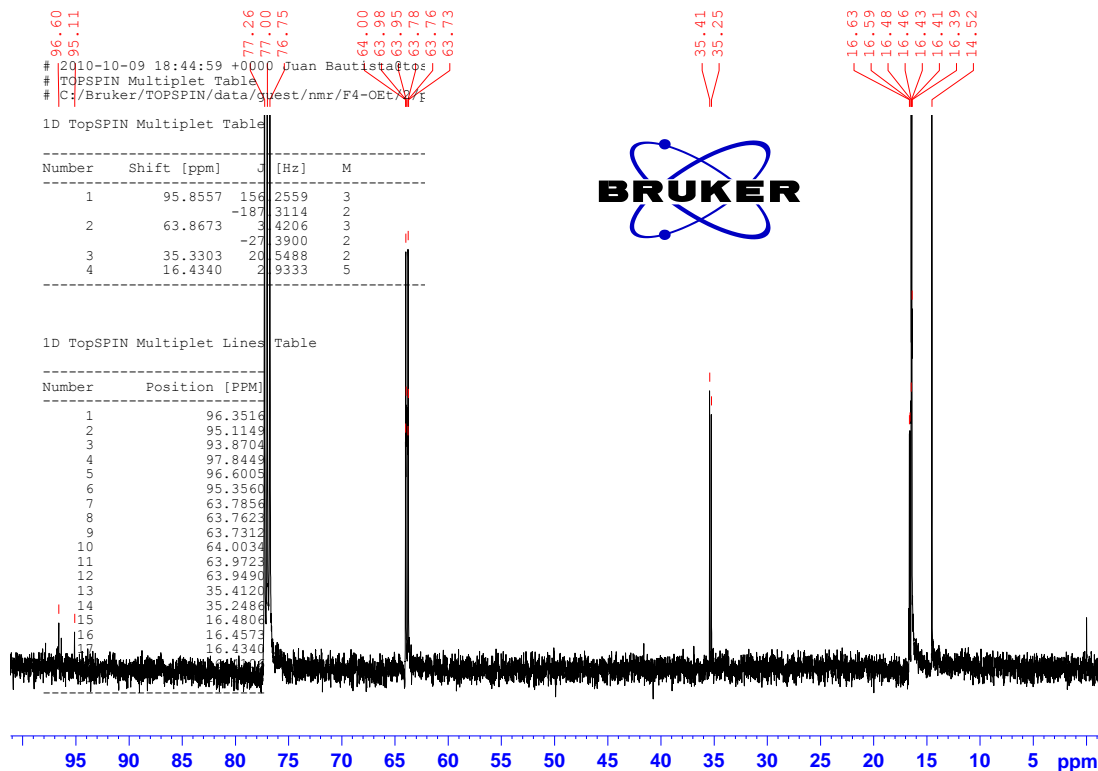
³¹P NMR spectrum of compound **37**

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 CCCl3



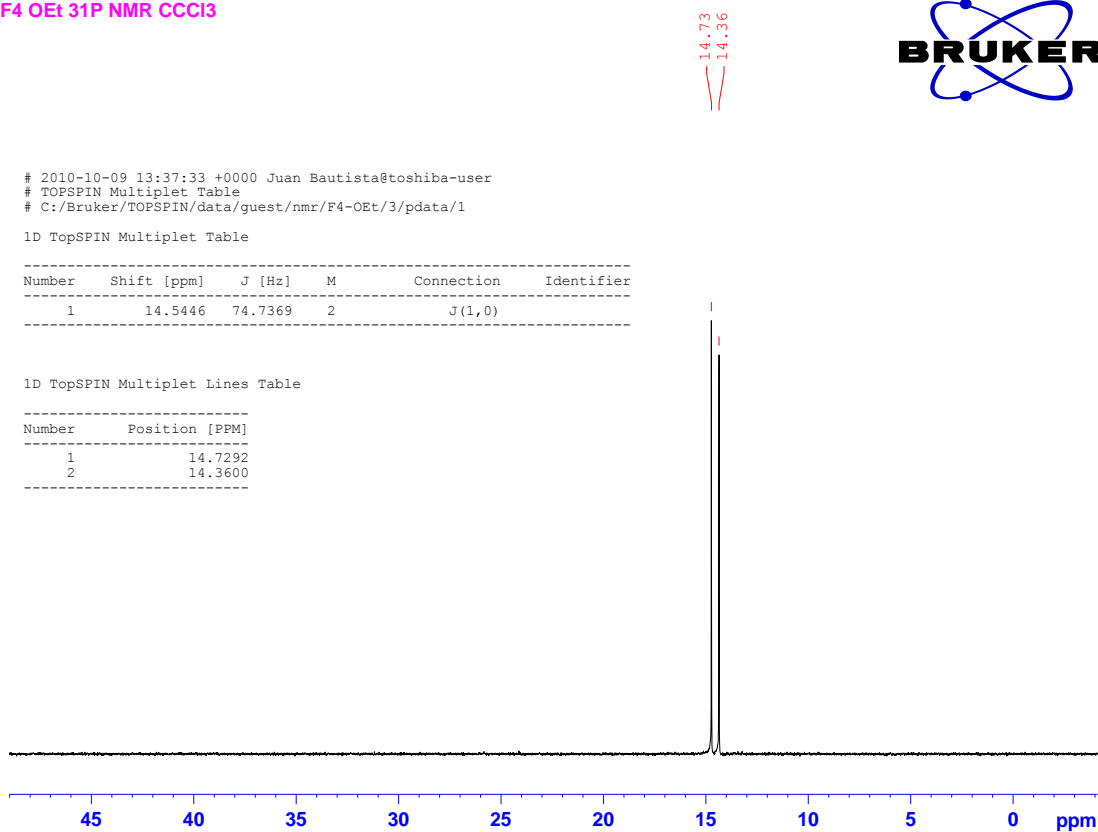
2010-10-09 13:37:33 +0000 Juan Bautista@toshiba-user
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/F4-OEt/3/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	14.5446	74.7369	2	J(1,0)	

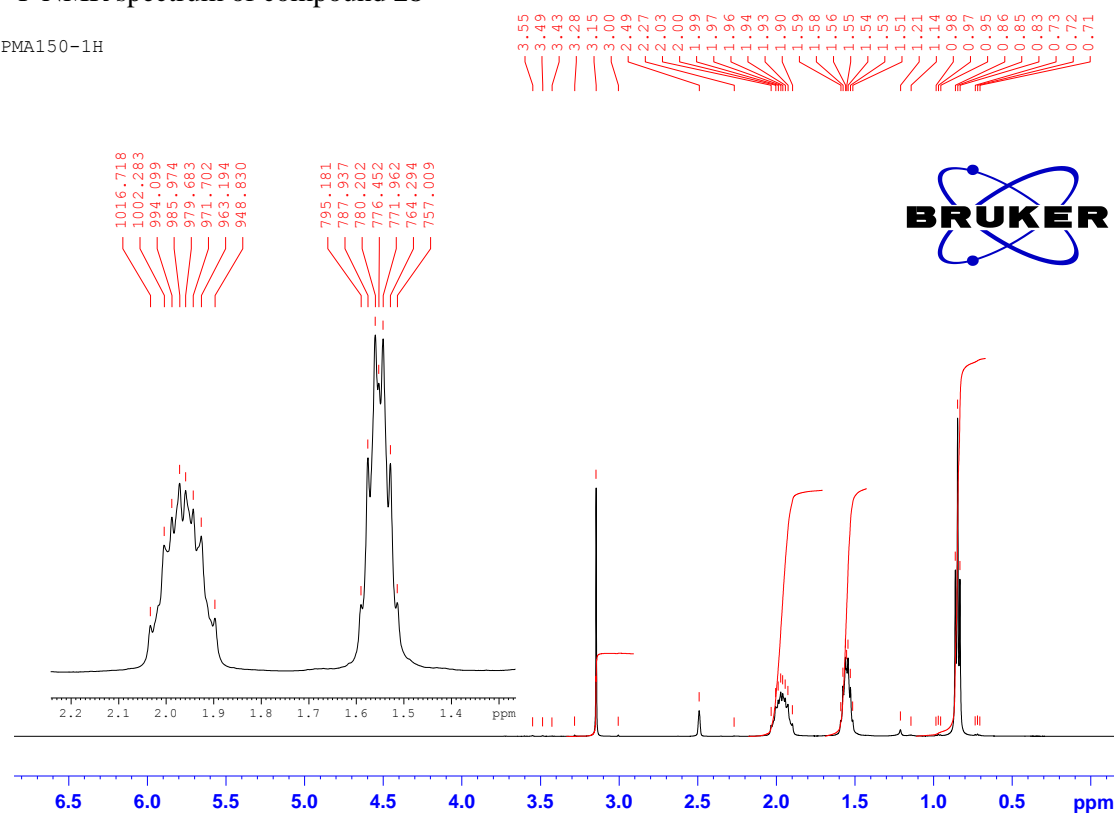
1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	14.7292
2	14.3600



