

Supplementary Materials: Antiparasitic Activity of Sulfur- and Fluorine-Containing Bisphosphonates against Trypanosomatids and Apicomplexan Parasites

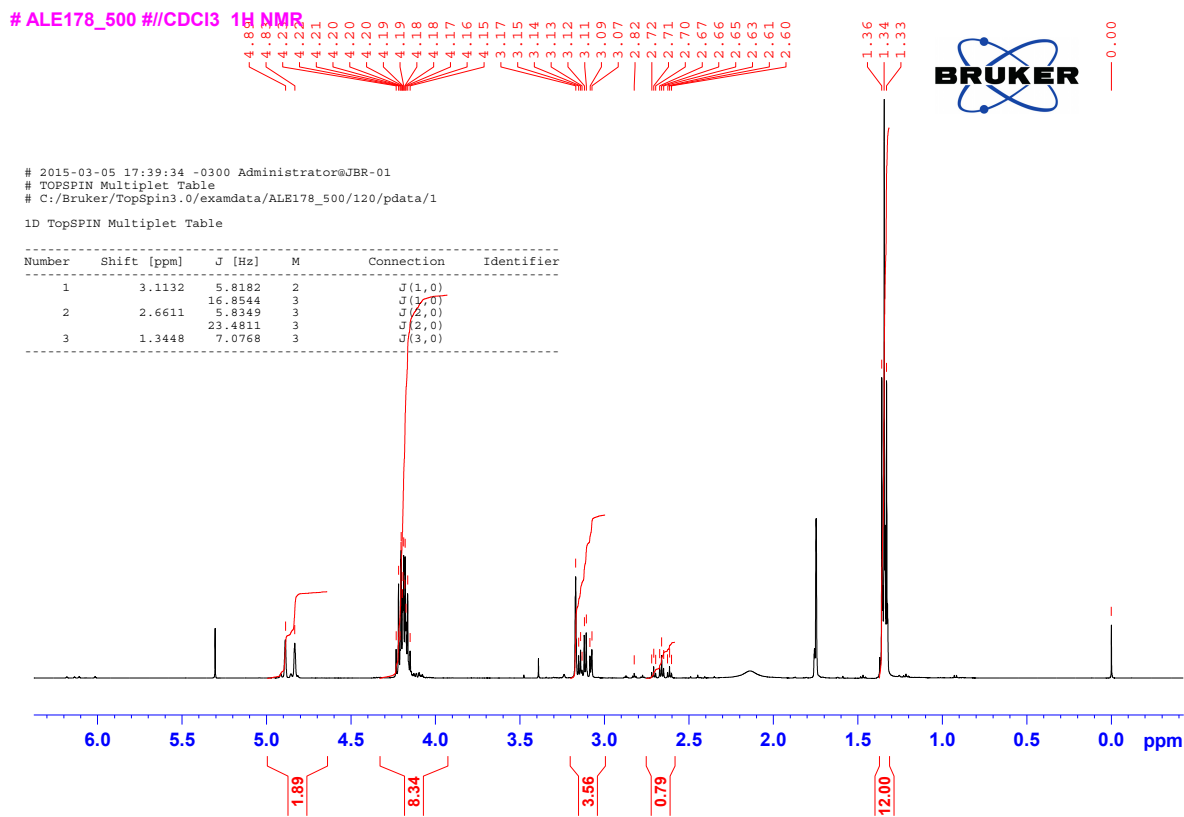
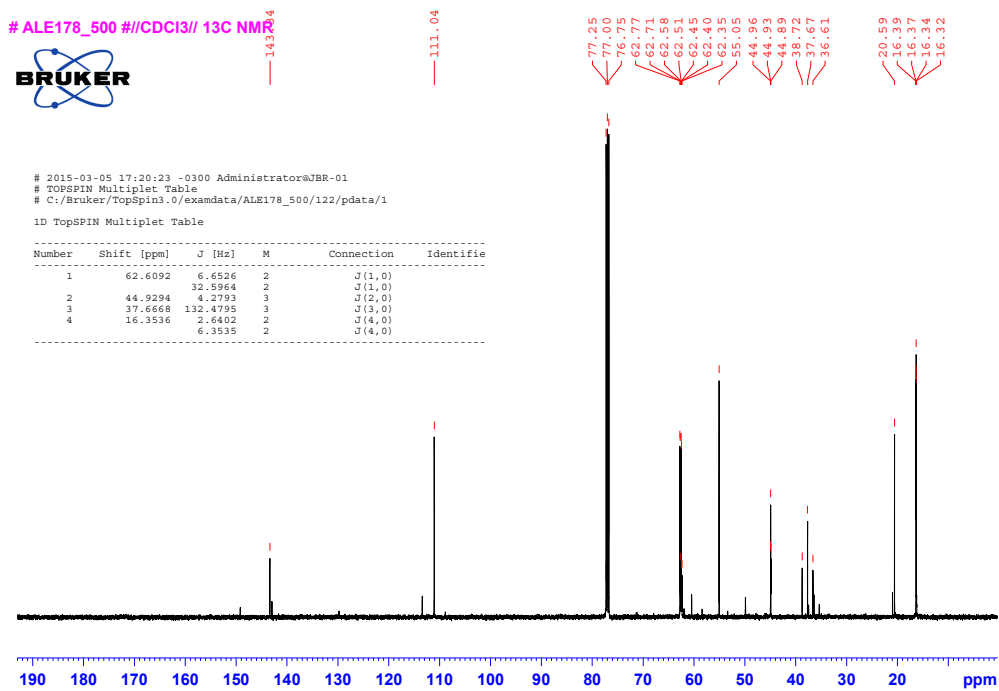
Tamila Galaka, Mariana Ferrer Casal, Melissa Storey, Catherine Li, María N. Chao, Sergio H. Szajnman, Roberto Docampo, Silvia N. J. Moreno, and Juan B. Rodriguez

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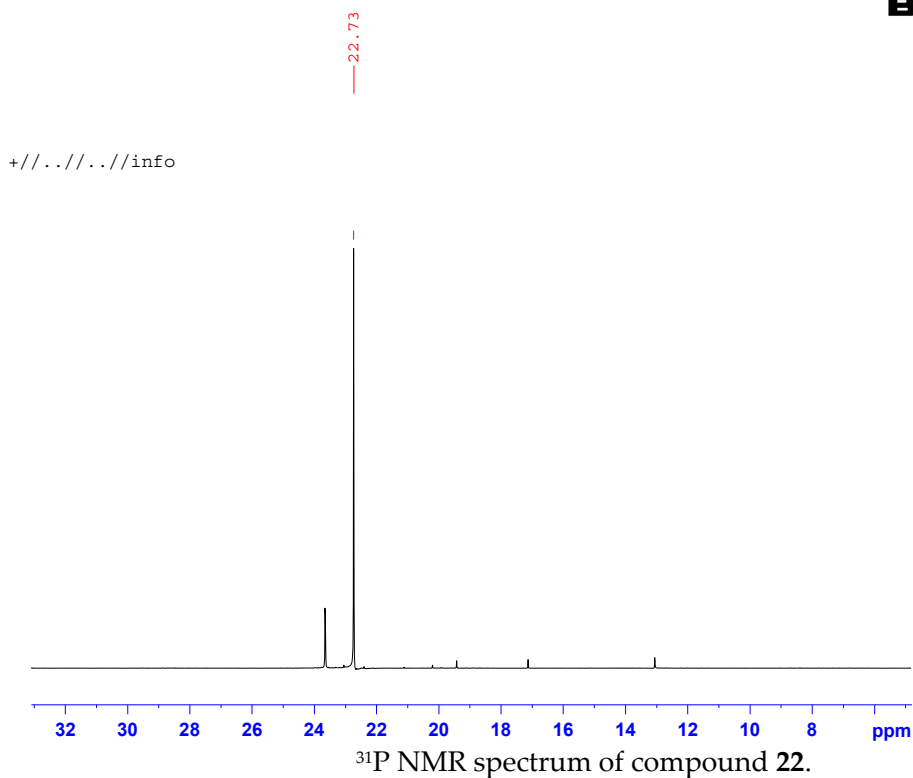
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¹ H NMR spectrum of compound 52	S24
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³¹ P NMR spectrum of compound 52	S25
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¹ H NMR spectrum of compound 45	S30
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³¹ P NMR spectrum of compound 45	S31
¹ H NMR spectrum of compound 67	S32
¹³ C NMR spectrum of compound 67	S32
³¹ P NMR spectrum of compound 67	S33
¹ H NMR spectrum of compound 68	S33
¹³ C NMR spectrum of compound 68	S34
³¹ P NMR spectrum of compound 68	S34
¹ H NMR spectrum of compound 69	S35
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³¹ P NMR spectrum of compound 73	S42
¹ H NMR spectrum of compound 74	S42
¹³ C NMR spectrum of compound 74	S43
³¹ P NMR spectrum of compound 74	S43

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³¹ P NMR spectrum of compound 75	S45
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¹⁹ F NMR spectrum of compound 76	S47
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¹⁹ F NMR spectrum of compound 77	S49
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¹⁹ F NMR spectrum of compound 56	S65
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¹³ C NMR spectrum of compound 57	S66
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¹⁹ F NMR spectrum of compound 57	S67
¹ H NMR spectrum of compound 58	S68
¹³ C NMR spectrum of compound 58	S68
³¹ P NMR spectrum of compound 58	S69
¹⁹ F NMR spectrum of compound 58	S69
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³¹ P NMR spectrum of compound 59	S71
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¹ H NMR spectrum of compound 60	S72
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³¹ P NMR spectrum of compound 60	S73
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¹³ C NMR spectrum of compound 61	S74
³¹ P NMR spectrum of compound 61	S75
¹⁹ F NMR spectrum of compound 61	S75

¹H NMR spectrum of compound 22.¹³C NMR spectrum of compound 22.