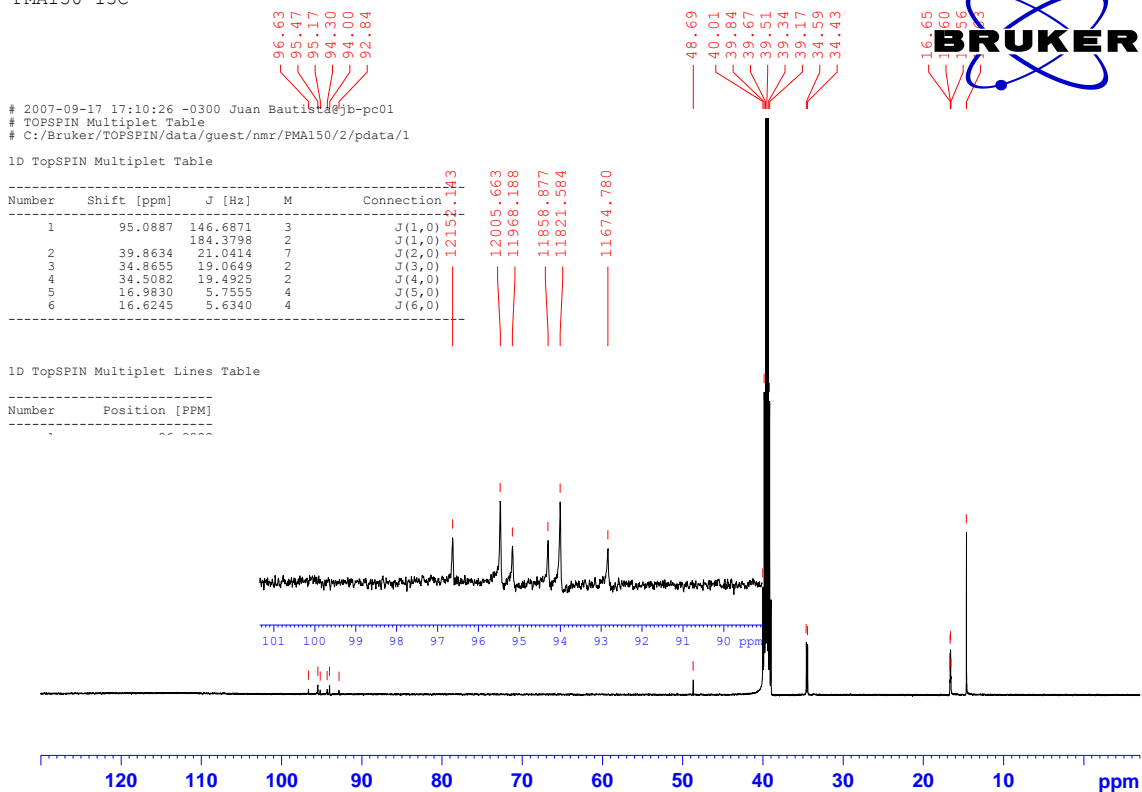
³¹P NMR spectrum of compound 28

PMA150-1H



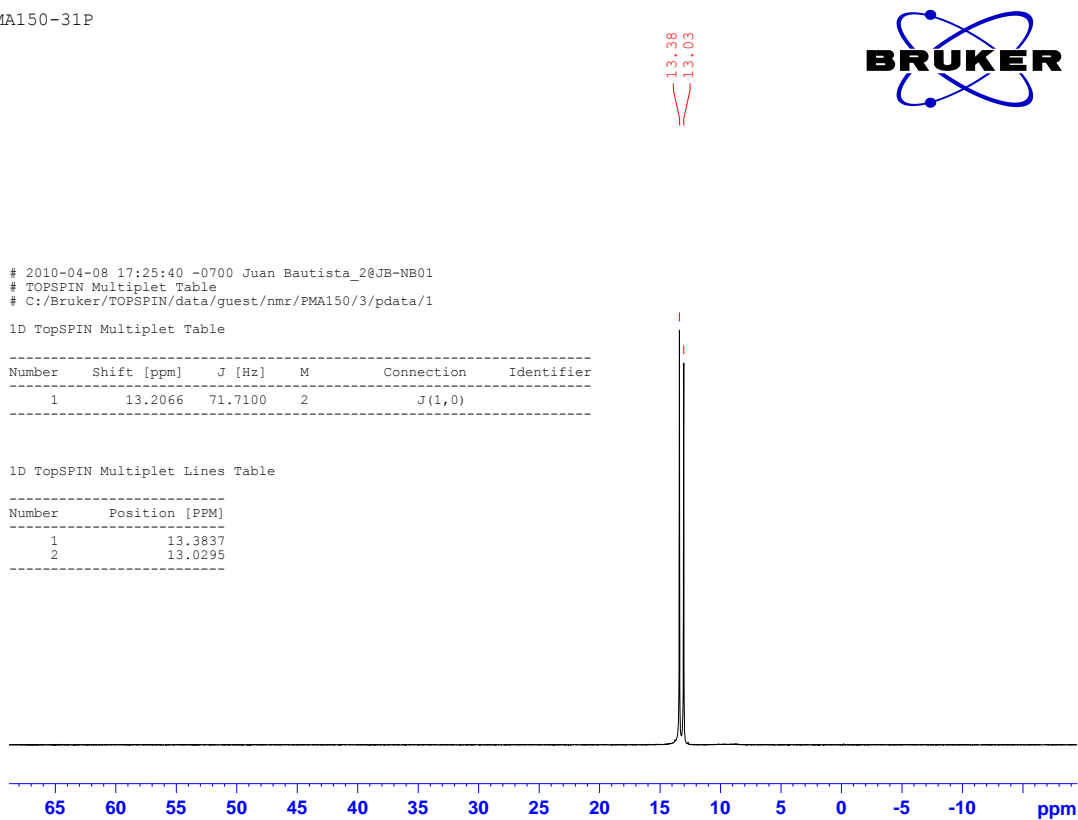
¹H NMR spectrum of compound 38

PMA150-13C

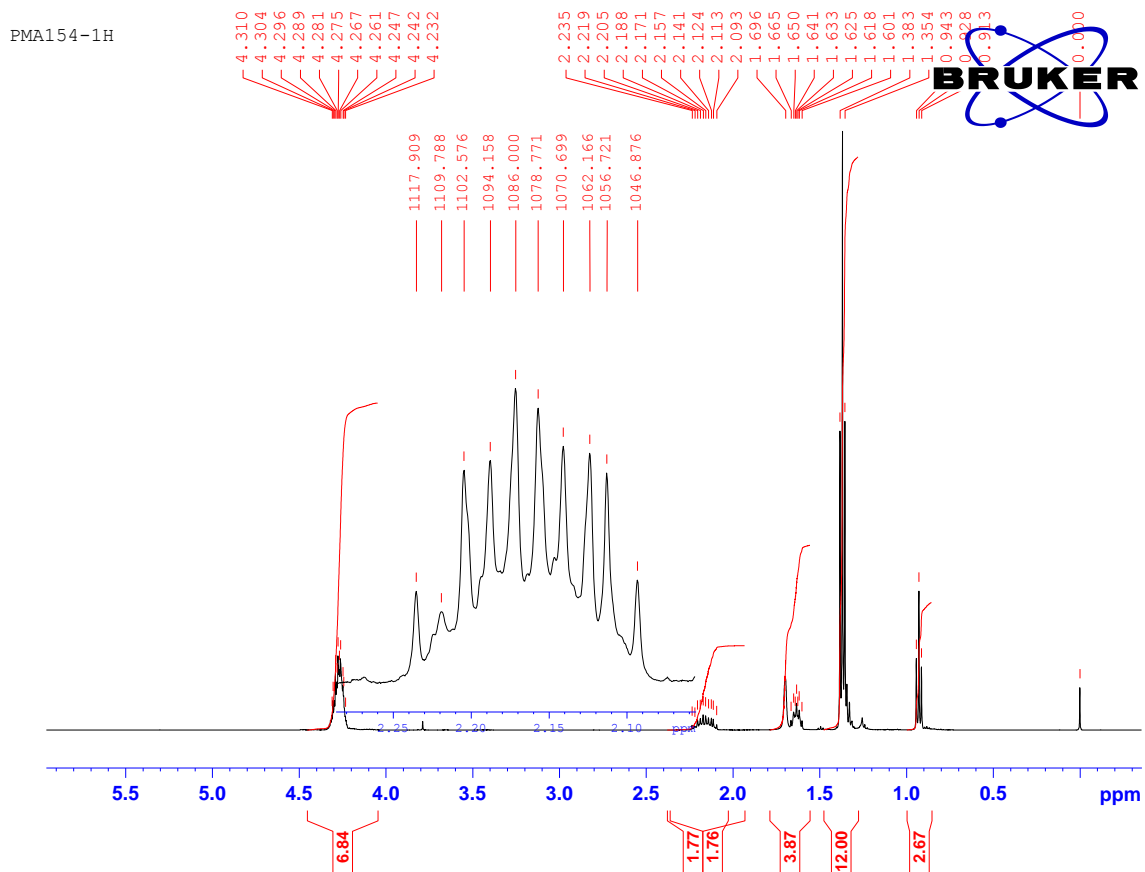


¹³C NMR spectrum of compound 38

PMA150-31P

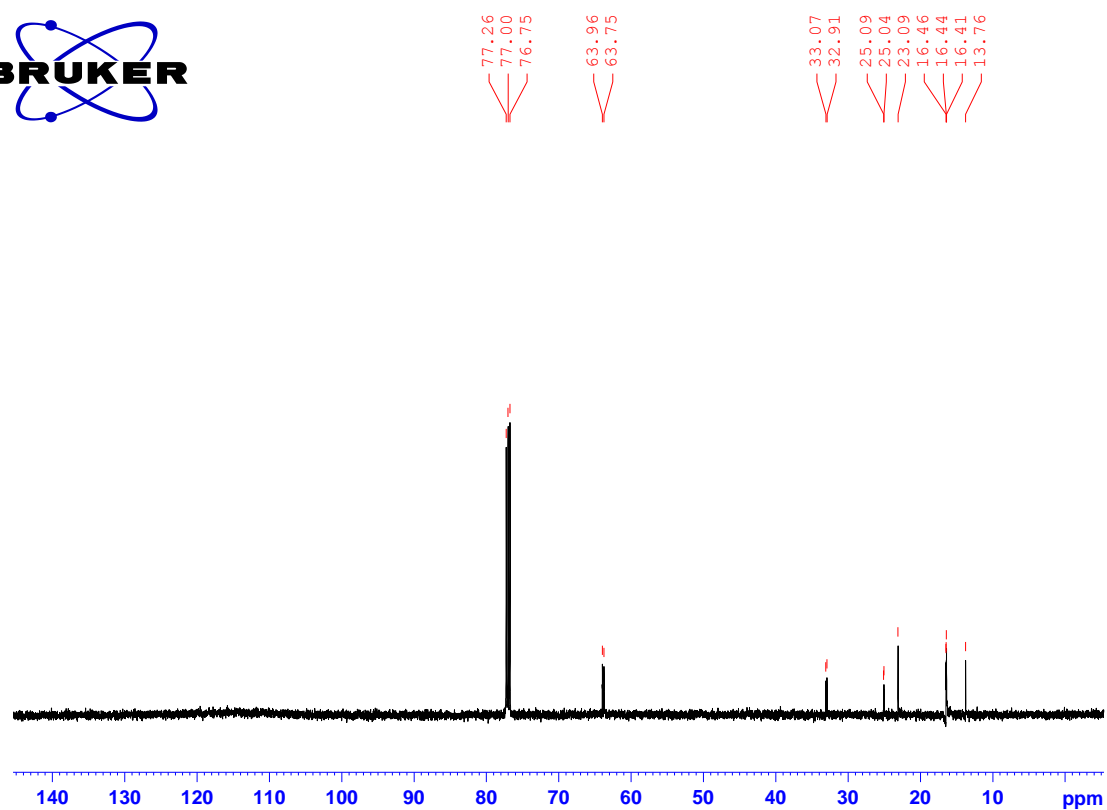


³¹P NMR spectrum of compound 38



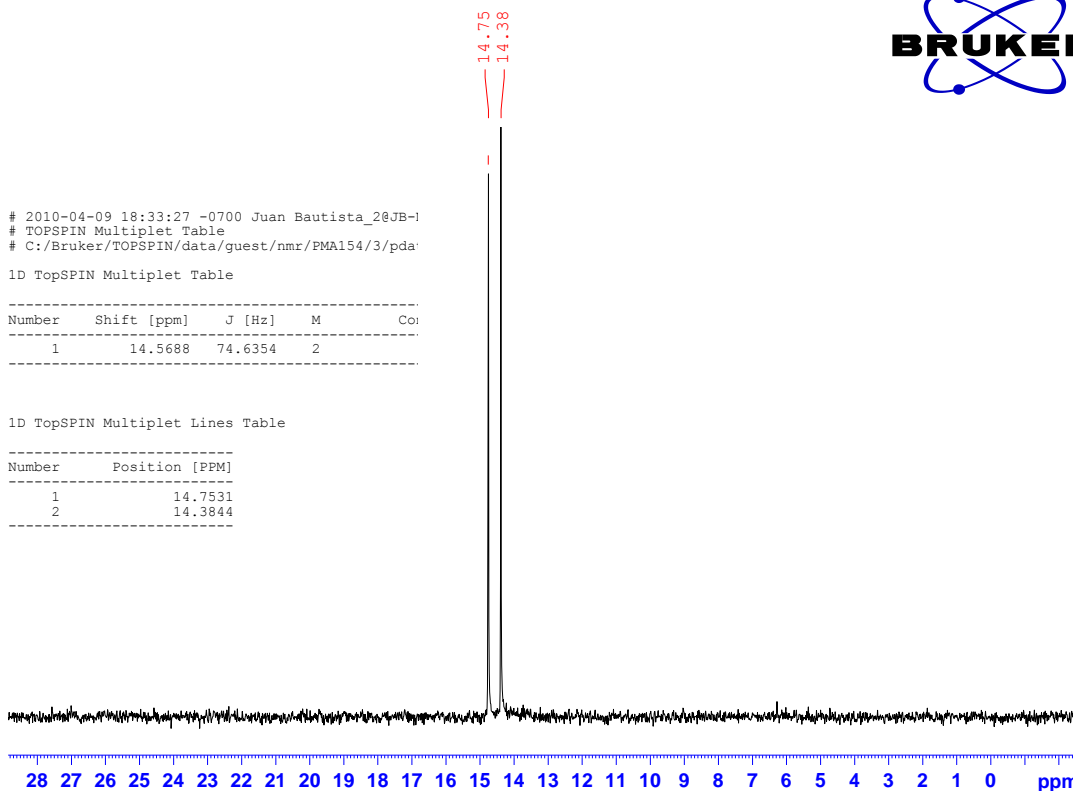
¹H NMR spectrum of compound **29**

PMA154-13C



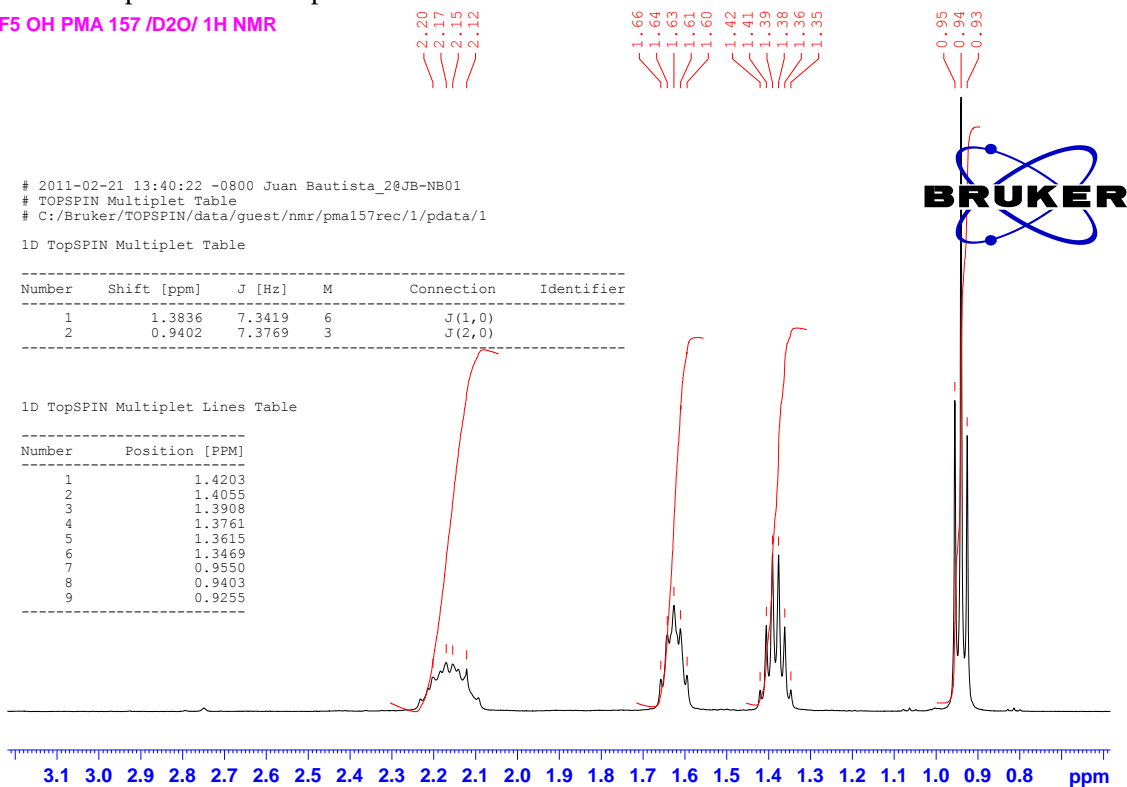
¹³C NMR spectrum of compound **29**

PMA154-31P



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..



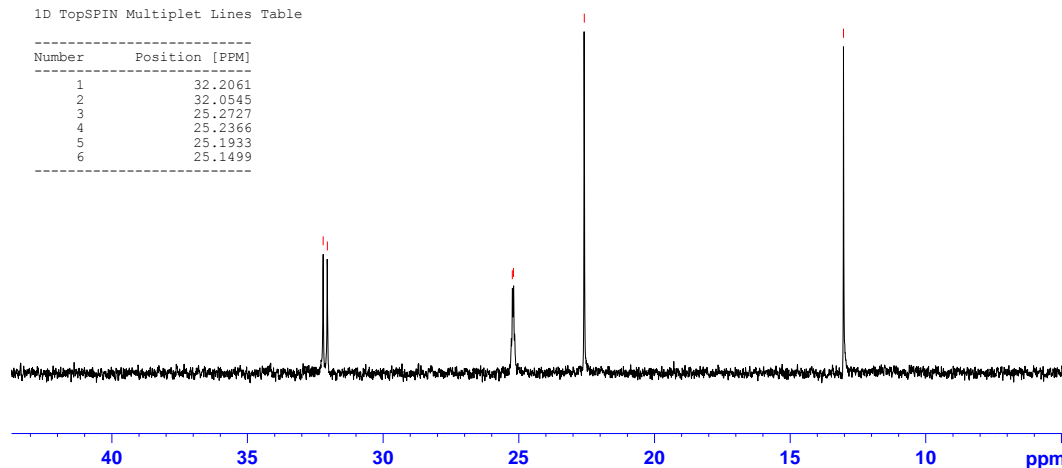
2011-02-21 13:48:35 -0800 Juan Bautista_2@JB-NB01
 # TOPSPIN Multiplet Table
 # C:/Bruker/TOPSPIN/data/guest/nmr/pma157rec/2/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	32.1303	19.0735	2	J(1,0)	
2	25.2113	5.1477	4	J(2,0)	

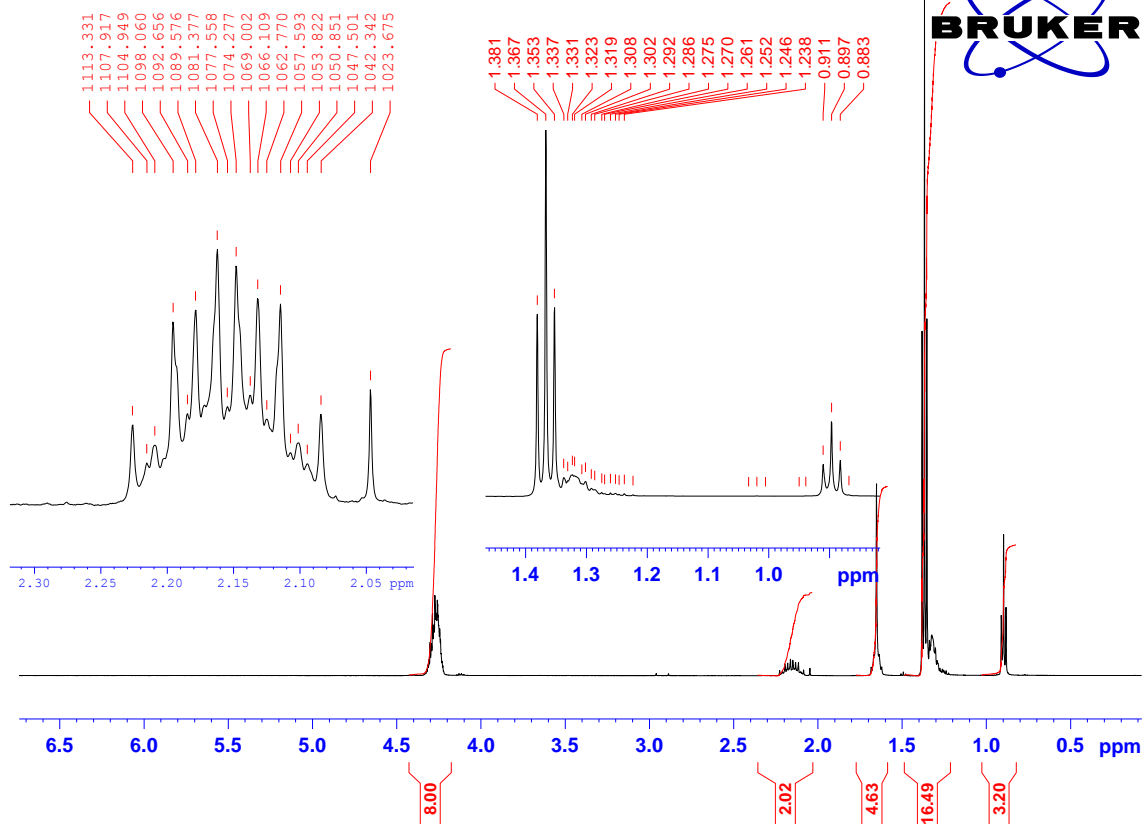
1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	32.2061
2	32.0545
3	25.2727
4	25.2366
5	25.1933
6	25.1499



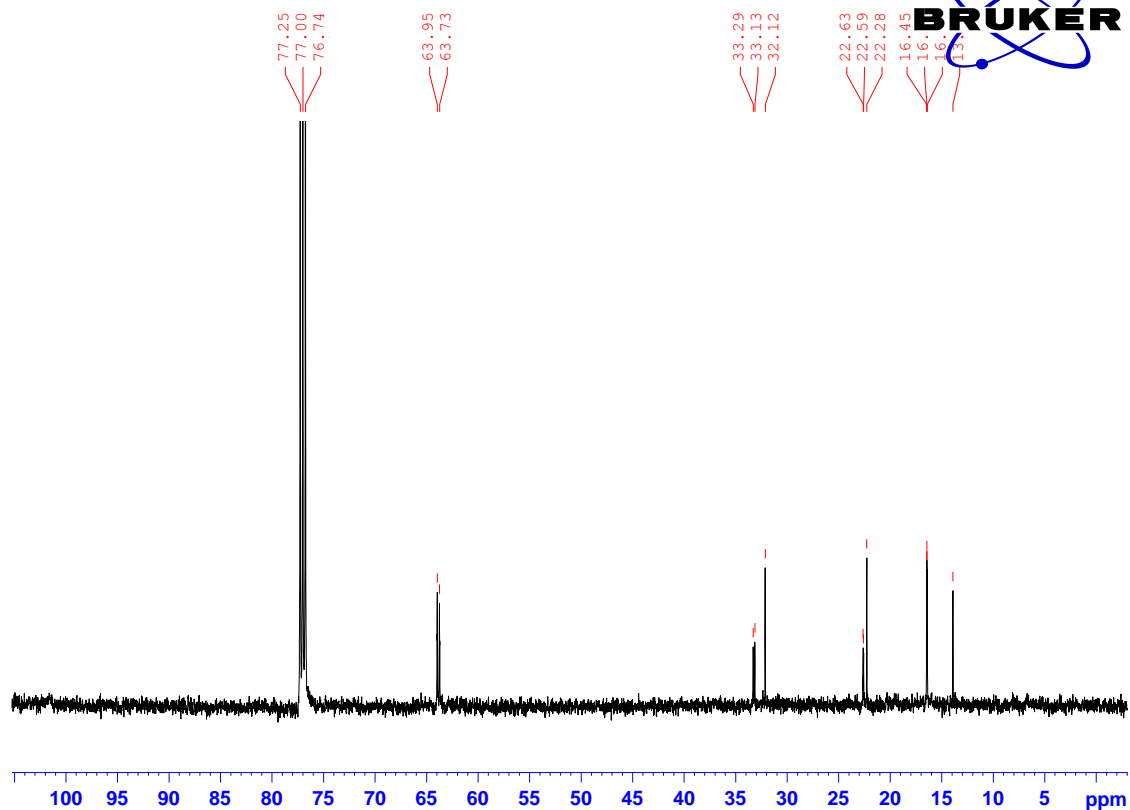
¹³C NMR spectrum of compound 39

F-6 (OEt)₃ # //CDCl₃//



¹H NMR spectrum of compound 30

PMA-156 - #1 # //CDCl3//, 13C NMR*



¹³C NMR spectrum of compound **30**

PMA-156 - #1 # //CDCl3//, 31P NMR

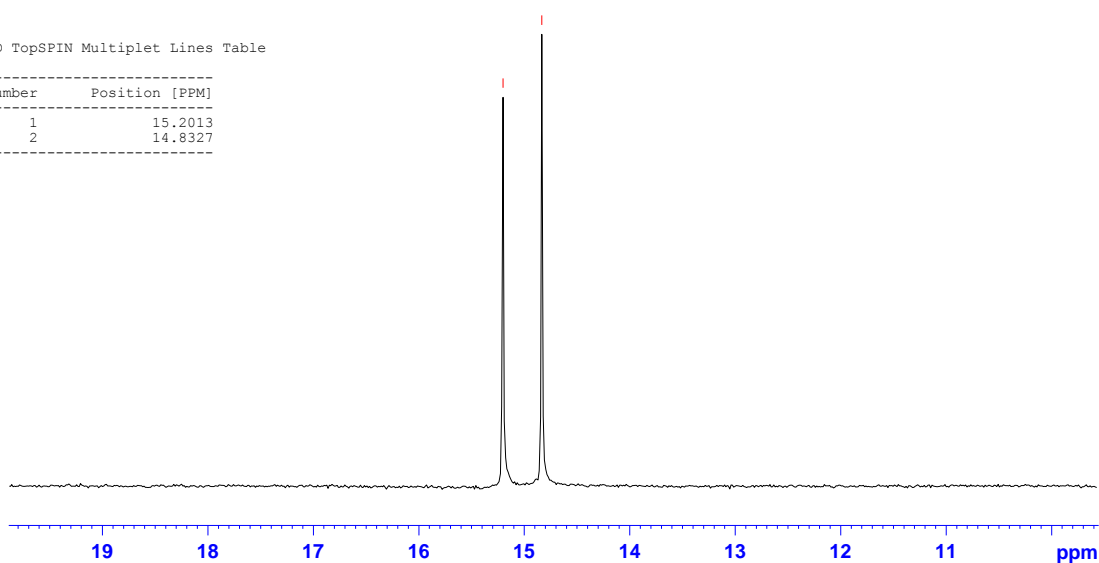
2010-06-01 10:54:02 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/pma156_1/3/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	15.0170	74.6354	2	J(1,0)	

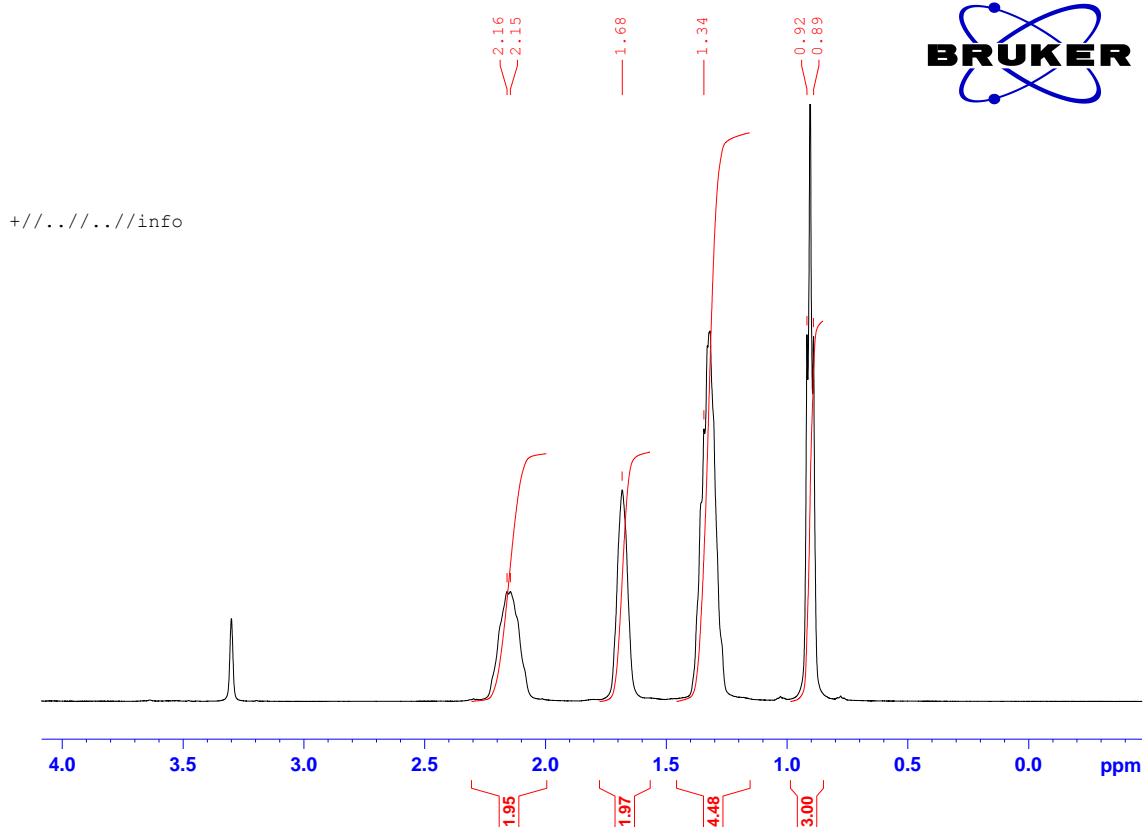
1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	15.2013
2	14.8327