ALE178_500 #//CDCl3// 31P NMR



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PROCNO    1

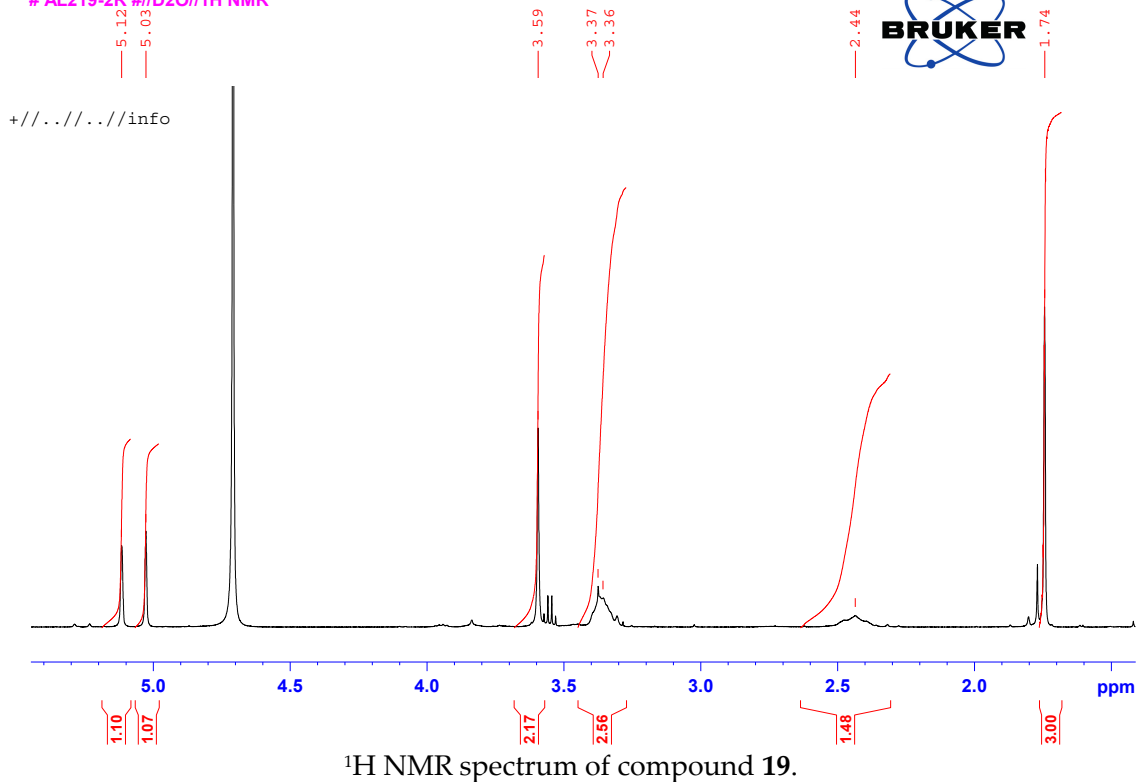
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FIDRES     1.243923 Hz
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RG         2050
DW         6.133 usec
DE         10.00 usec
TE         298.6 K
D1         1.0000000 sec
D11        0.0300000 sec
TD0        1

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PL1        -2.00 dB
PL1W       79.62143707 W
SFO1       202.4532982 MHz

===== CHANNEL f2 =====
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PL2         1.00 dB
PL12        16.92 dB
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ALE219-2R #//D2O// ¹³C NMR

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117.41

52.54

44.30

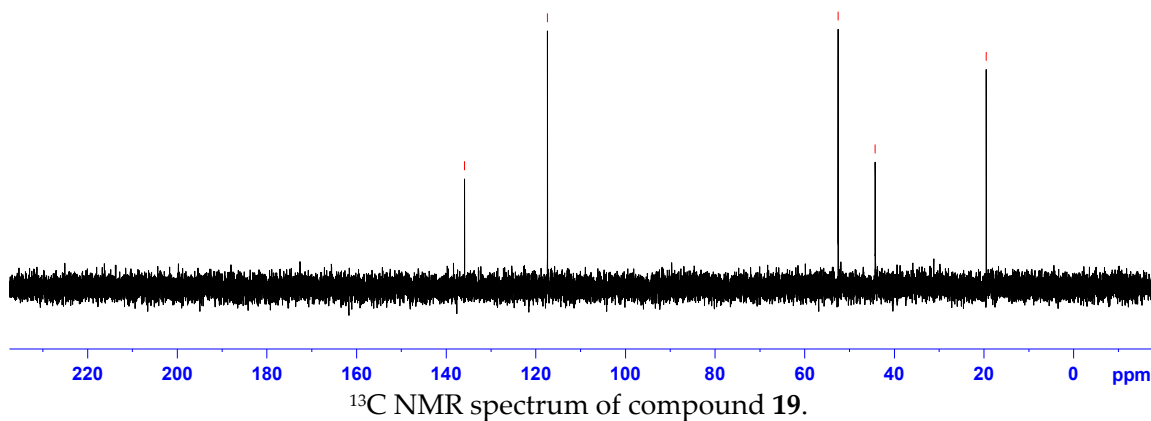
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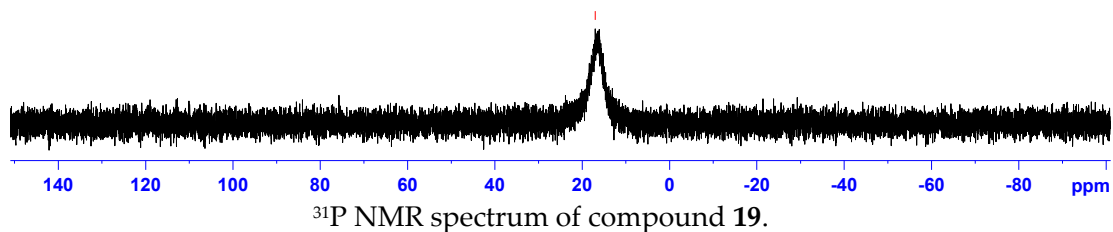
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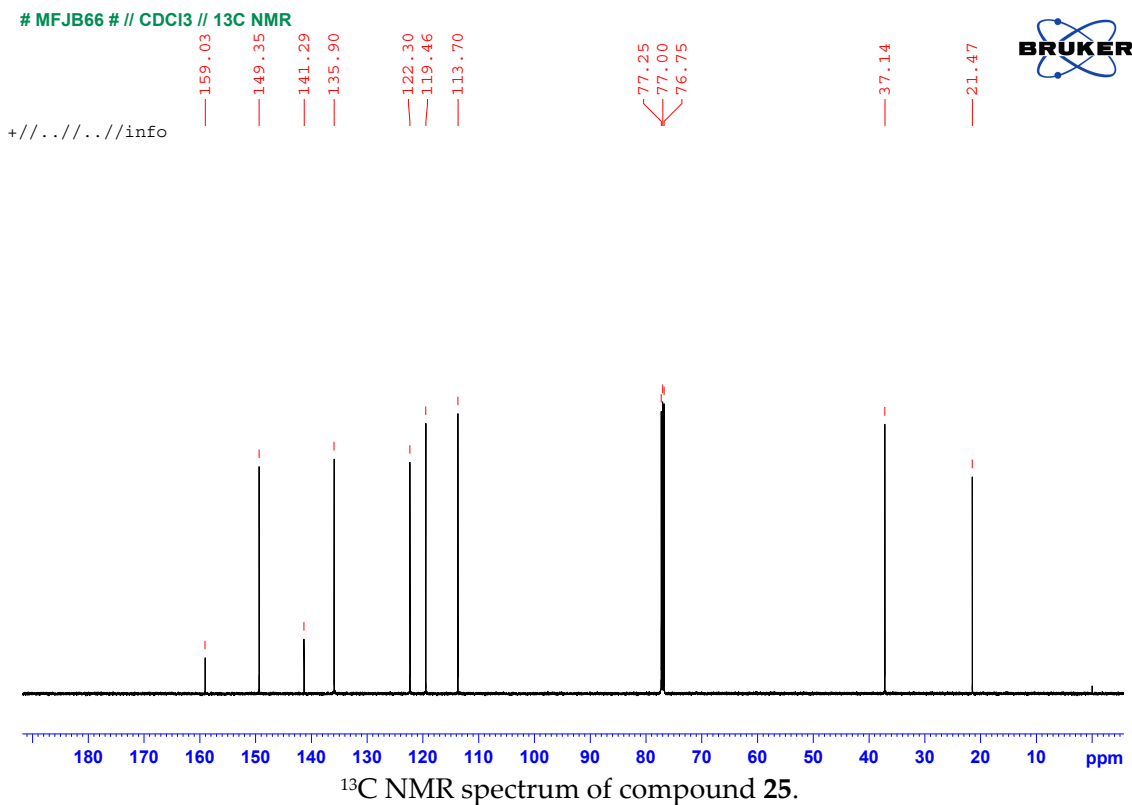
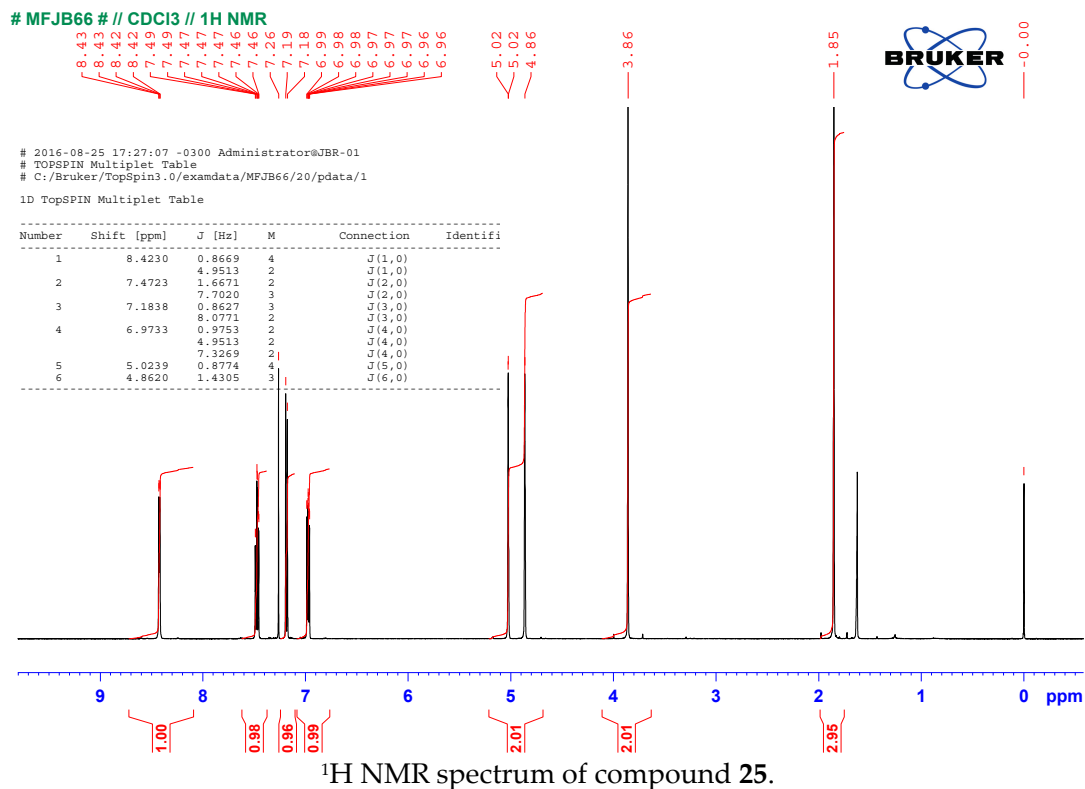
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16.96