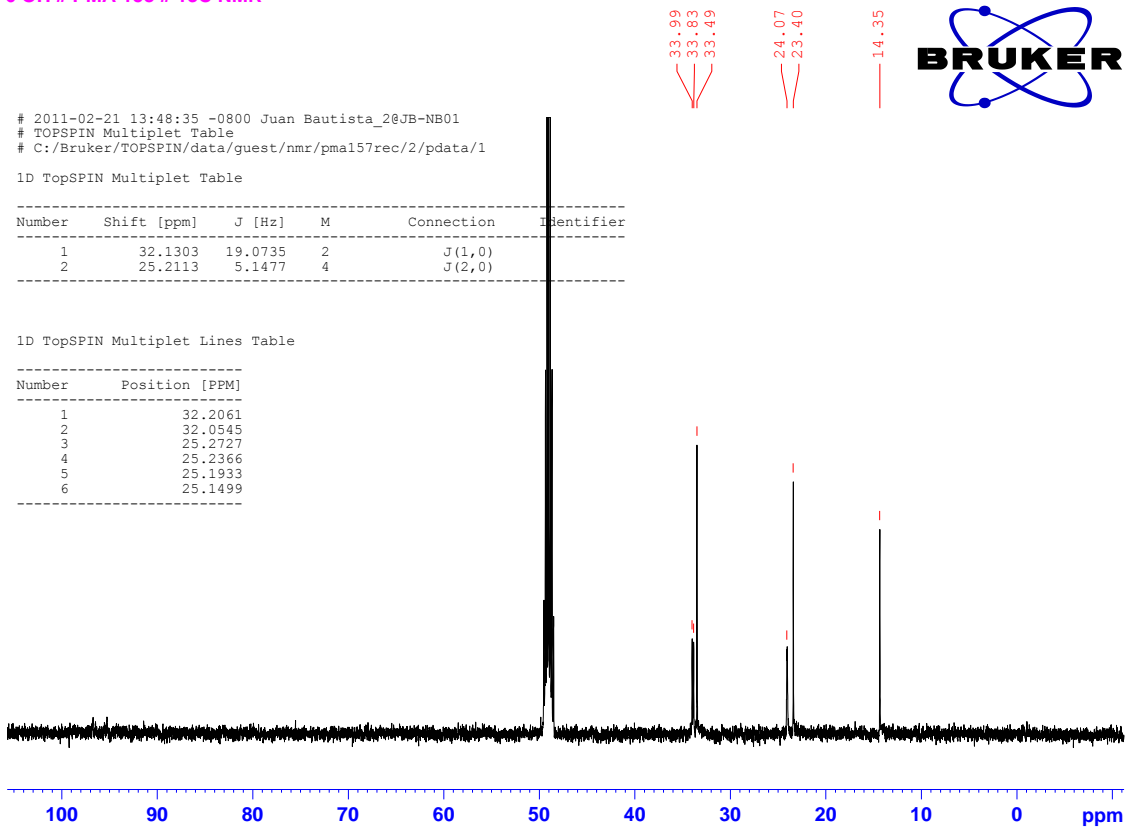
³¹P NMR spectrum of compound **30**

F6 OH PMA-158 # 1H NMR



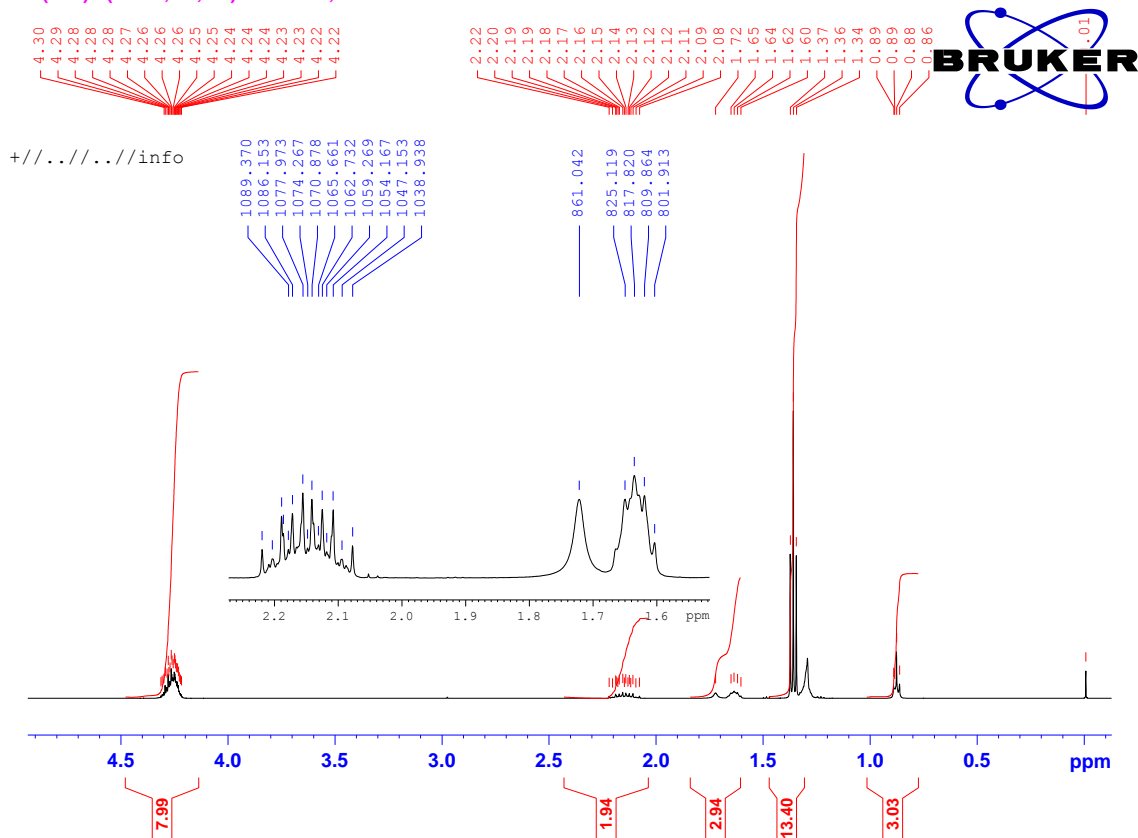
¹H NMR spectrum of compound 40

F6 OH # PMA-158 # 13C NMR



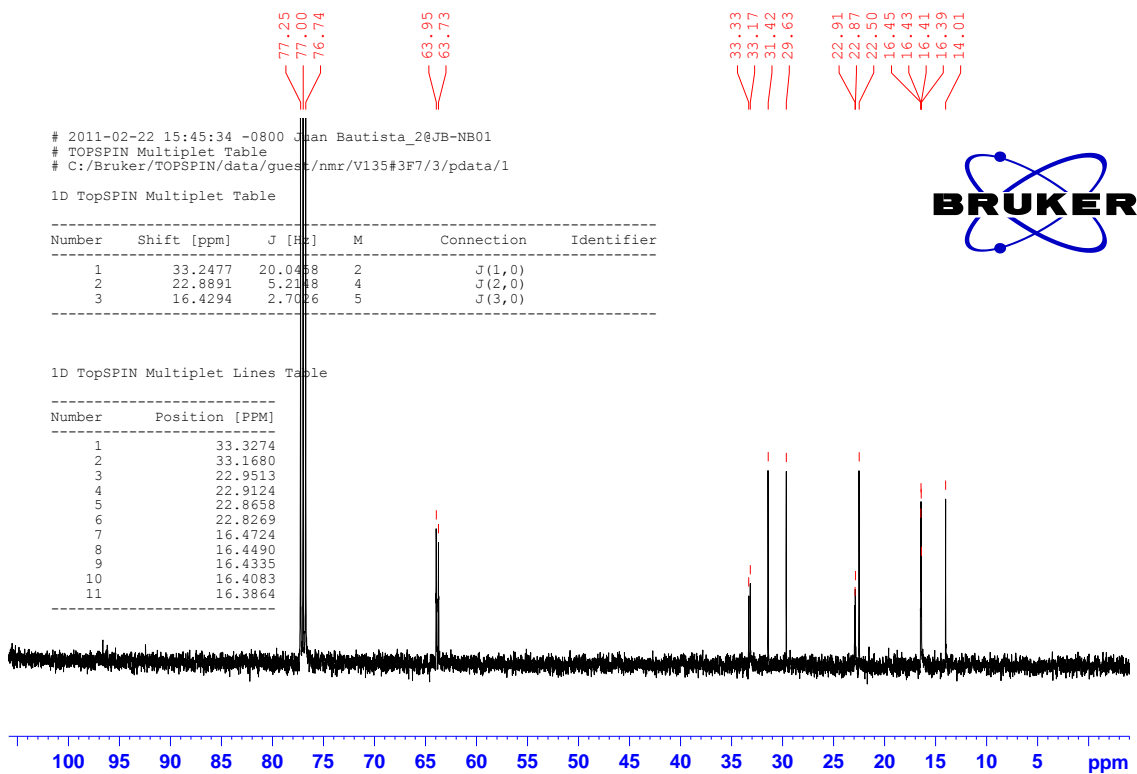
¹³C NMR spectrum of compound 40

F7 (OEt)₂ (V 135, #3, F7) //CDCl₃//, ¹H NMR 2/6/10.



¹H NMR spectrum of compound 31

F7 (OEt)₂ (V 135, #3, F7) # //CDCl₃//, ¹³C NMR 2/6/10.



2011-02-22 15:45:34 -0800 Juan Bautista_2@JB-NB01
 # TOPSPIN Multiplet Table
 # C:/Bruker/TOPSPIN/data/guest/nmr/V135#3F7/3/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	33.2477	20.0468	2	J(1,0)	
2	22.8891	5.2148	4	J(2,0)	
3	16.4294	2.7086	5	J(3,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	33.3274
2	33.1680
3	22.9513
4	22.9124
5	22.8658
6	22.8269
7	16.4724
8	16.4490
9	16.4335
10	16.4083
11	16.3864

¹³C NMR spectrum of compound 31

F7 (OEt)₂ # (V 135, #3, F7) # //CDCl₃//, 31PNMR 2/6/10.

14.77
14.40



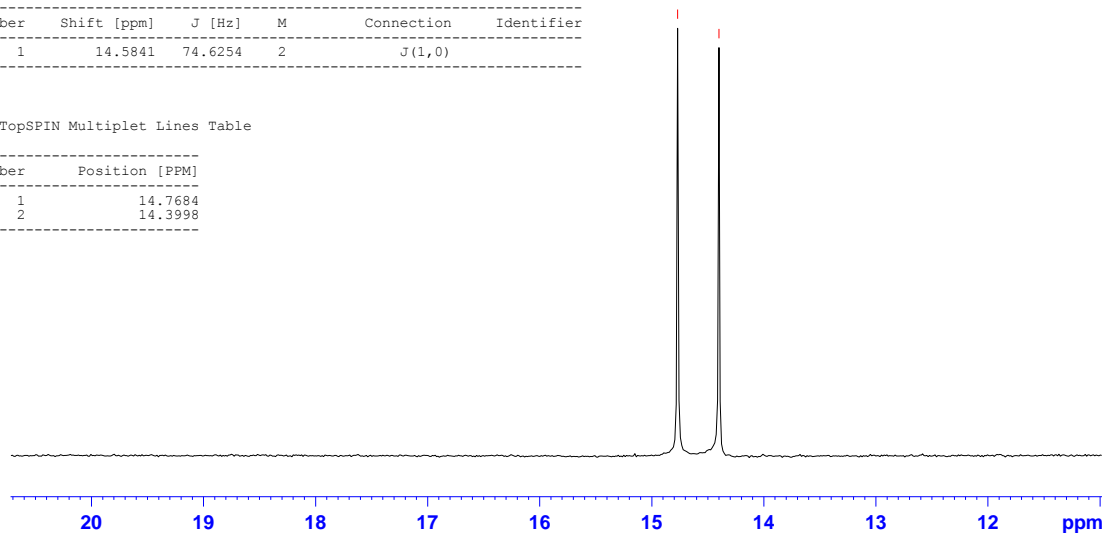
2011-02-22 15:50:27 -0800 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/V135#3F7/2/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
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
1.20

0.78
0.77
0.76

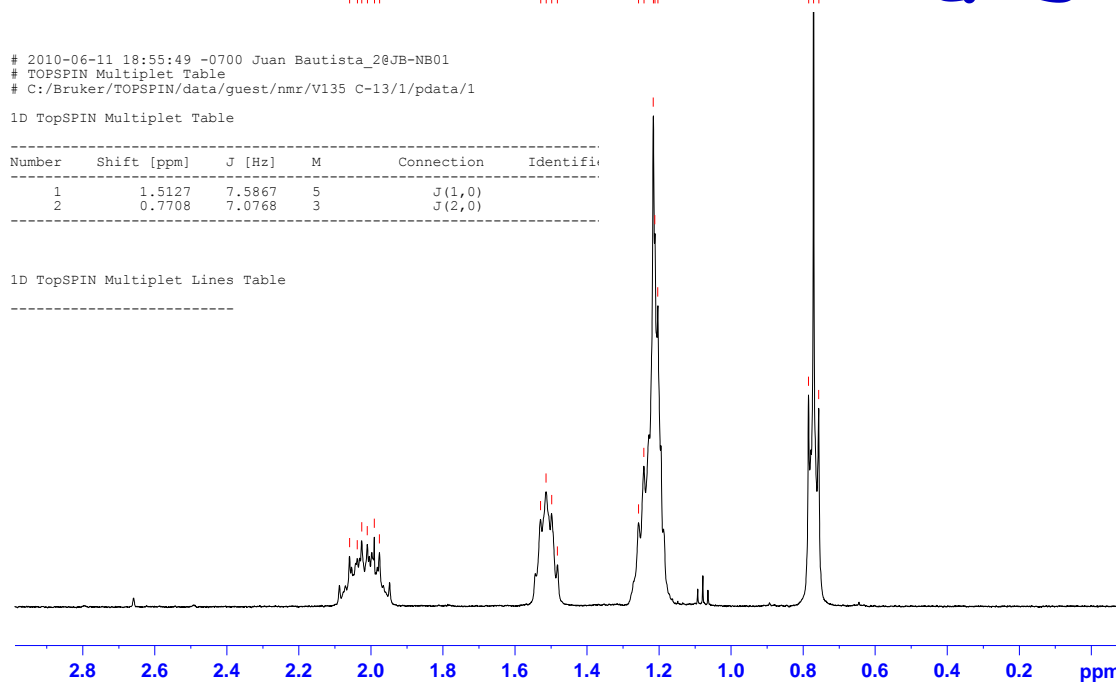


2010-06-11 18:55:49 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/V135 C-13/1/pdata/1

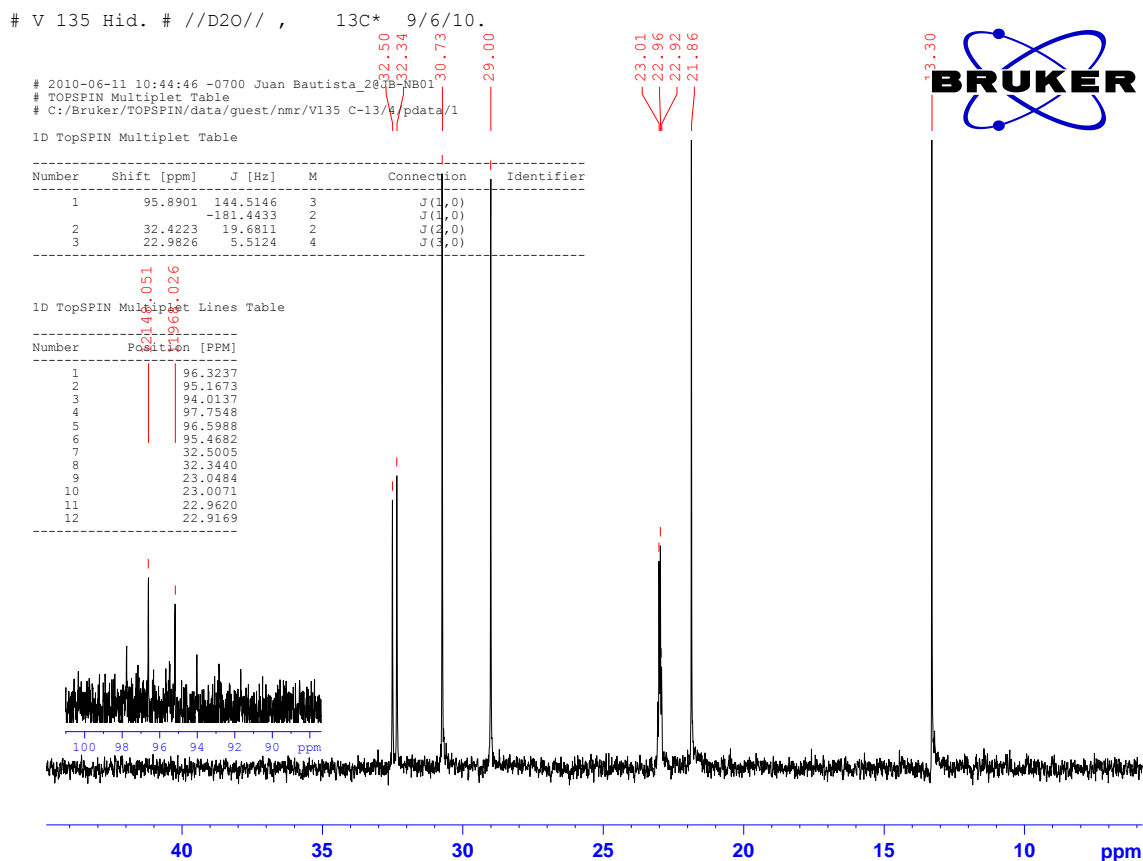
1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifi
1	1.5127	7.5867	5	J(1,0)	
2	0.7708	7.0768	3	J(2,0)	

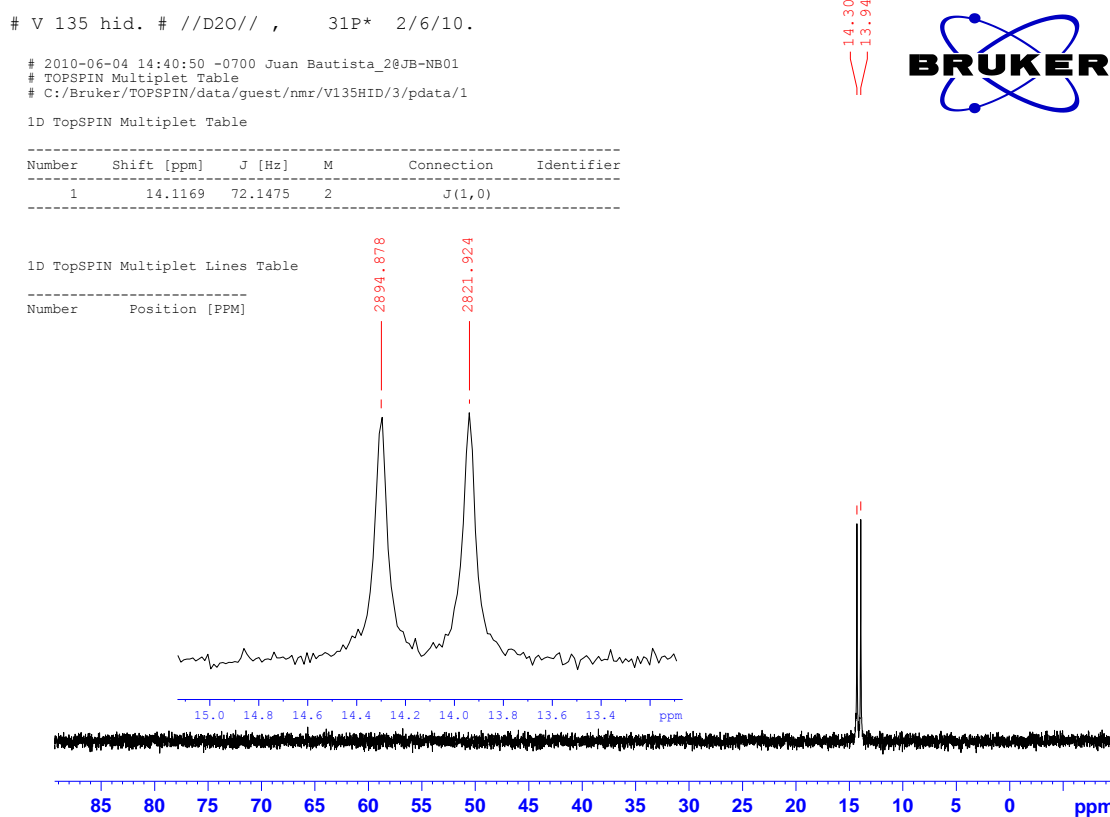
1D TopSPIN Multiplet Lines Table



¹H NMR spectrum of compound **41**

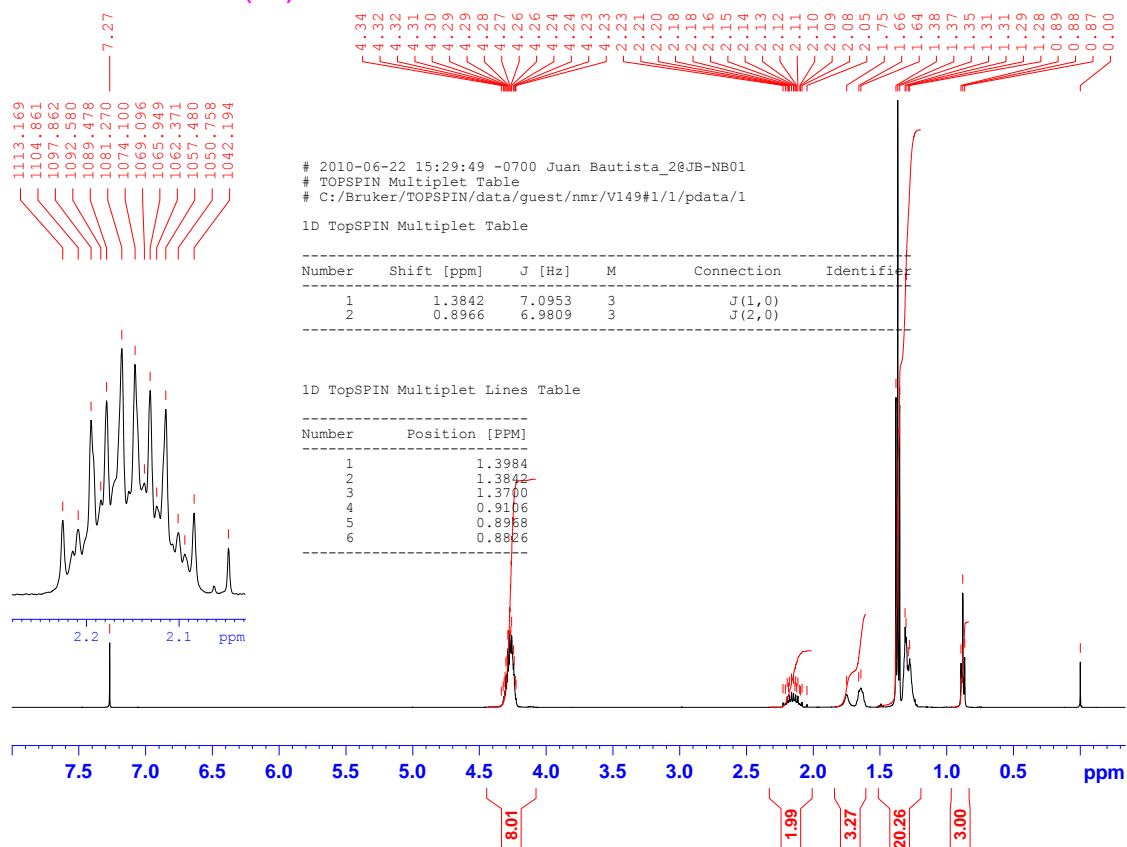


¹³C NMR spectrum of compound 41



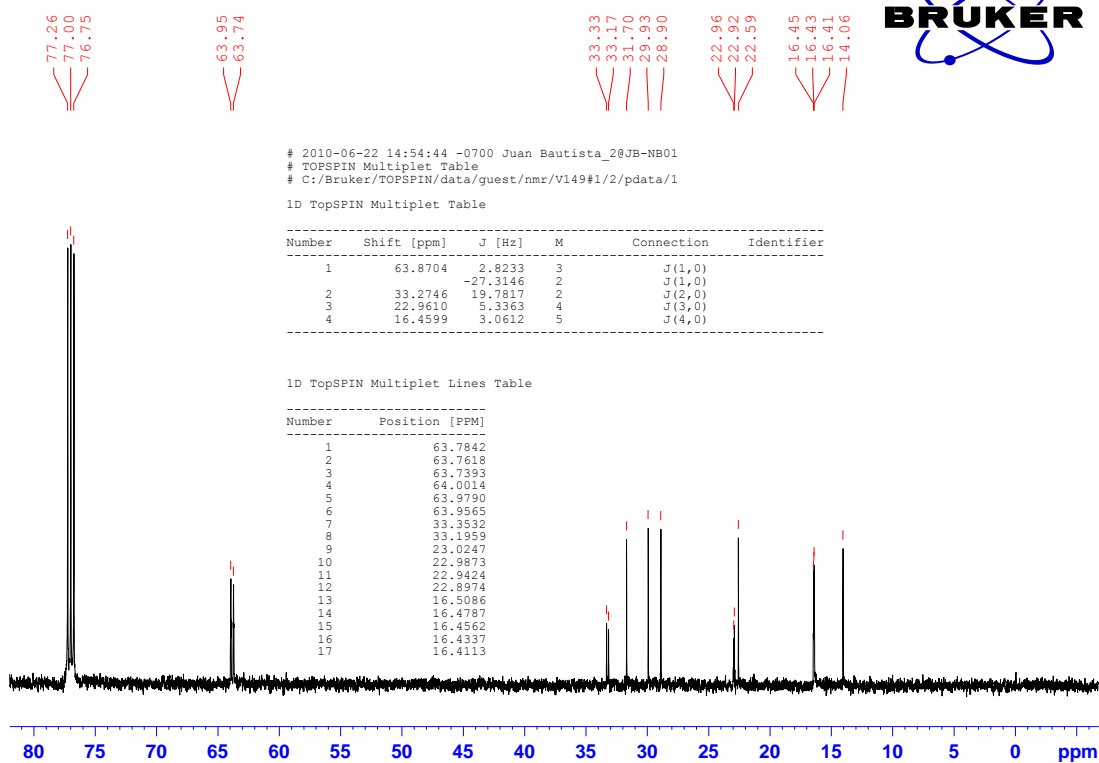
³¹P NMR spectrum of compound 41

V149 /CDCl₃/ ¹H NMR F8 (OEt) 18/6/10.