+//...//info





SSC73 # // CDCl3 // 1H NMR

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8.74
8.04
8.02
7.93
7.93
7.91
7.91
7.90
7.53
7.52
7.52
7.51
7.51
7.51
7.50
7.26

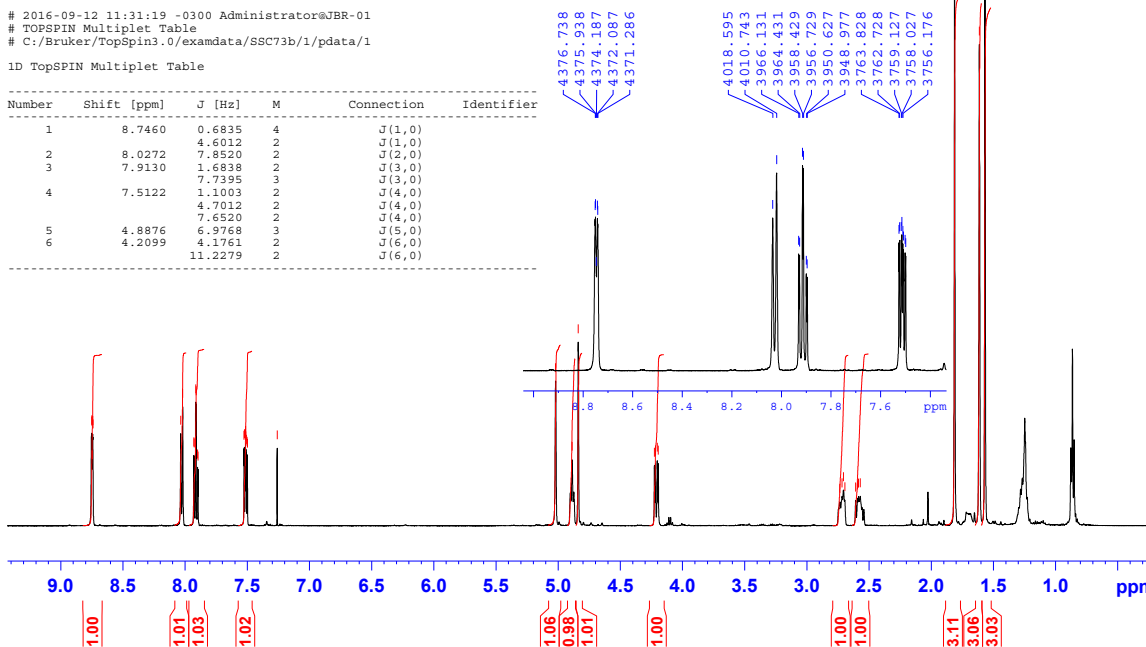
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4.20
4.19

2.73
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2.69
2.61
2.59
2.58
2.57



2016-09-12 11:31:19 -0300 Administrator@JBR-01
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4	7.5122	1.1003	2	J(3,0)	
		4.7012	2	J(4,0)	
		4.6520	2	J(4,0)	
5	4.8876	6.9768	3	J(5,0)	
6	4.2099	4.1761	2	J(6,0)	
		11.2279	2	J(6,0)	



¹H NMR spectrum of compound 29.