¹H NMR spectrum of compound 32

V149 # 1 /CDCl₃/ ¹³C NMR F8 OEt 18/6/10.



¹³C NMR spectrum of compound 32

V149 # 1 /CDCI3/ 31P NMR F8 OEt 18/6/10.



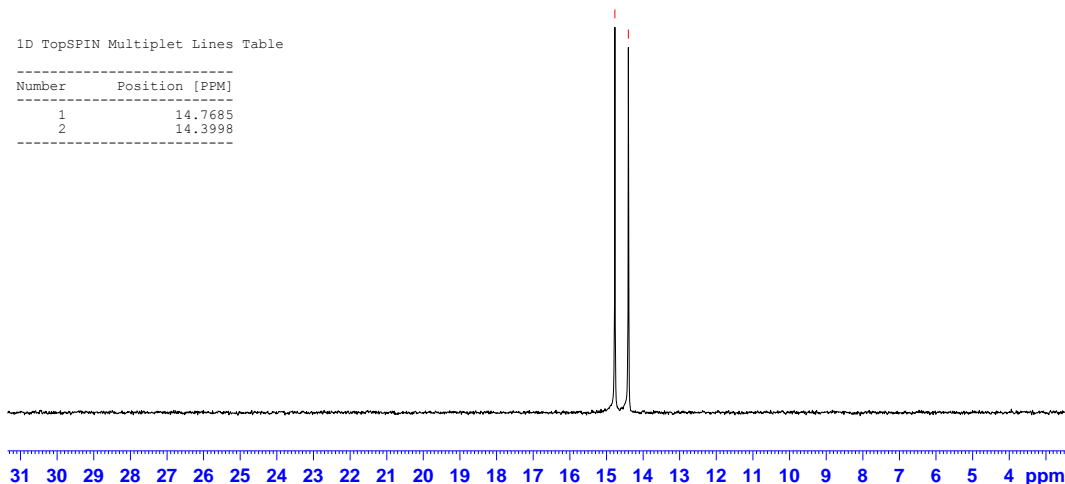
2010-06-22 14:27:58 -0700 Juan Bautista_2@JB-NB01
 # TOPSPIN Multiplet Table
 # C:/Bruker/TOPSPIN/data/guest/nmr/V149#1/3/pdata/1

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 **32**

V149HID /D2O/ 1H NMR F8 OH 18/6/10.



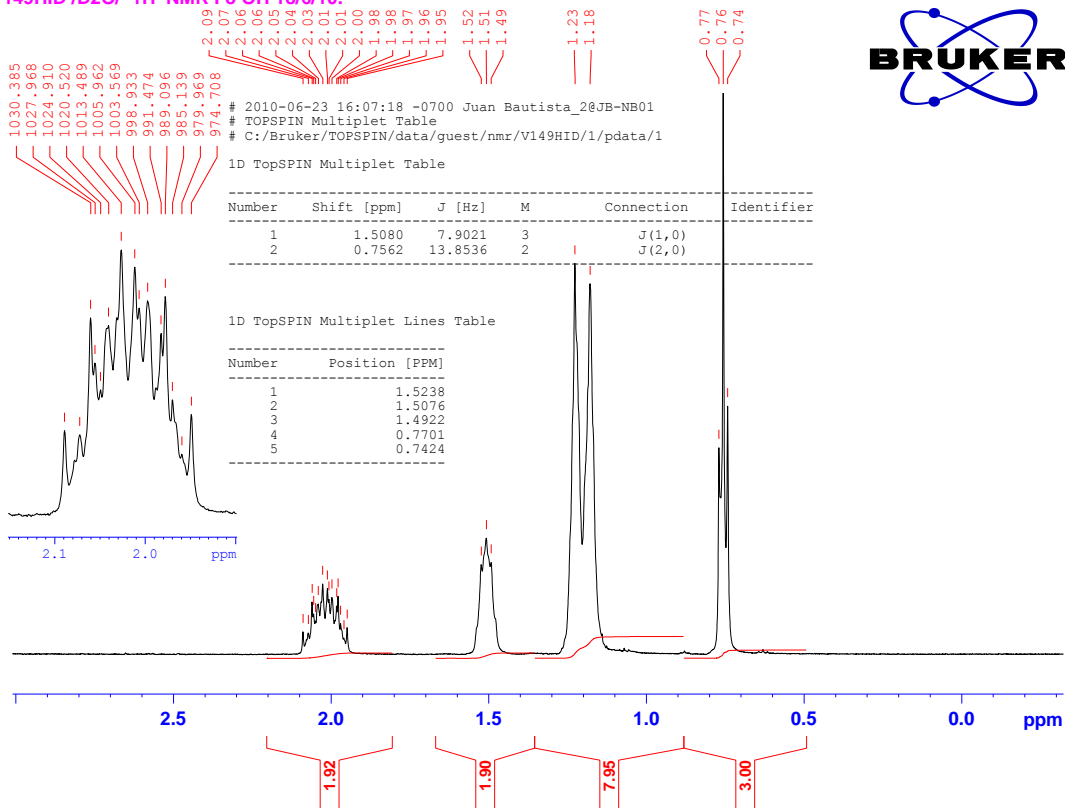
2010-06-23 16:07:18 -0700 Juan Bautista_2@JB-NB01
 # TOPSPIN Multiplet Table
 # C:/Bruker/TOPSPIN/data/guest/nmr/V149HID/1/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	1.5080	7.9021	3	J(1,0)	
2	0.7562	13.8536	2	J(2,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	1.5238
2	1.5076
3	1.4922
4	0.7701
5	0.7424



¹H NMR spectrum of compound **42**

V149HID /D2O/ ¹³C NMR F8 OH 18/6/10.



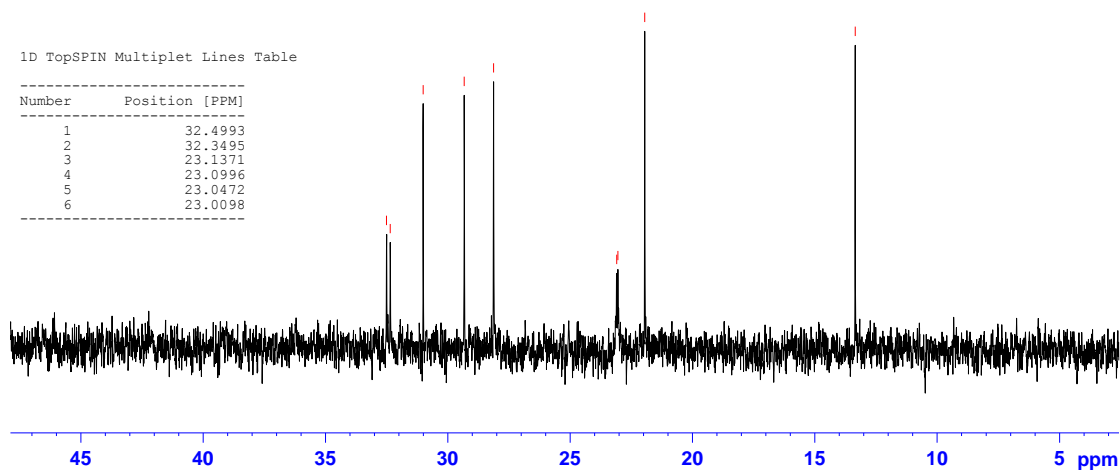
2010-06-23 16:53:09 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/V149HID/2/pdata/1

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 42

V149HID /D2O/ F8 OH ³¹P NMR 18/6/10.



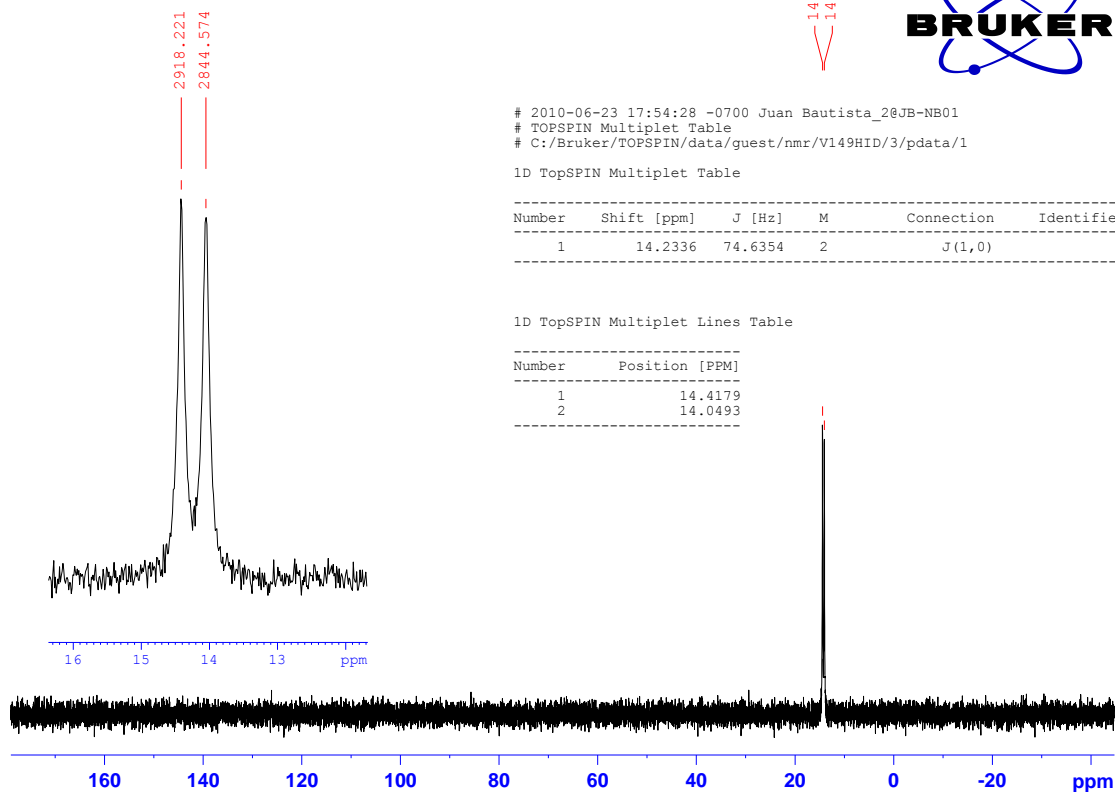
2010-06-23 17:54:28 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/V149HID/3/pdata/1

1D TopSPIN Multiplet Table

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

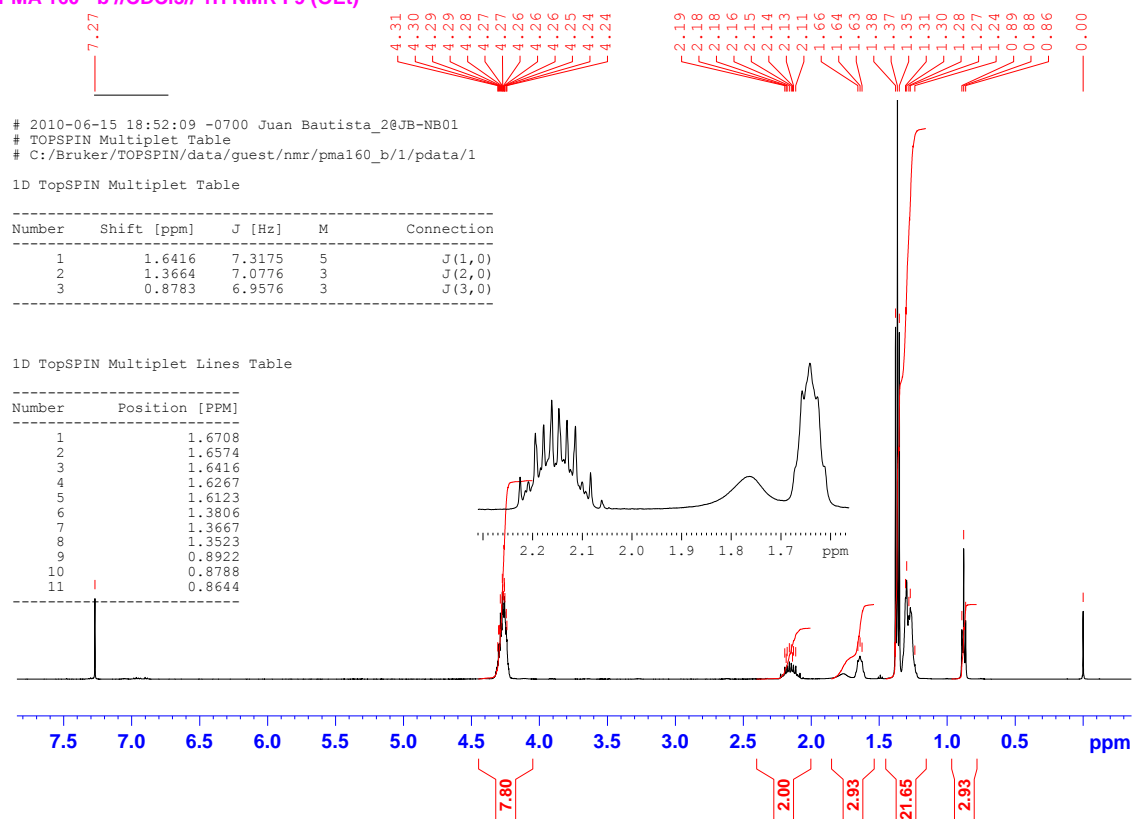
1D TopSPIN Multiplet Lines Table

Number	Position [PPM]
1	14.4179
2	14.0493



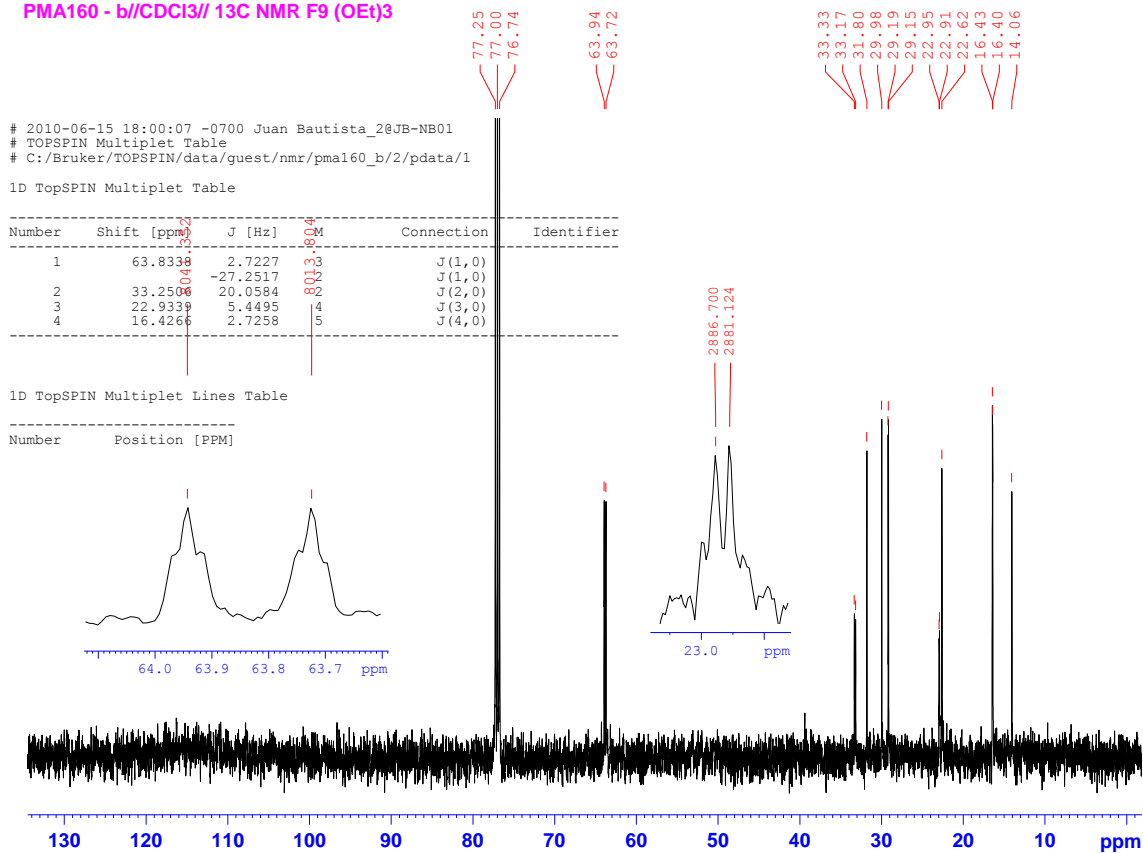
³¹P NMR spectrum of compound 42

PMA 160 - b //CDCl3// 1H NMR F9 (OEt)



¹H NMR spectrum of compound 33

PMA160 - b//CDCl3// 13C NMR F9 (OEt)3



¹³C NMR spectrum of compound 33

PMA160 - b //CDCl3// 31P NMR

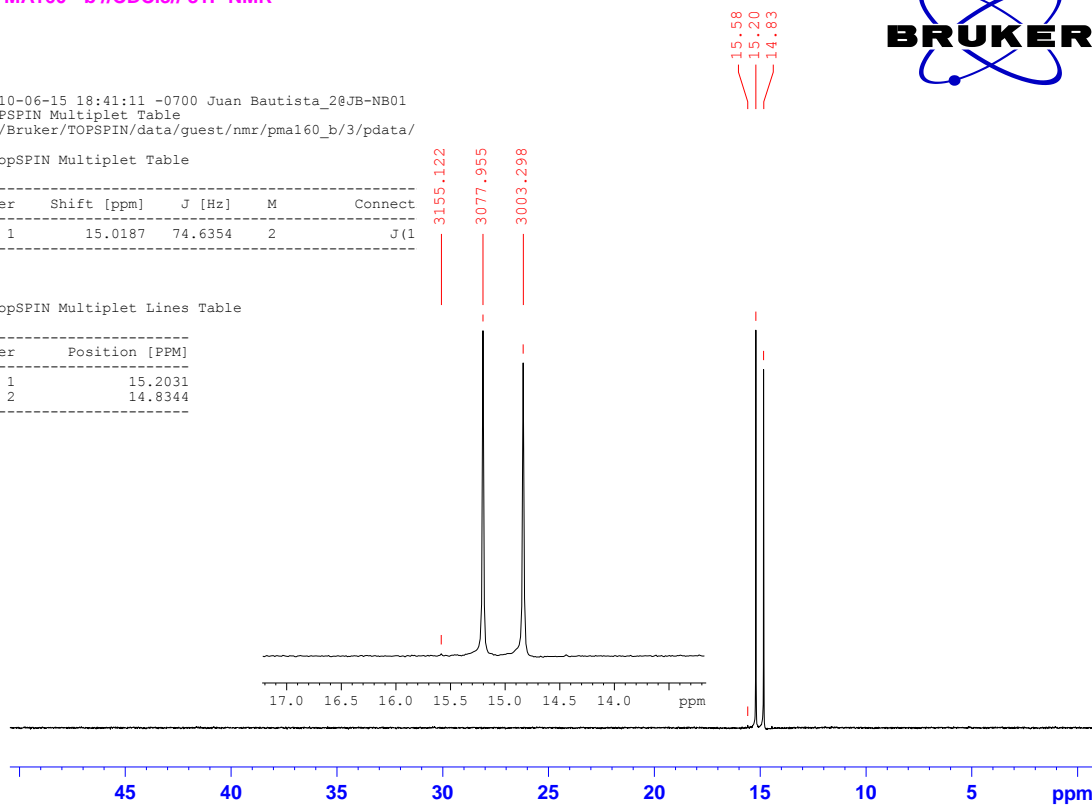
2010-06-15 18:41:11 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/pma160_b/3/pdata/

1D TopSPIN Multiplet Table

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

1D TopSPIN Multiplet Lines Table

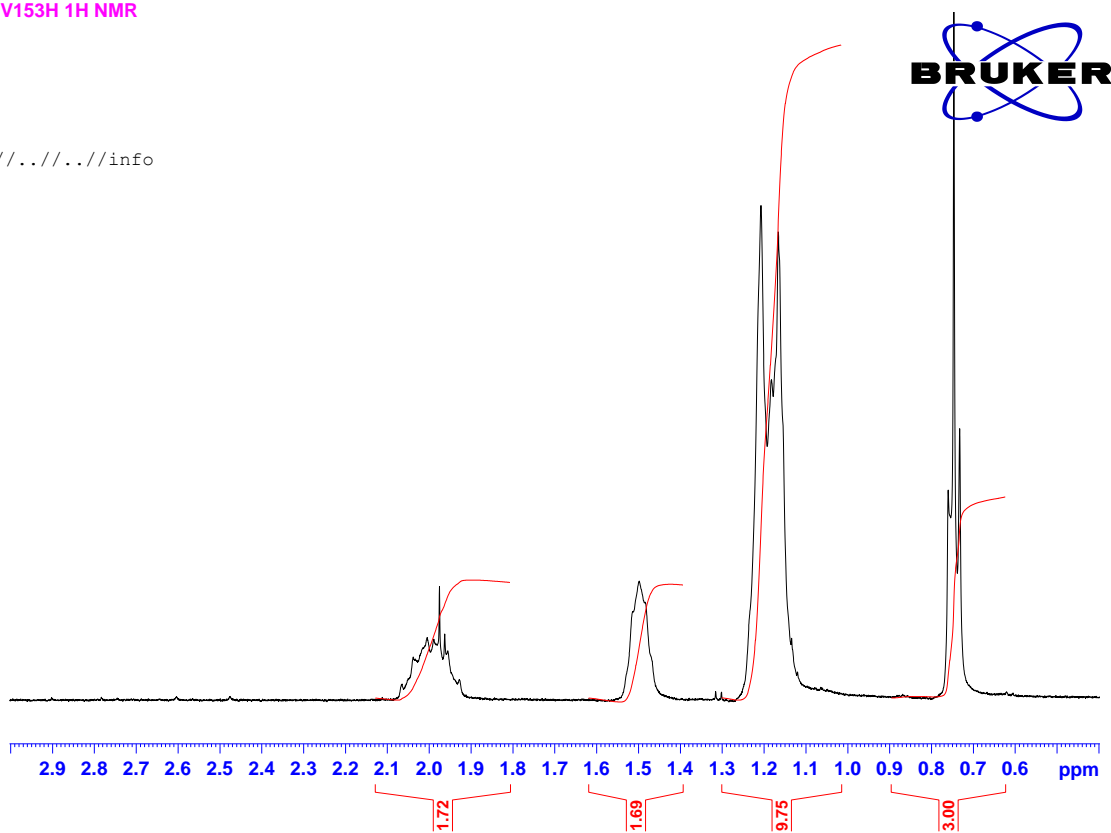
Number	Position [PPM]
1	15.2031
2	14.8344



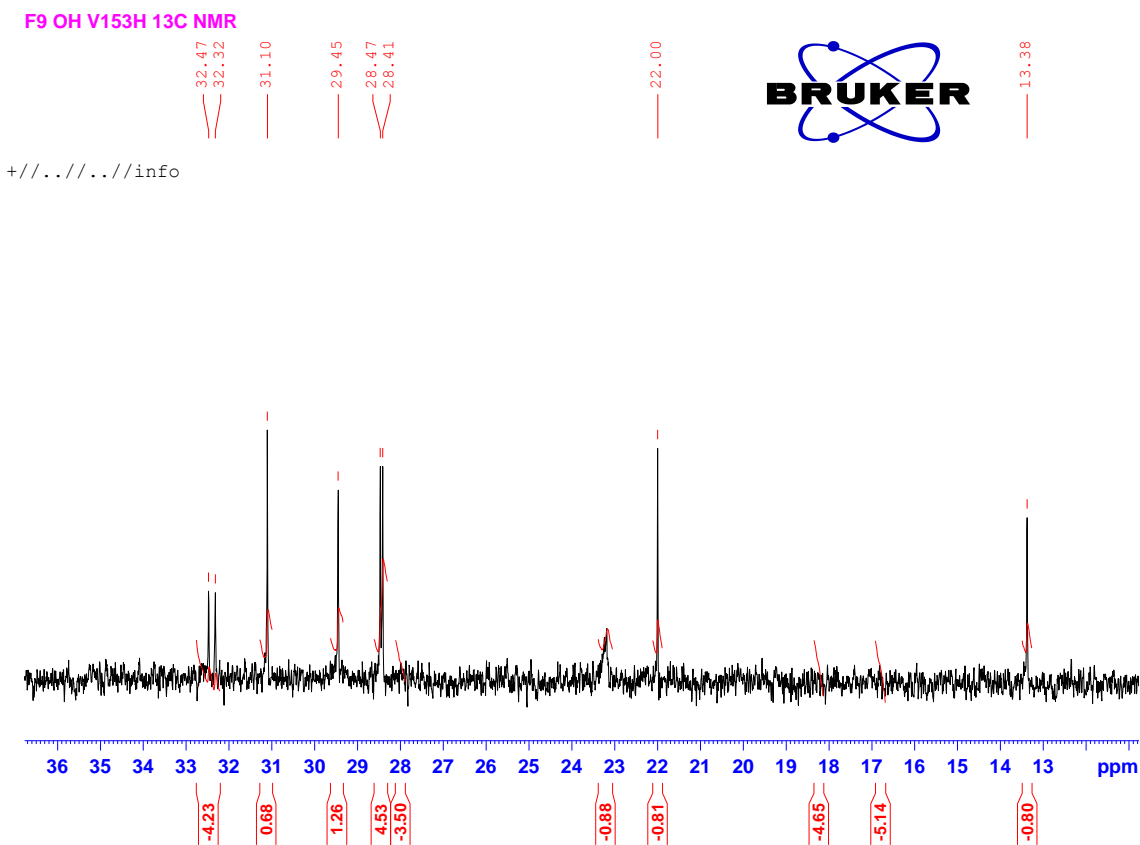
³¹P NMR spectrum of compound 33

V153H 1H NMR

+//.....//info

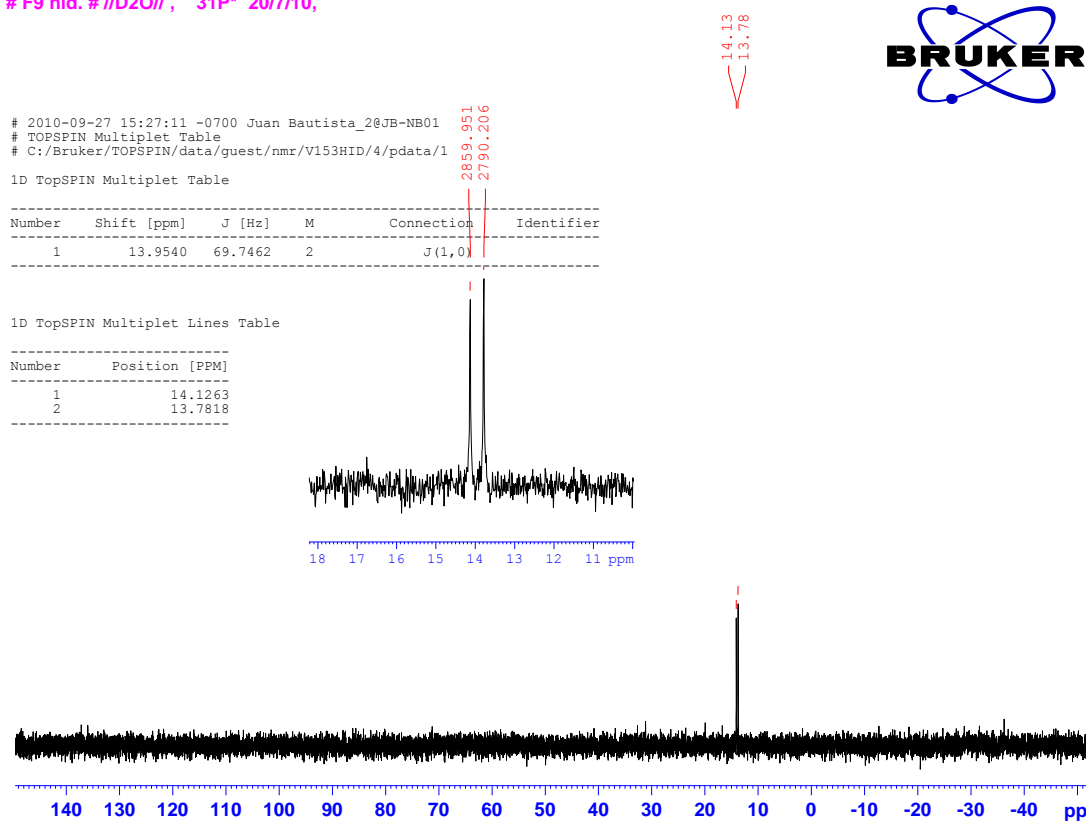


¹H NMR spectrum of compound 43

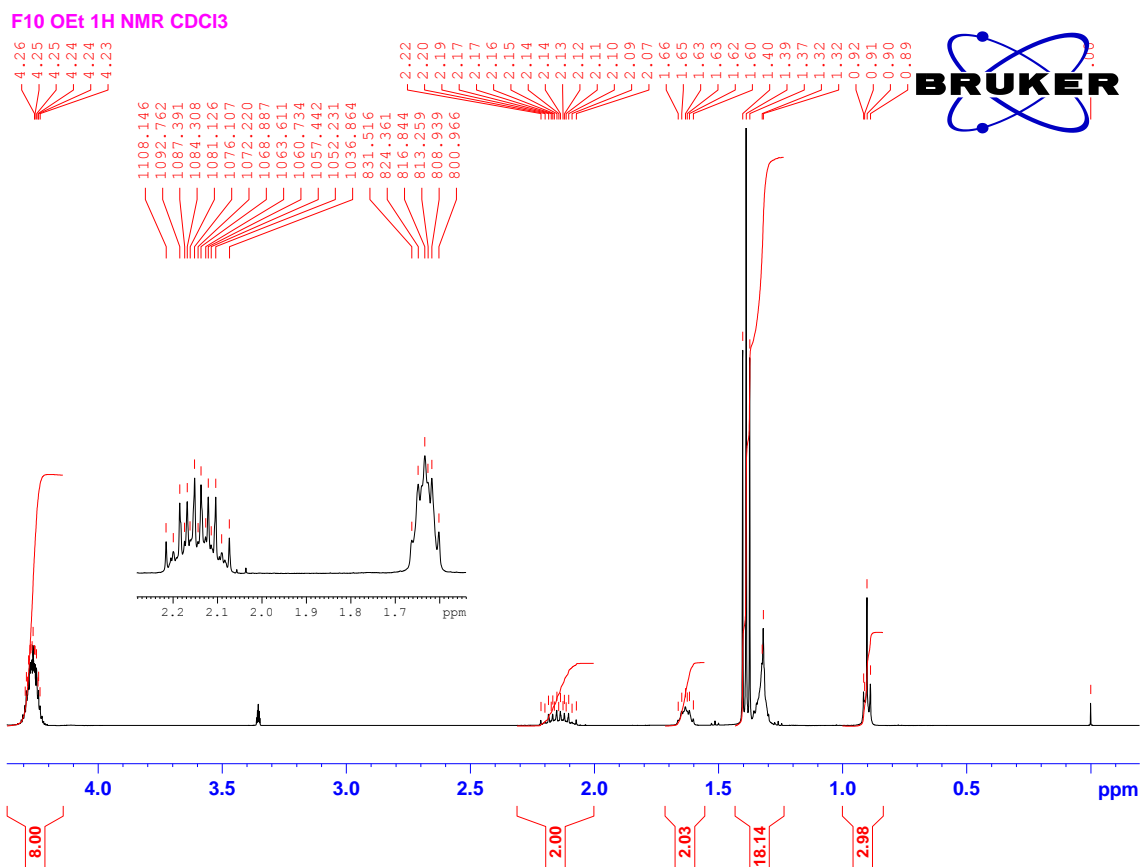


¹³C NMR spectrum of compound 43

F9 hid. # //D2O//, 31P* 207/10,

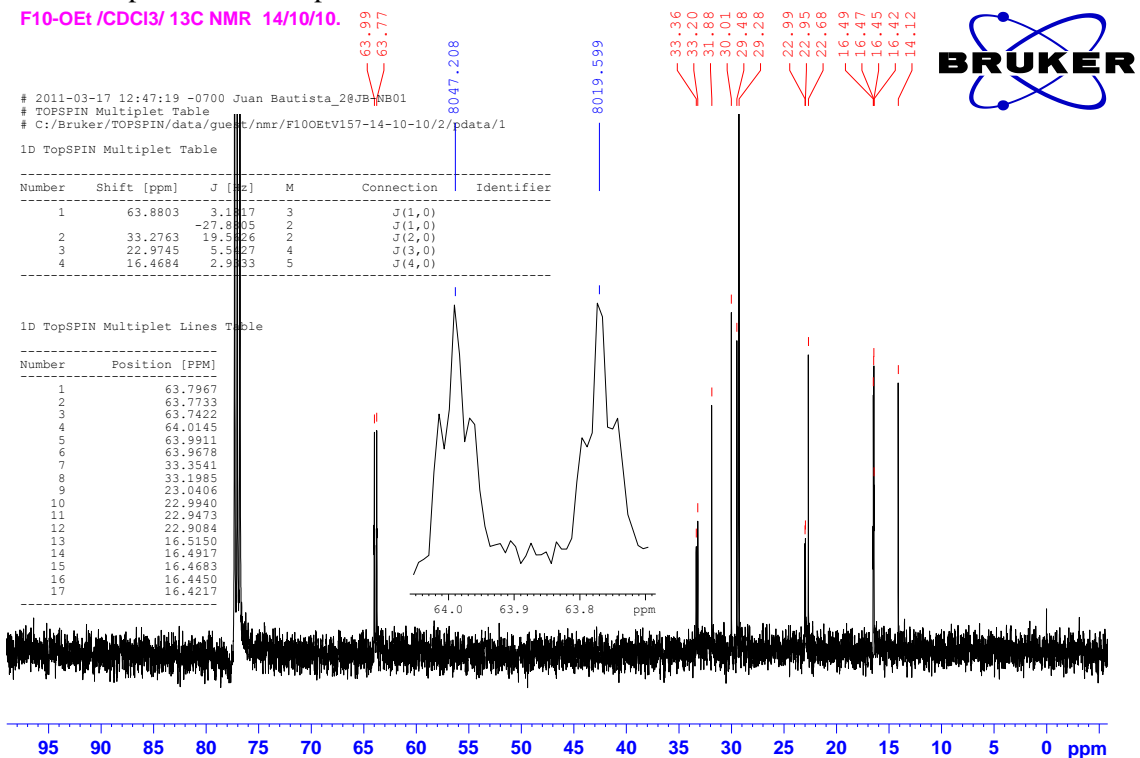


³¹P NMR spectrum of compound 43



¹H NMR spectrum of compound 34

F10-OEt /CDCl₃/ 13C NMR 14/10/10.



¹³C NMR spectrum of compound 34

³¹P F10 (OEt) CDCl₃

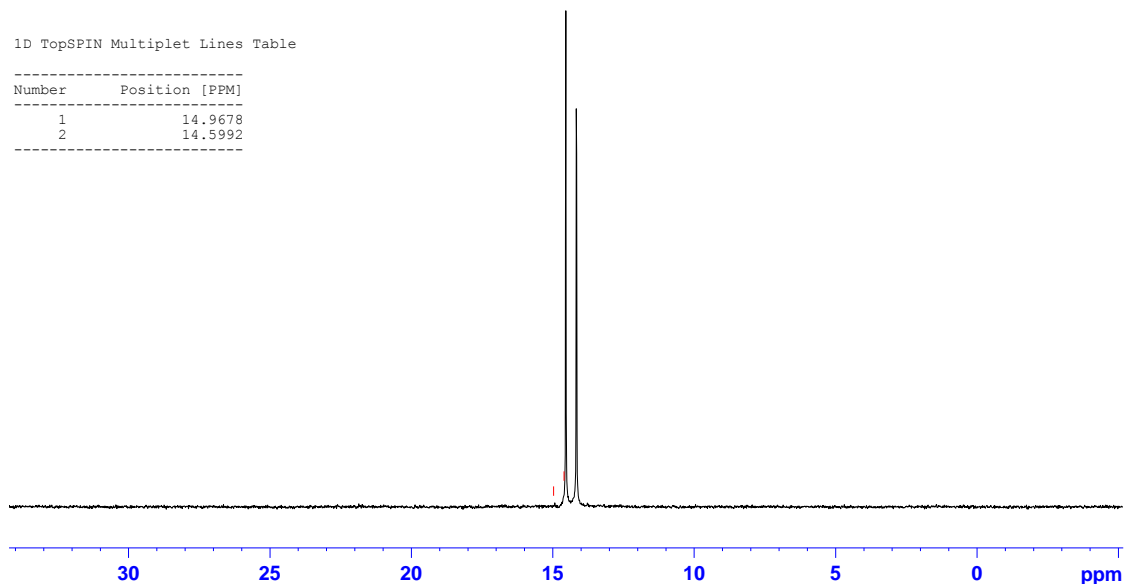


1D TopSPIN Multiplet Table

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



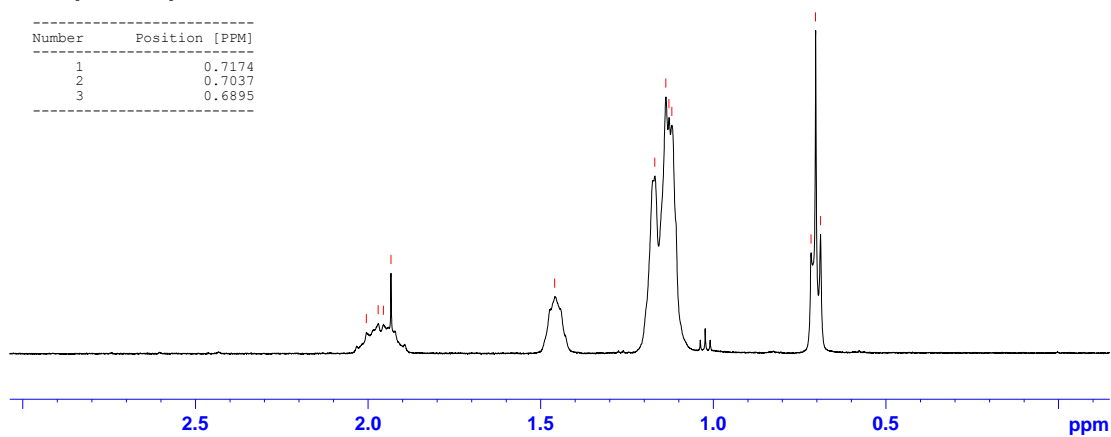
2010-09-29 17:33:20 -0700 Juan Bautista_2@JB-NB01
 # TOPSPIN Multiplet Table
 # C:/Bruker/TOPSPIN/data/guest/nmr/V157HID/1/pdata/1

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



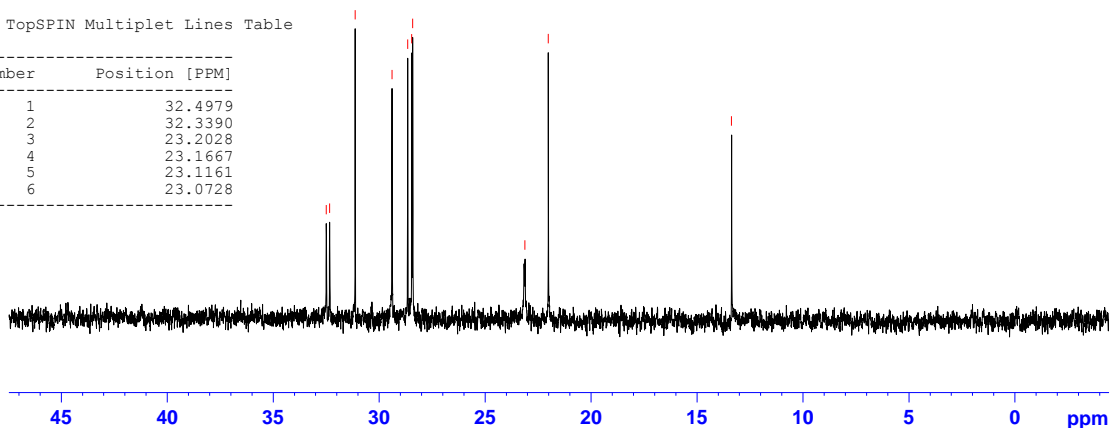
2010-09-29 17:47:42 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/V157HID/3/pdata/1

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"



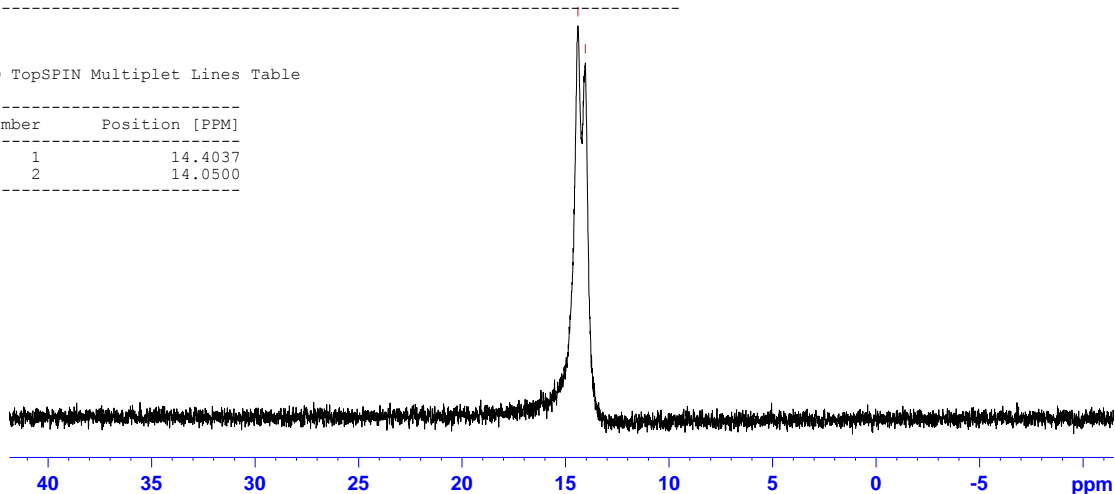
2010-09-29 17:54:53 -0700 Juan Bautista_2@JB-NB01
TOPSPIN Multiplet Table
C:/Bruker/TOPSPIN/data/guest/nmr/V157HID/2/pdata/1