SSC73-1 # // CDCl3 // 13C NMR

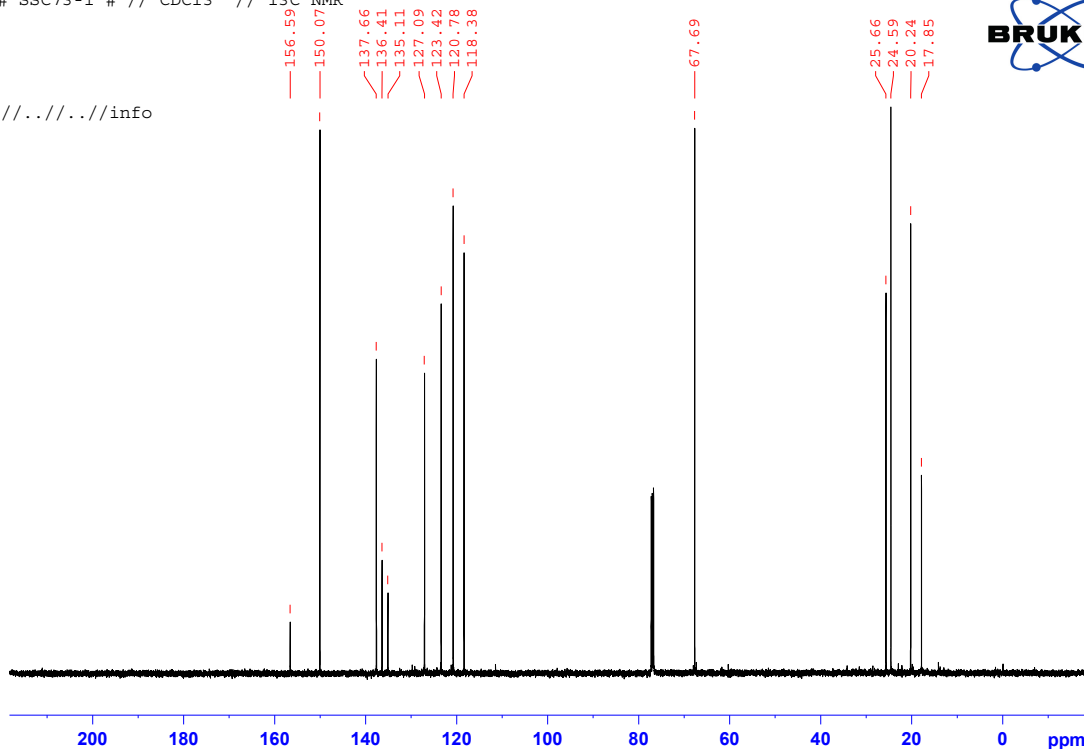
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136.41
135.11
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120.78
118.38

67.69

25.66
24.59
20.24
17.85



+//...//...//info



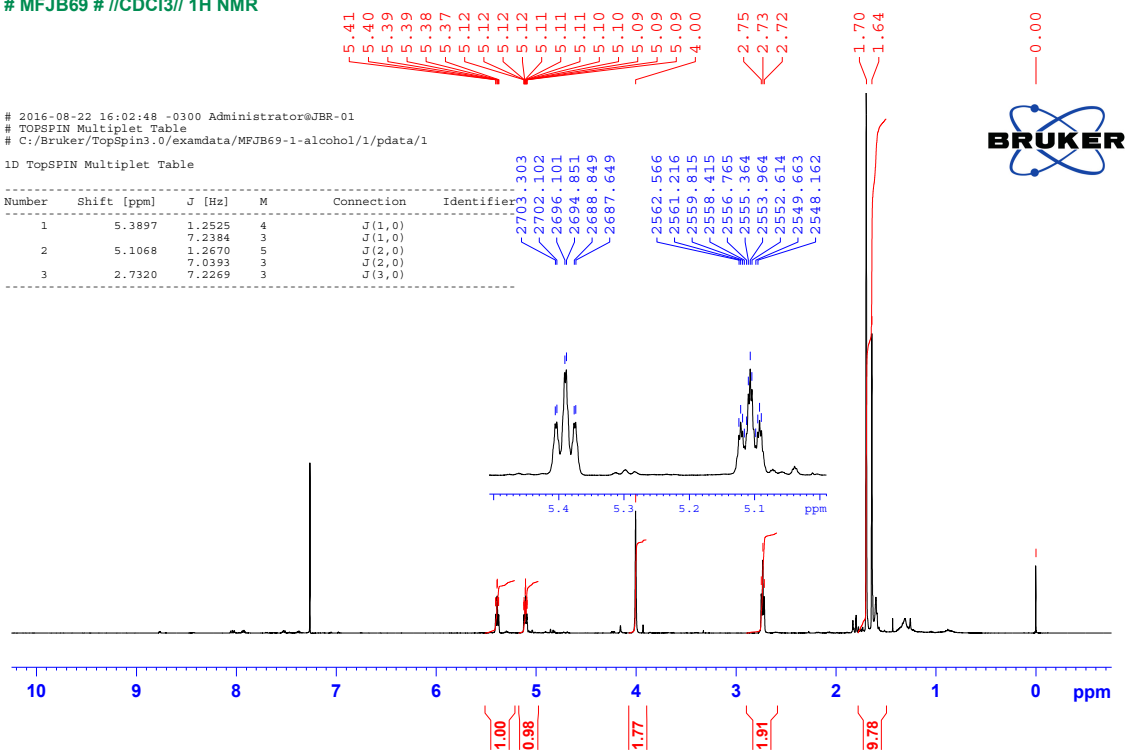
¹³C NMR spectrum of compound 29.