1D TopSPIN Multiplet Table

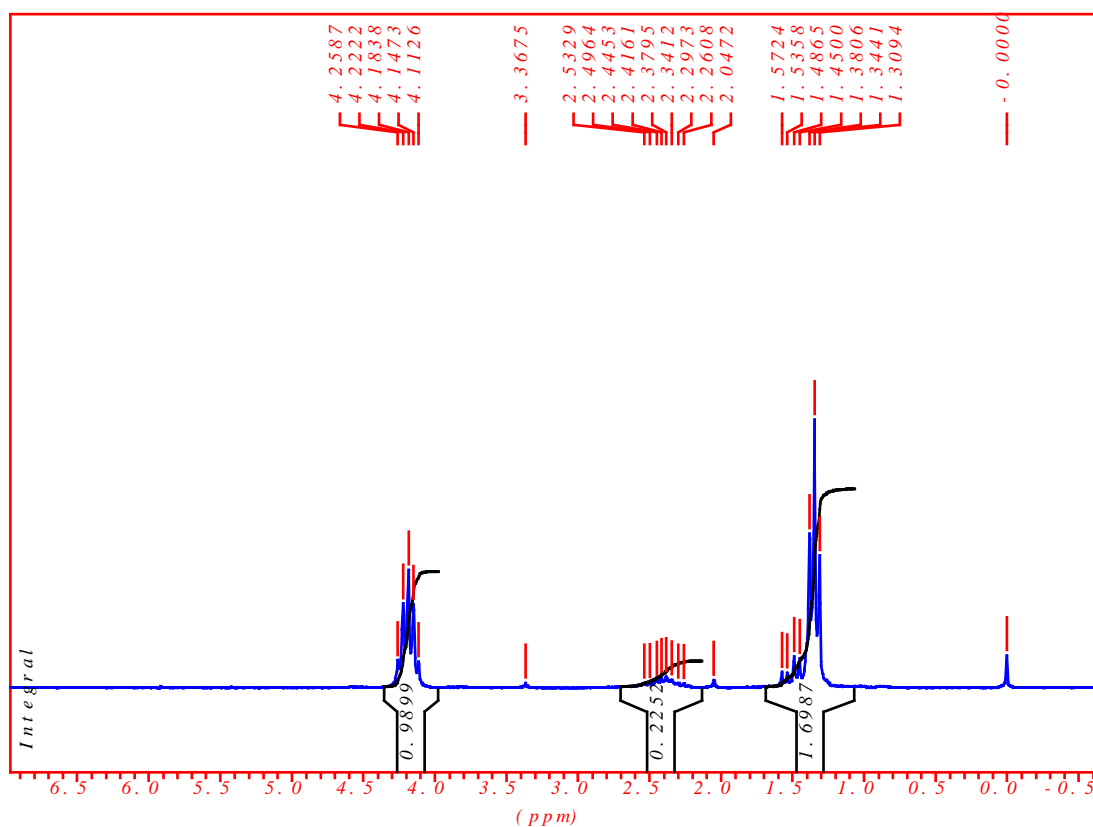
Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	14.2268	71.6229	2	J(1,0)	

1D TopSPIN Multiplet Lines Table

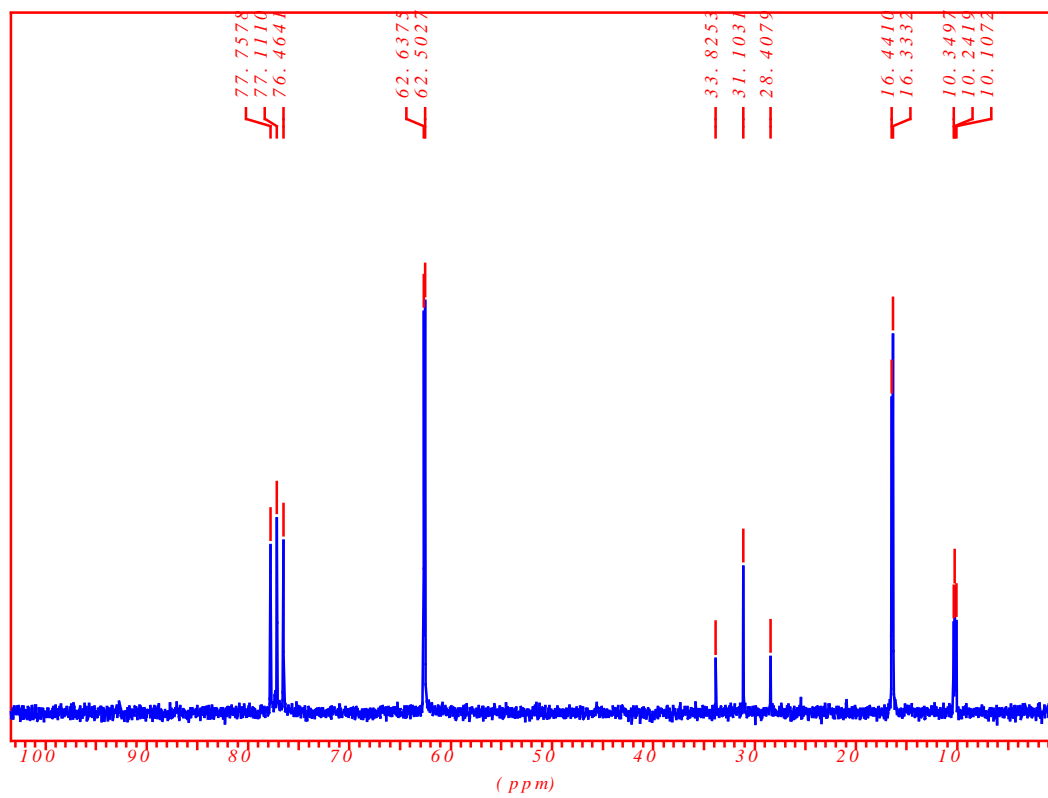
Number	Position [PPM]
1	14.4037
2	14.0500



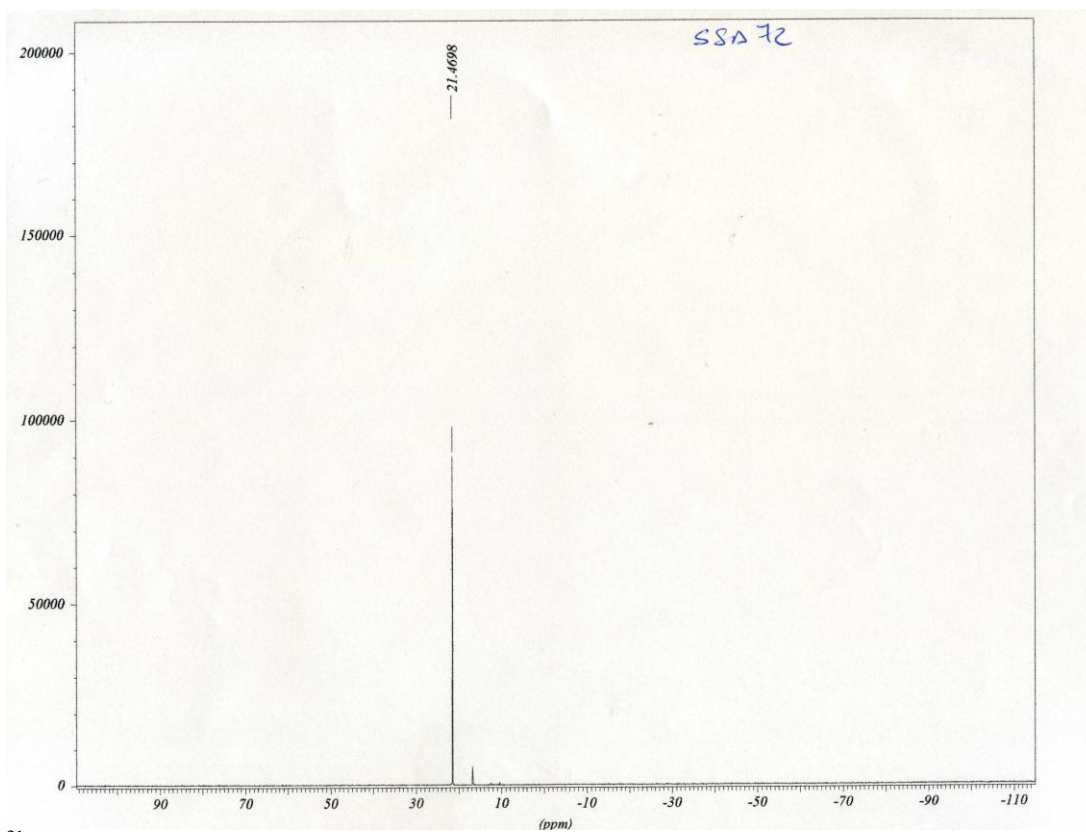
³¹P NMR spectrum of compound 44



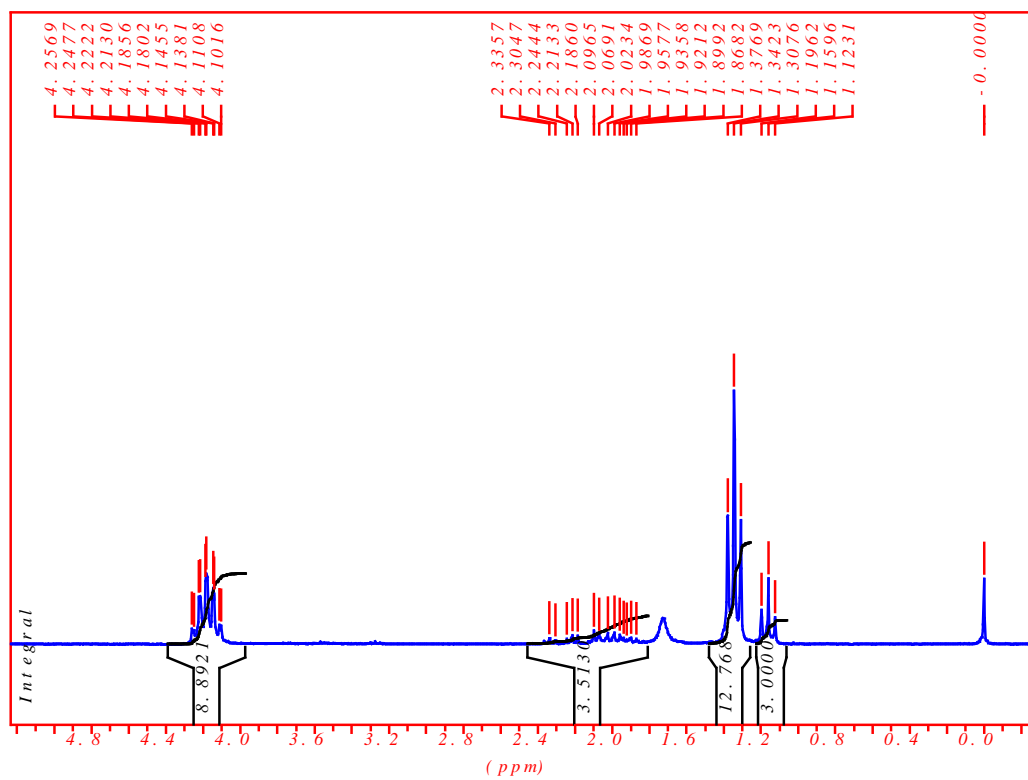
¹H NMR Spectrum of compound 16



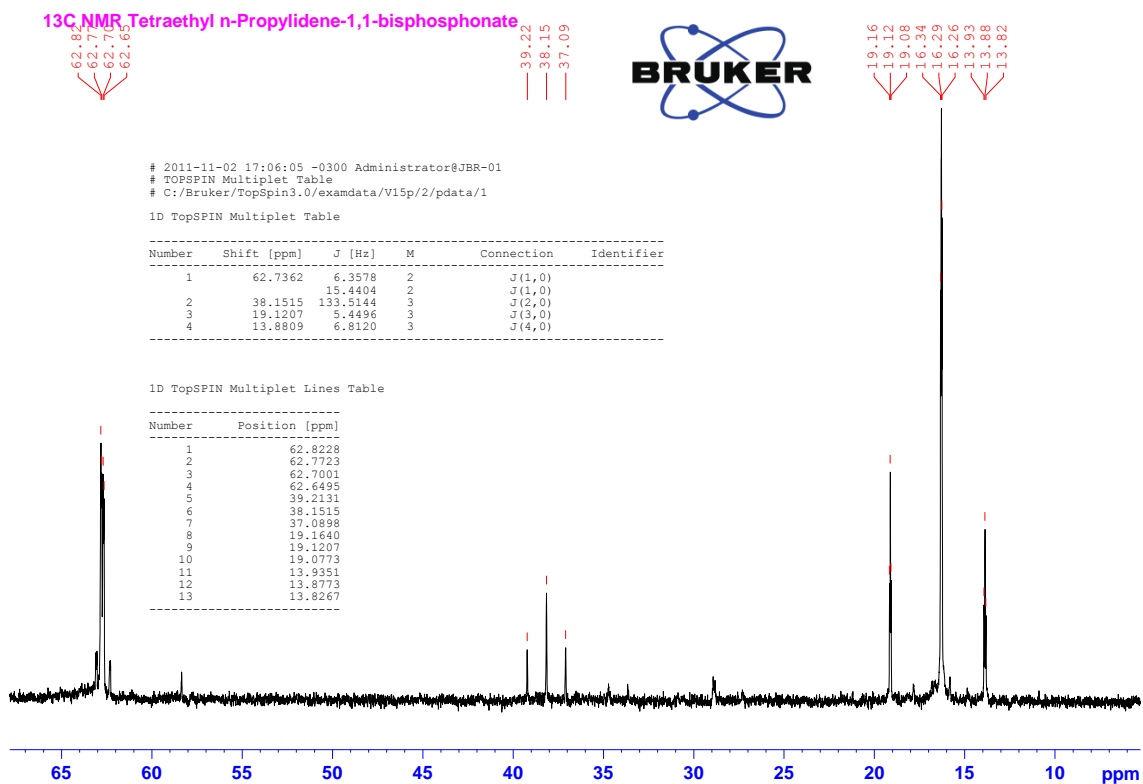
¹³C NMR Spectrum of compound 16



^{31}P NMR spectrum of compound 16

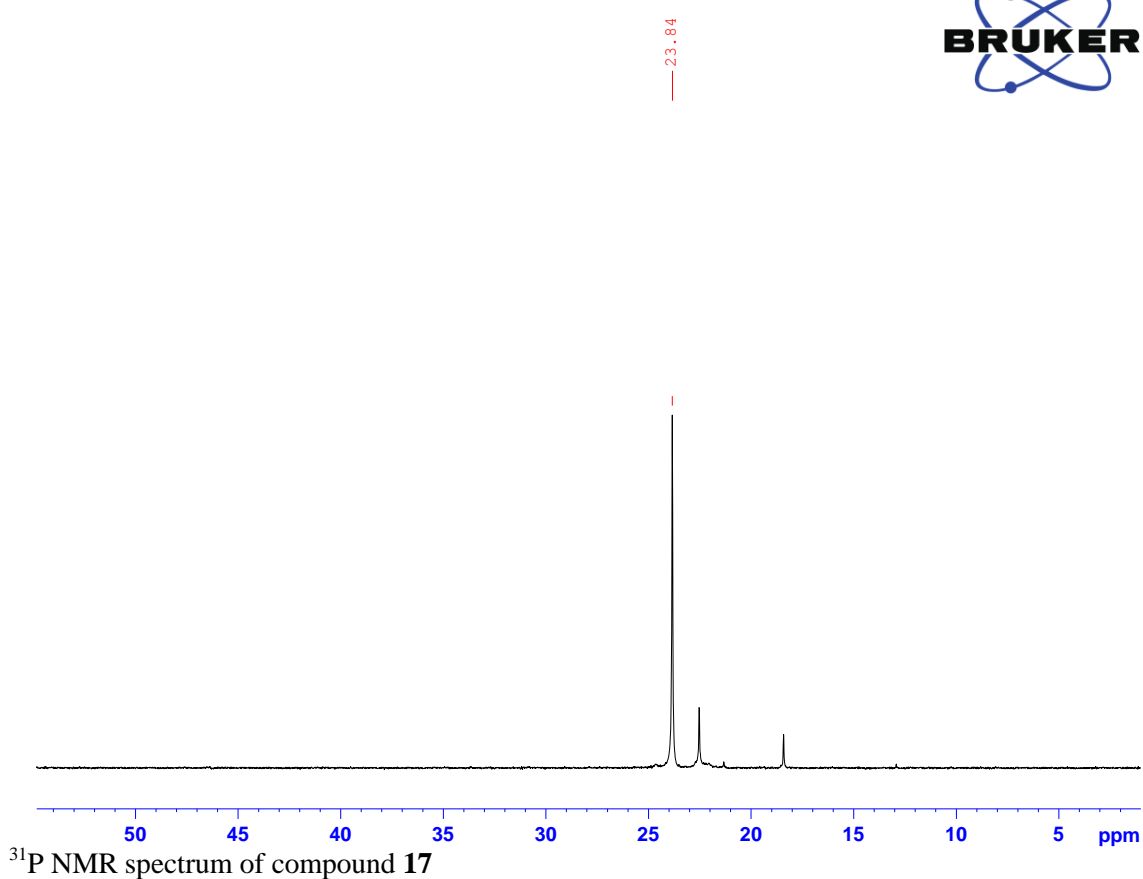


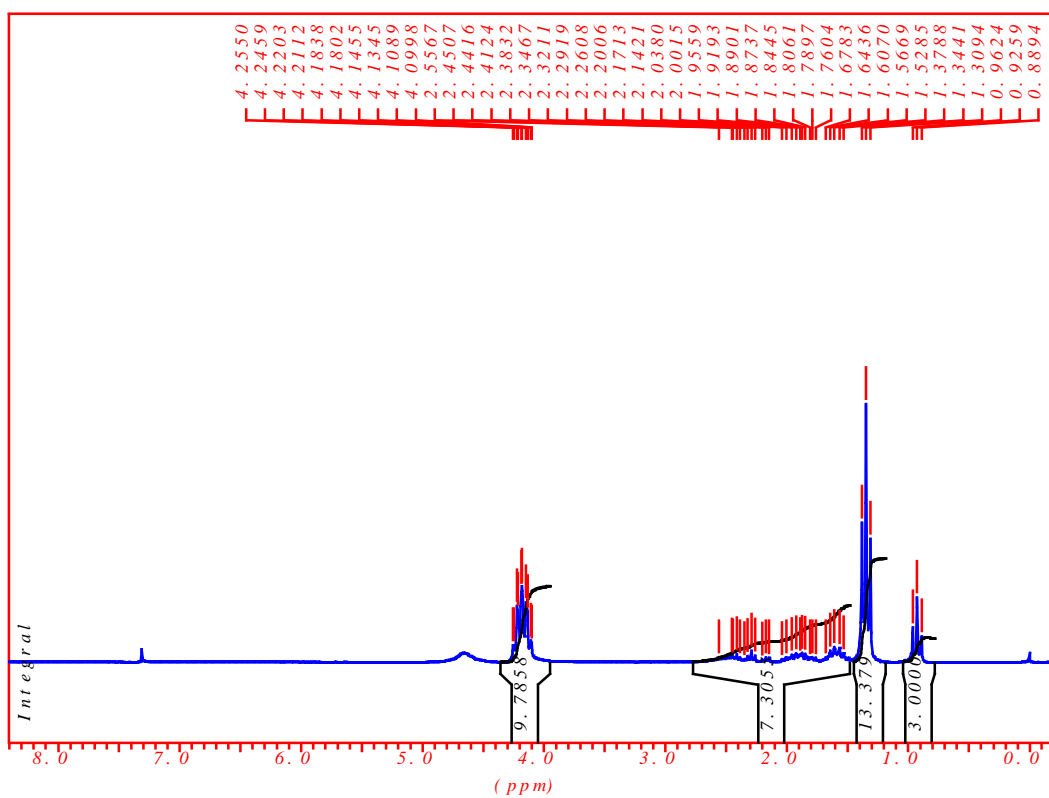
^1H NMR Spectrum of compound 17



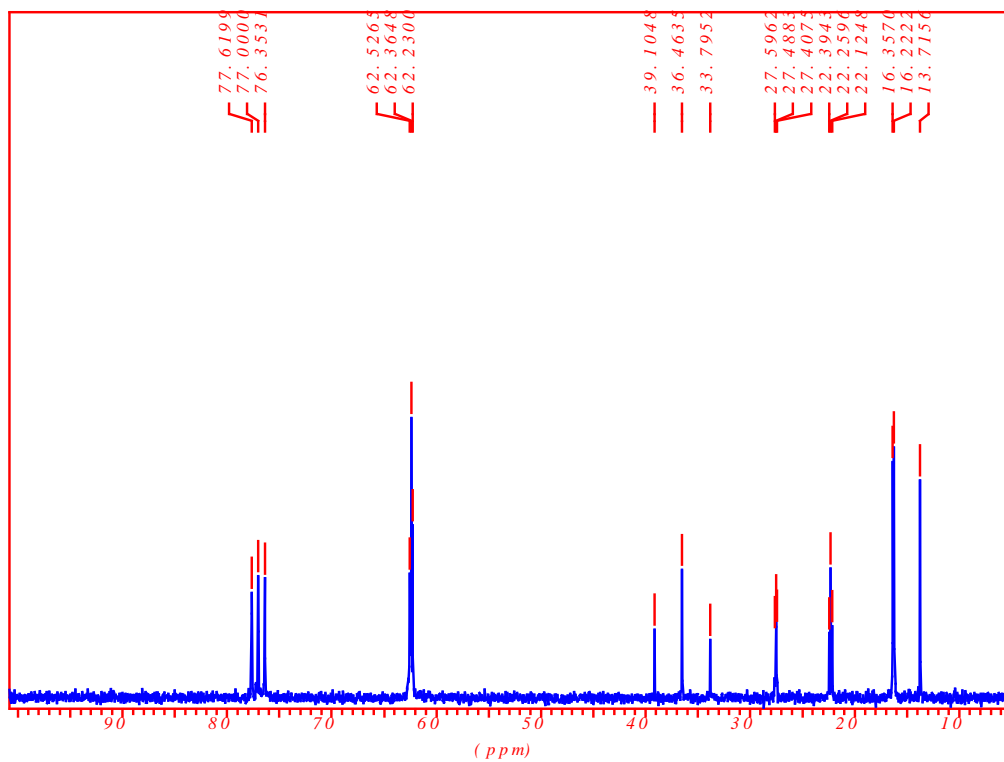
¹³C NMR Spectrum of compound **17**

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

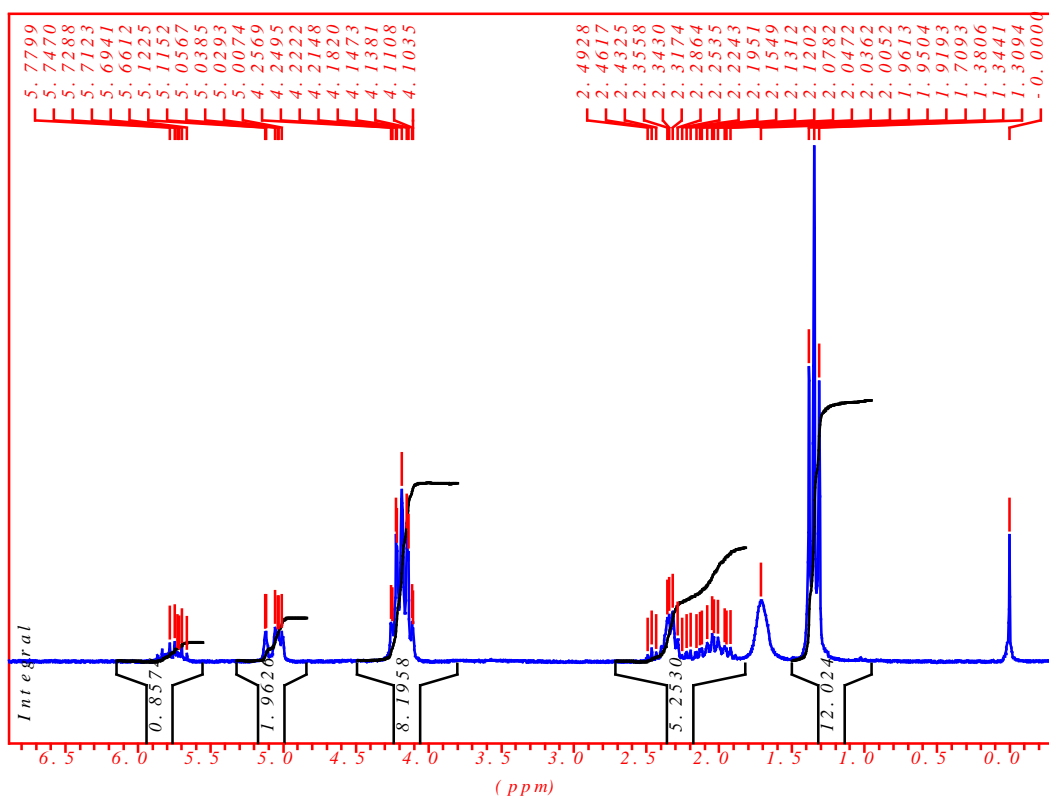




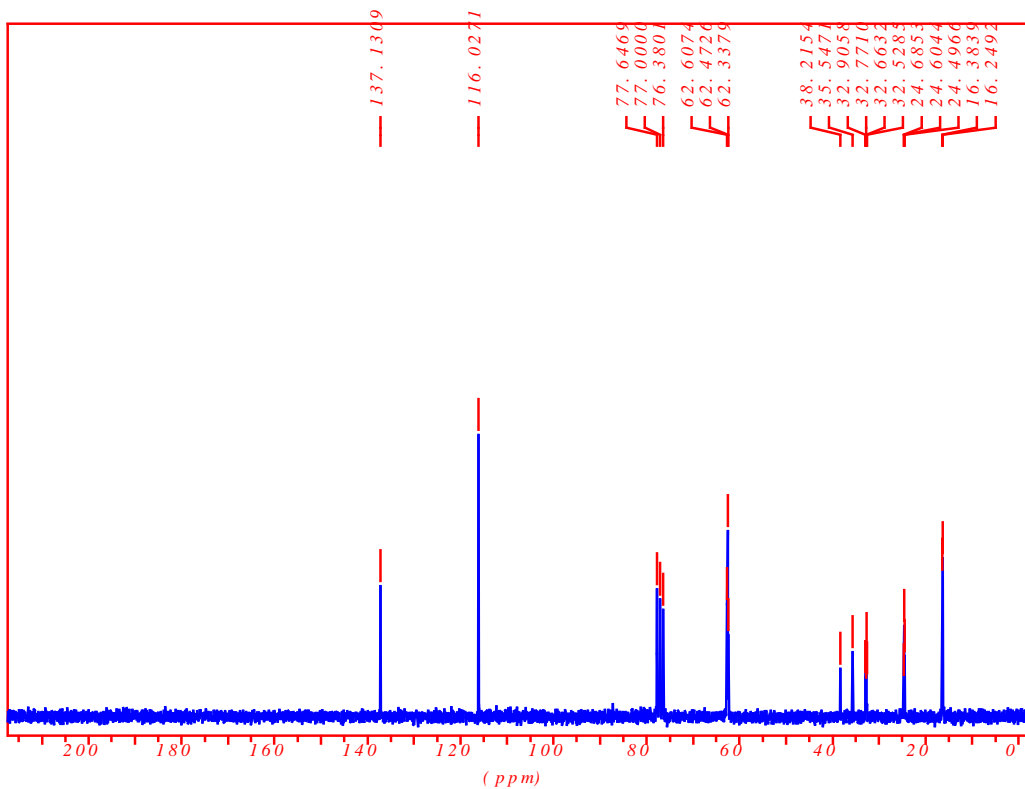
¹H NMR Spectrum of compound **18**



¹³C NMR Spectrum of compound **18**

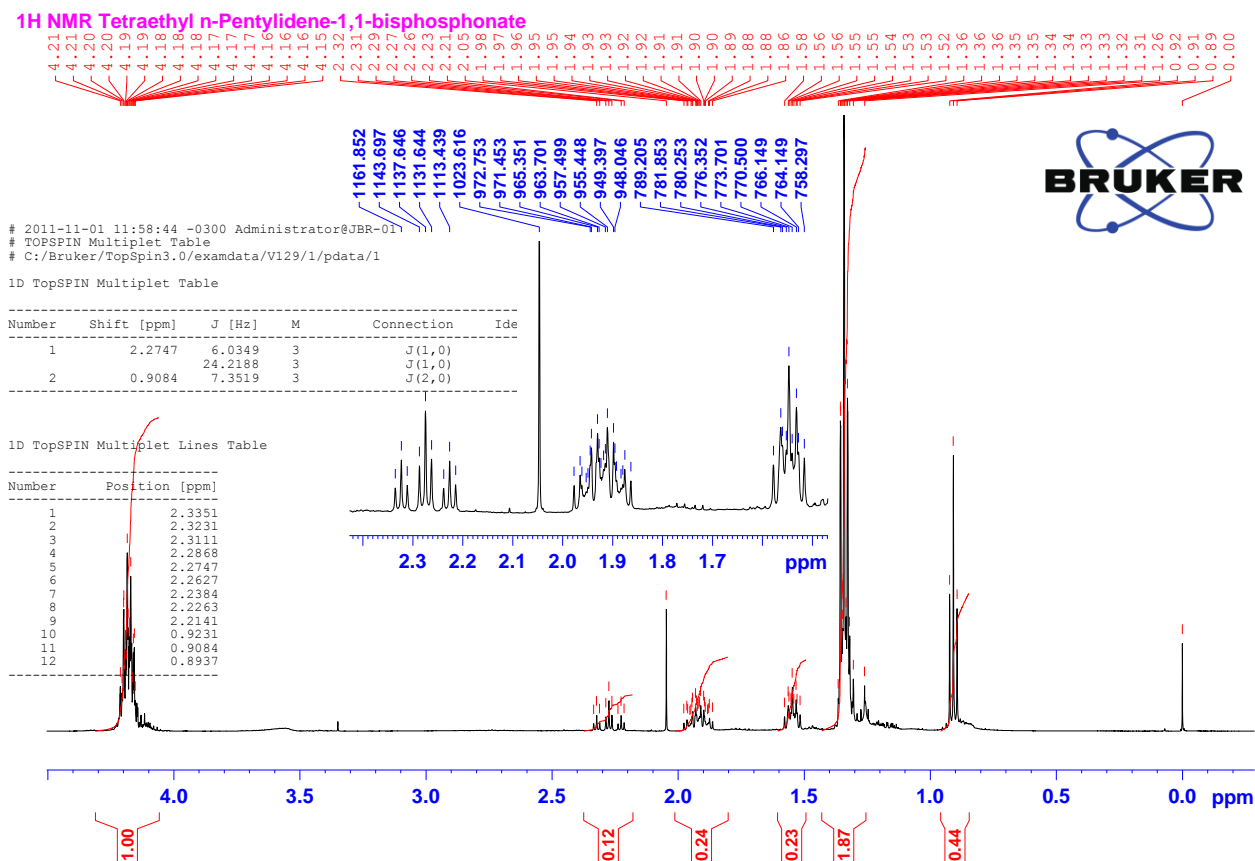


¹H NMR Spectrum of compound **19**



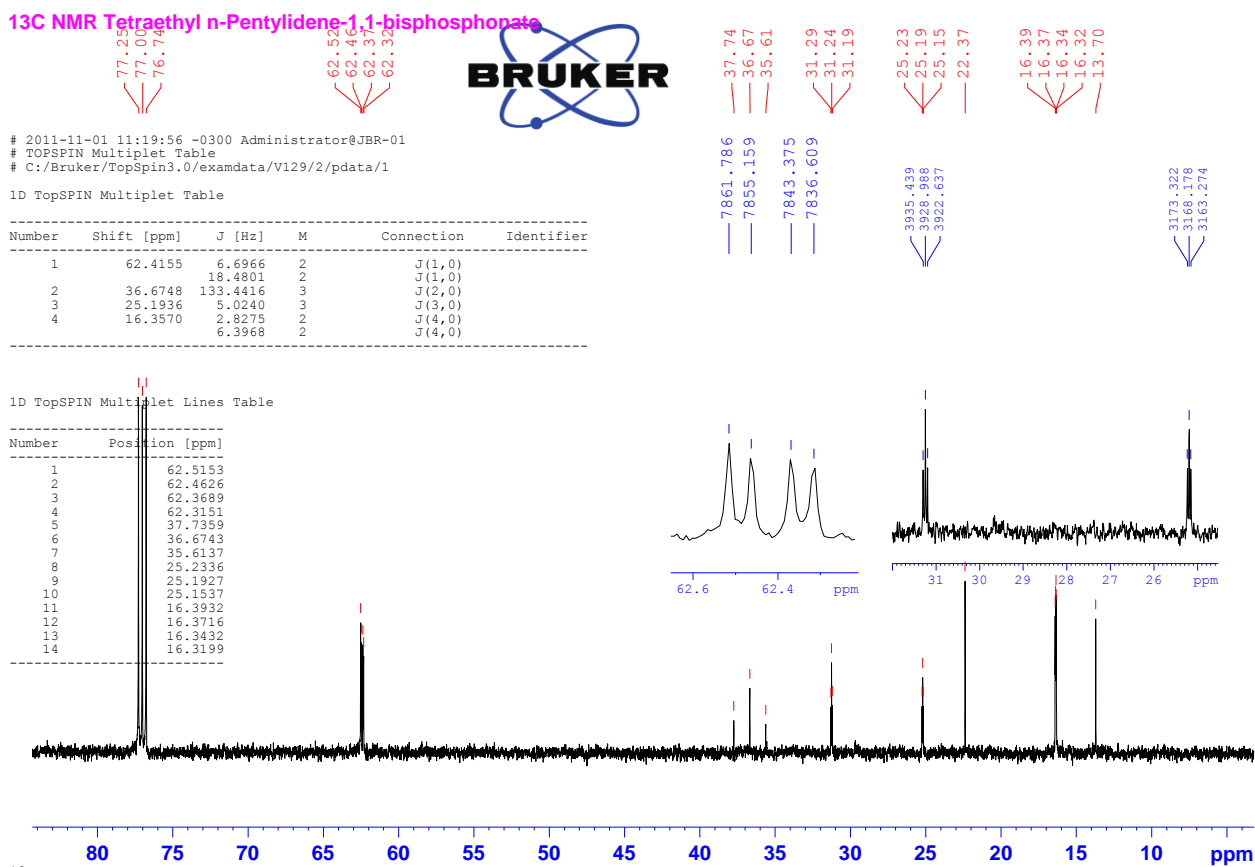
¹³C NMR Spectrum of compound **19**

¹H NMR Tetraethyl n-Pentylidene-1,1-bisphosphonate



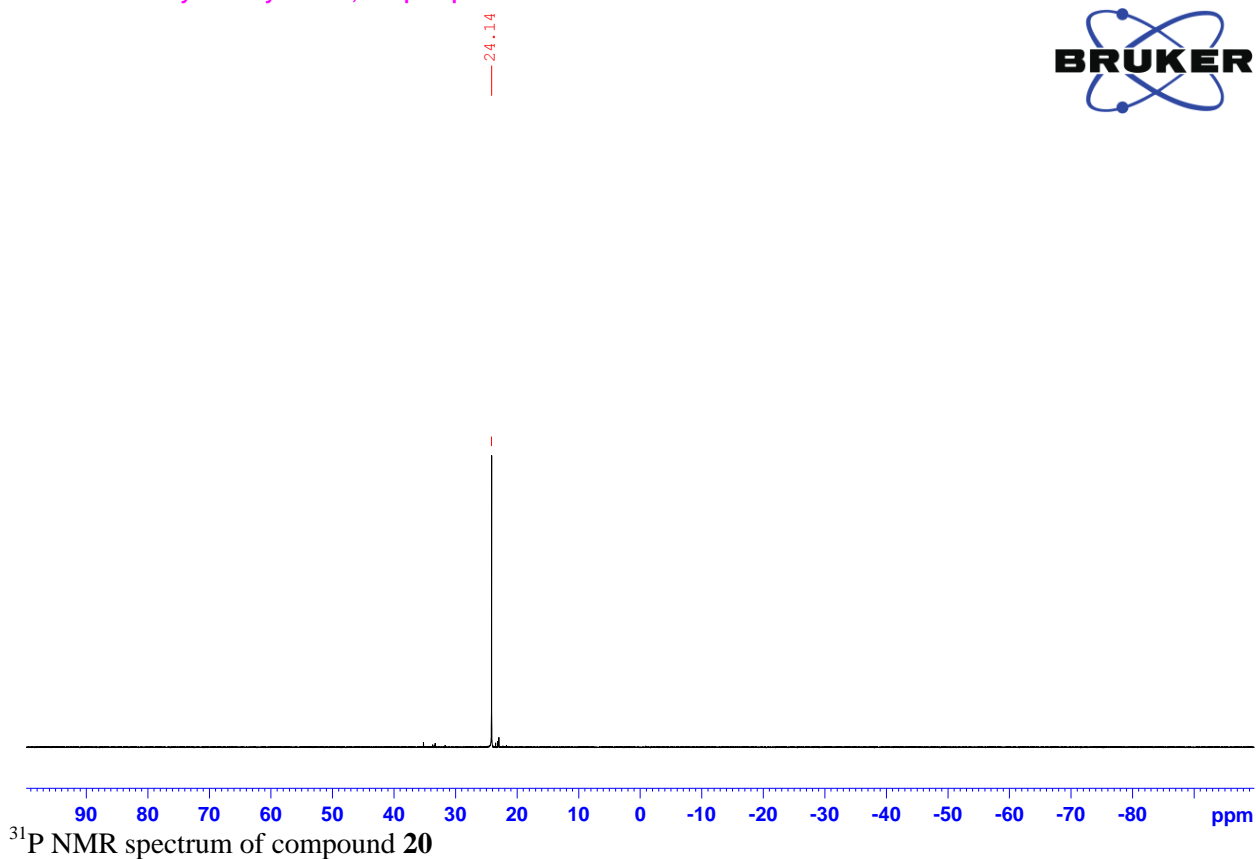
¹H NMR spectrum of compound 20

¹³C NMR Tetraethyl n-Pentylidene-1,1-bisphosphonate

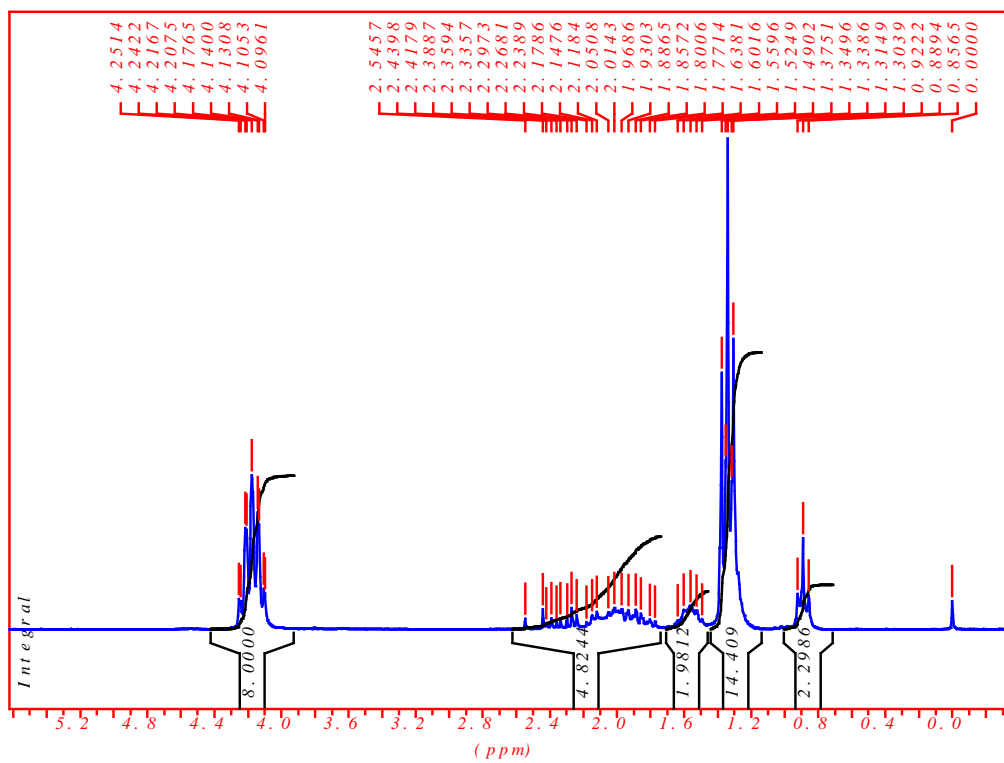


¹³C NMR spectrum of compound 20

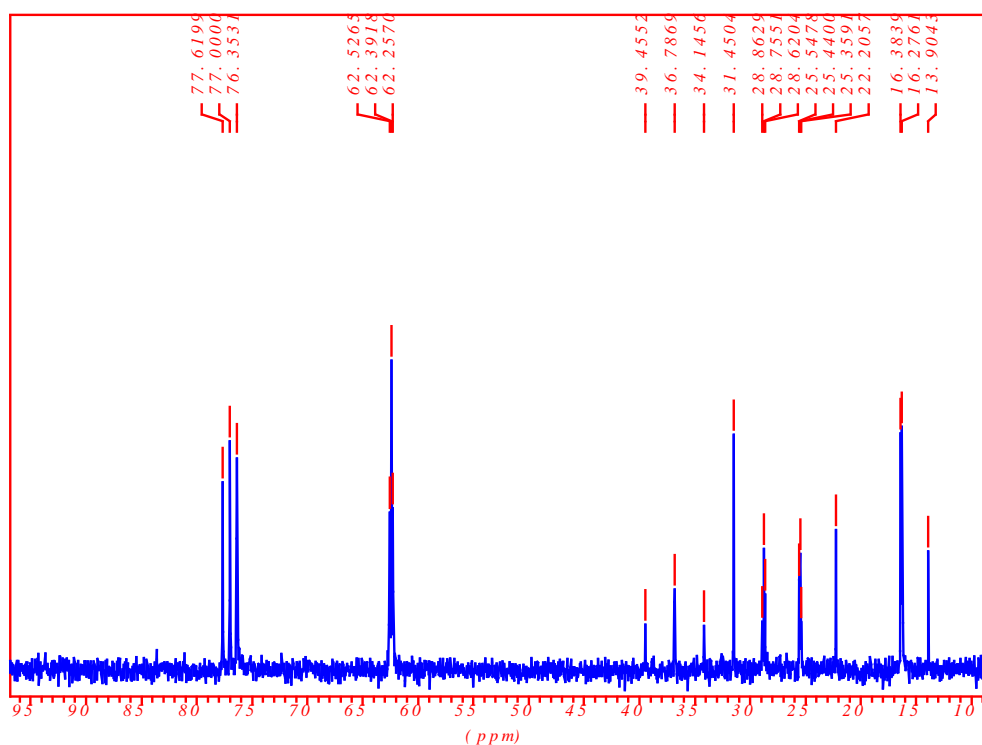
³¹P NMR Tetraethyl n-Pentylidene-1,1-bisphosphonate