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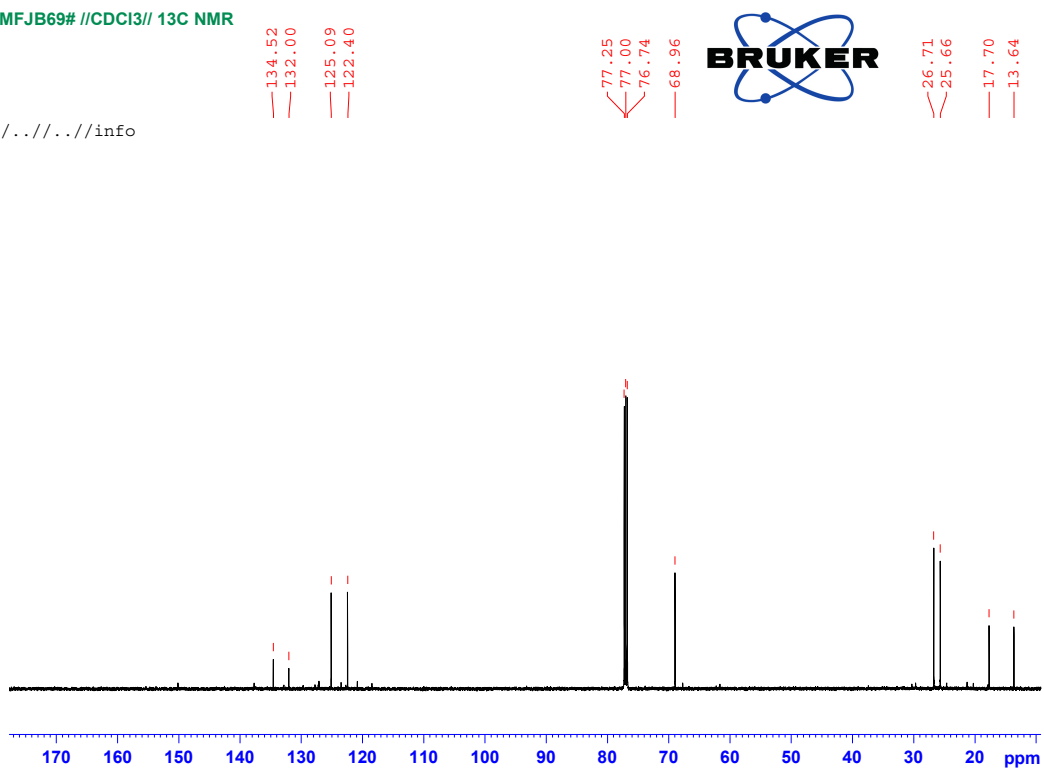
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		1.2670	5	J(2,0)	2696.101
3	2.7320	7.0393	3	J(2,0)	2694.851
		7.2269	3	J(3,0)	2688.849
					2687.649