³¹P NMR spectrum of compound 20

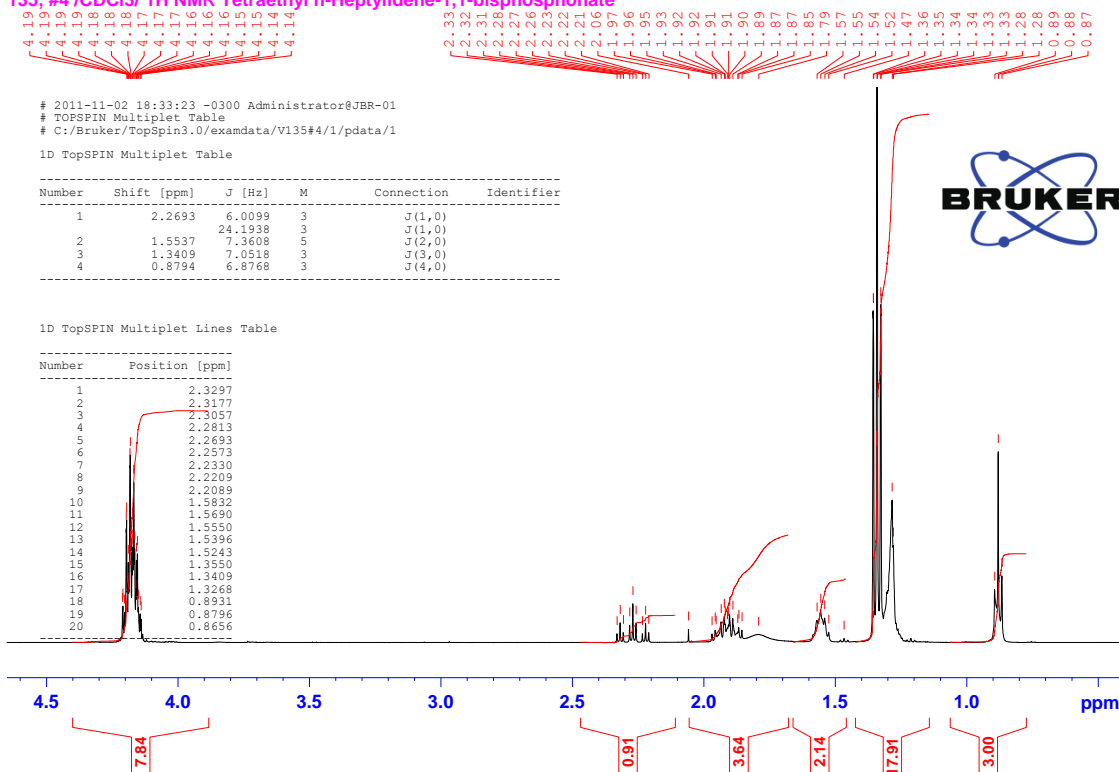


¹H NMR Spectrum of compound 21



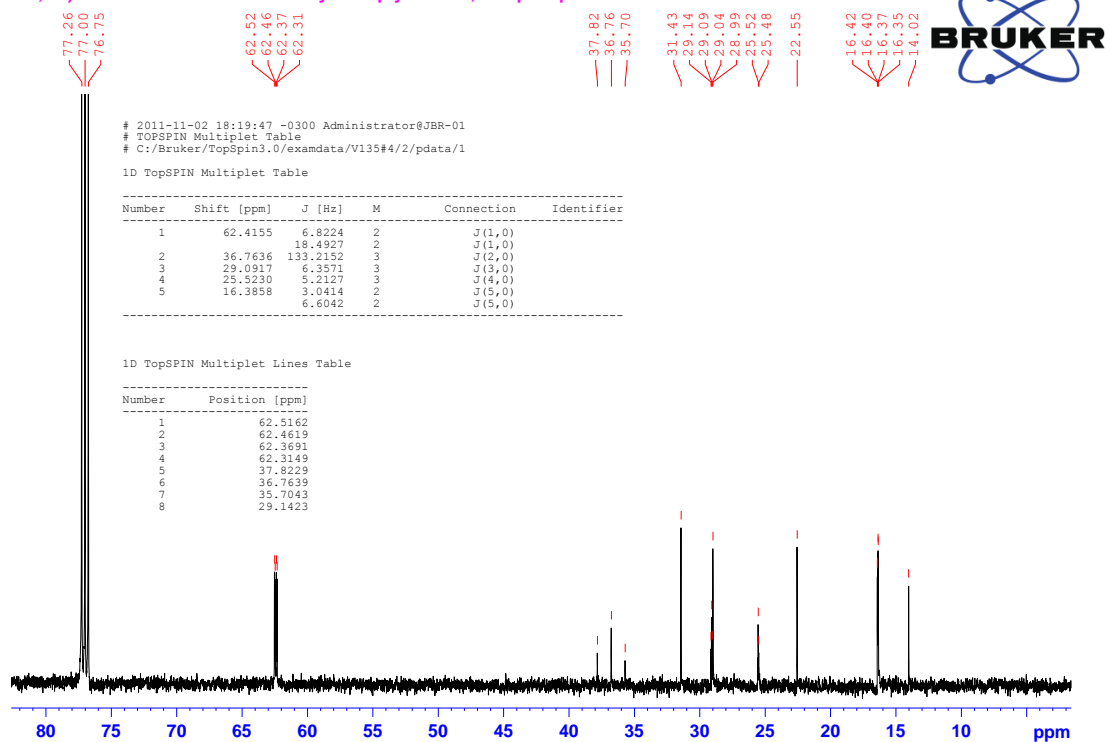
¹³C NMR Spectrum of compound 21

V 135_#4 /CDCl₃/ ¹H NMR Tetraethyl n-Heptylidene-1,1-bisphosphonate



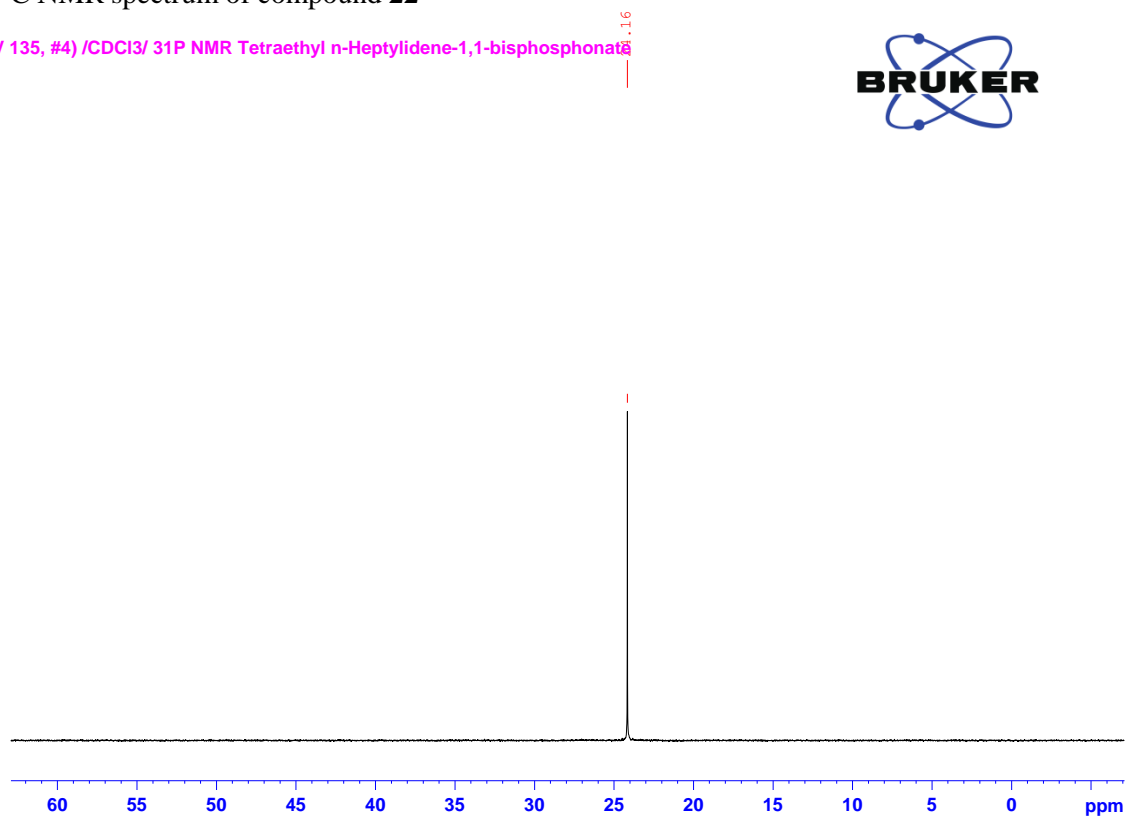
¹H NMR spectrum of compound 22

(V 135, #4) # /CDCl₃/ ¹³C NMR Tetraethyl n-Heptylidene-1,1-bisphosphonate



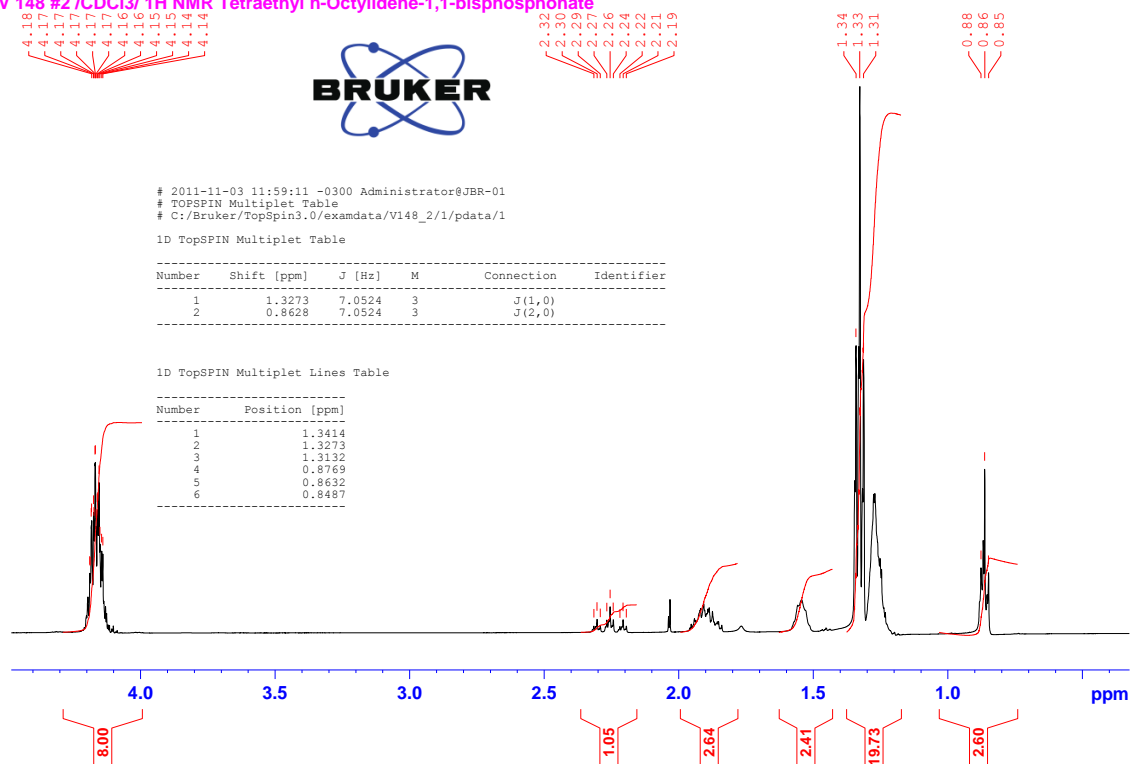
¹³C NMR spectrum of compound **22**

V 135, #4) /CDCl₃/ ³¹P NMR Tetraethyl n-Heptylidene-1,1-bisphosphonate

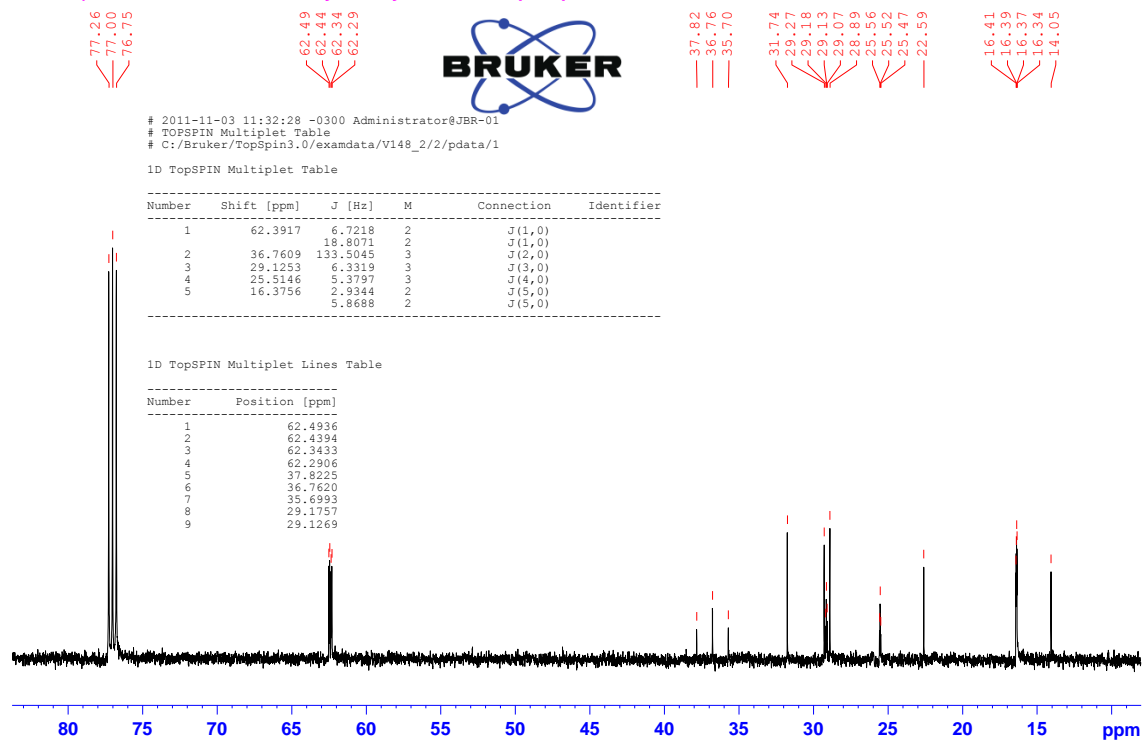


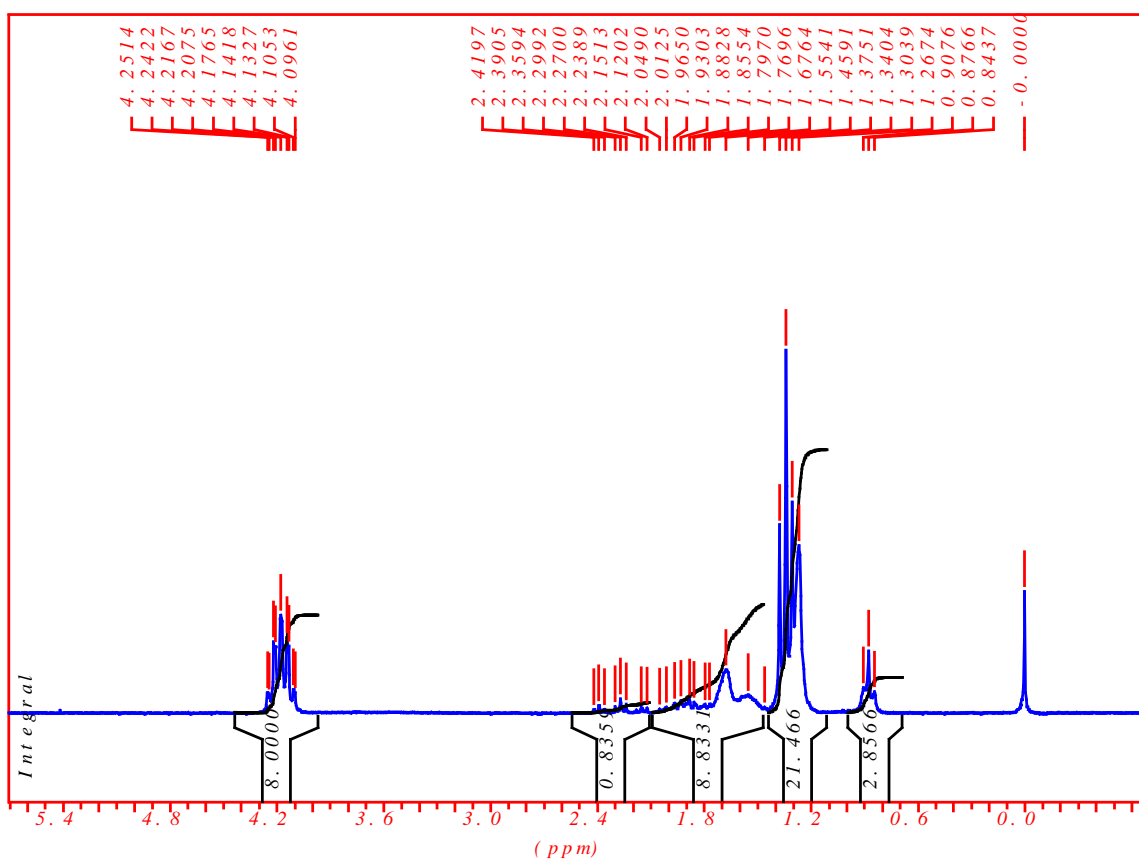
³¹P NMR spectrum of compound **22**

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

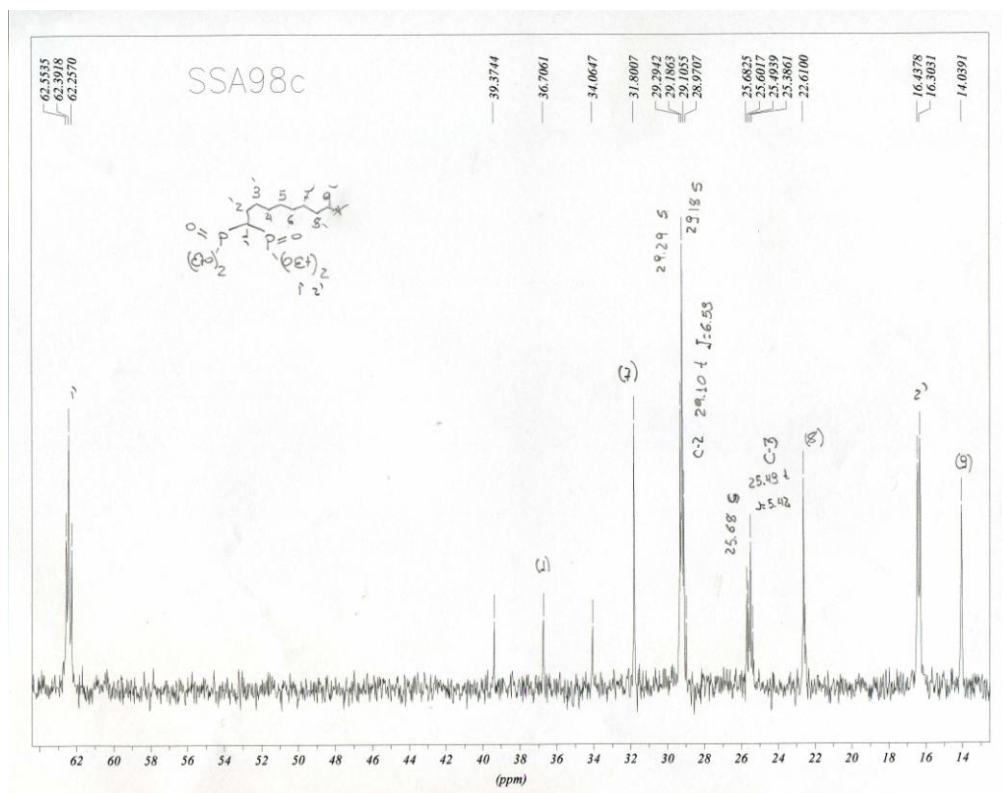


V 148 #2 /CDCI3/ 13C NMR Tetraethyl n-Octylidene-1,1-bisphosphonate





¹H NMR Spectrum of compound 24



¹³C NMR spectrum of compound 24

Sample No. SSA89 SUBMITTER
 Company / School Dr. Juan B. Rodriguez
 Address UNIVERSIDAD DE BUENOS AIRES
FACULTAD DE CIENCIAS EXACTAS Y NATURALES
DEPARTAMENTO DE QUIMICA ORGANICA
INSTITUTO DE QUIMICA ORGANICA
1100 BUENOS AIRES ARGENTINA

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

NO CHARGE FOR DUPLICATES

PROFESSOR/SUPERVISOR: P.O. #:
 NAME SEP 24, 2001 DATE

Element	Theory	Found	
C	46.92	45.05	44.97
H	9.00	8.69	8.71
P	17.29	OUR LAB DOES NOT PERFORM PHOSPHORUS ANALYSIS.	

Single Duplicate
 Elements C, H, O, P
 Present: C, H, P
 Analyze for: C, H, P
 Hygroscopic Explosive
 M.P. S.P.
 To be dried: Yes No
 Temp. rt vac Time 3h
 FAX Service 54114 804-1692
 Fax Phone # 54114 804-1692
 Return 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 21

Sample No. SSA87 SUBMITTER
 Company / School Dr. Juan B. Rodriguez
 Address UNIVERSIDAD DE BUENOS AIRES
FACULTAD DE CIENCIAS EXACTAS Y NATURALES
DEPARTAMENTO DE QUIMICA ORGANICA
INSTITUTO DE QUIMICA ORGANICA
1100 BUENOS AIRES ARGENTINA

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

NO CHARGE FOR DUPLICATES

PROFESSOR/SUPERVISOR: P.O. #:
 NAME SEP 24, 2001 DATE

Element	Theory	Found	
C	46.38	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: C, H, P
 Analyze for: C, H, P
 Hygroscopic Explosive
 M.P. S.P.
 To be dried: Yes No
 Temp. rt vac Time 3h
 FAX Service 54114 804-1692
 Fax Phone # 54114 804-1692
 Return 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. SSA86 SUBMITTER
 Company / School Dr. Juan B. Rodriguez
 Address UNIVERSIDAD DE BUENOS AIRES
FACULTAD DE CIENCIAS EXACTAS Y NATURALES
DEPARTAMENTO DE QUIMICA ORGANICA
INSTITUTO DE QUIMICA ORGANICA
1100 BUENOS AIRES ARGENTINA

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

NO CHARGE FOR DUPLICATES

PROFESSOR/SUPERVISOR: P.O. #:
 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: C, H, P
 Analyze for: C, H, P
 Hygroscopic Explosive
 M.P. S.P.
 To be dried: Yes No
 Temp. rt vac Time _____
 FAX Service 54114 804-1692
 Fax Phone # 54114 804-1692
 Return 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.