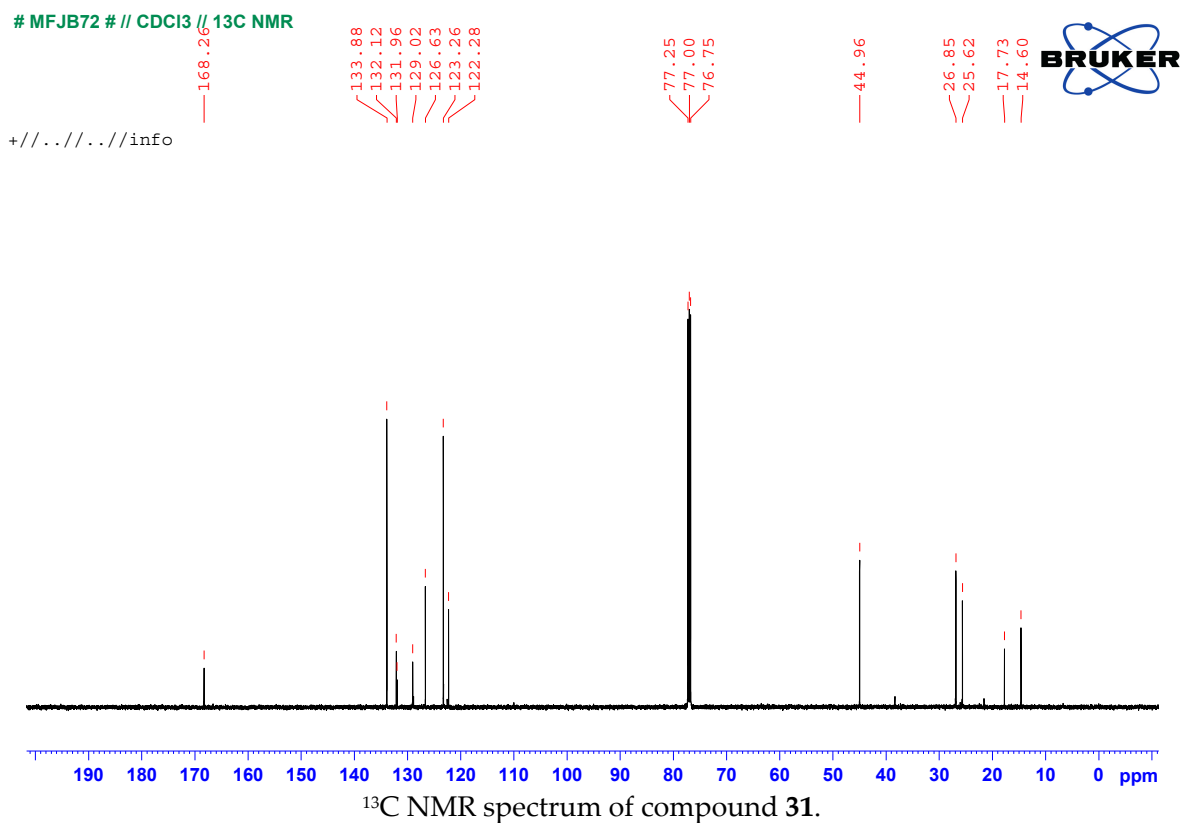
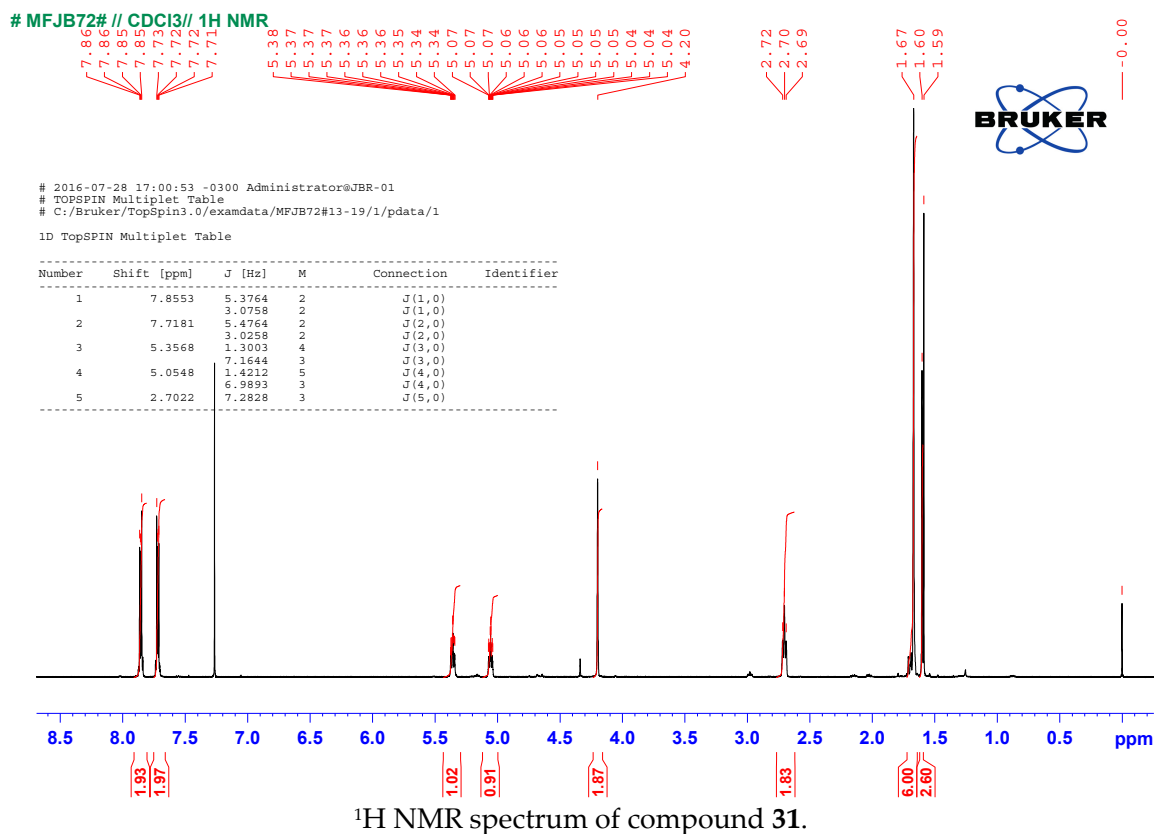
¹H NMR spectrum of compound 30.

MFJB69# //CDCl3// 13C NMR

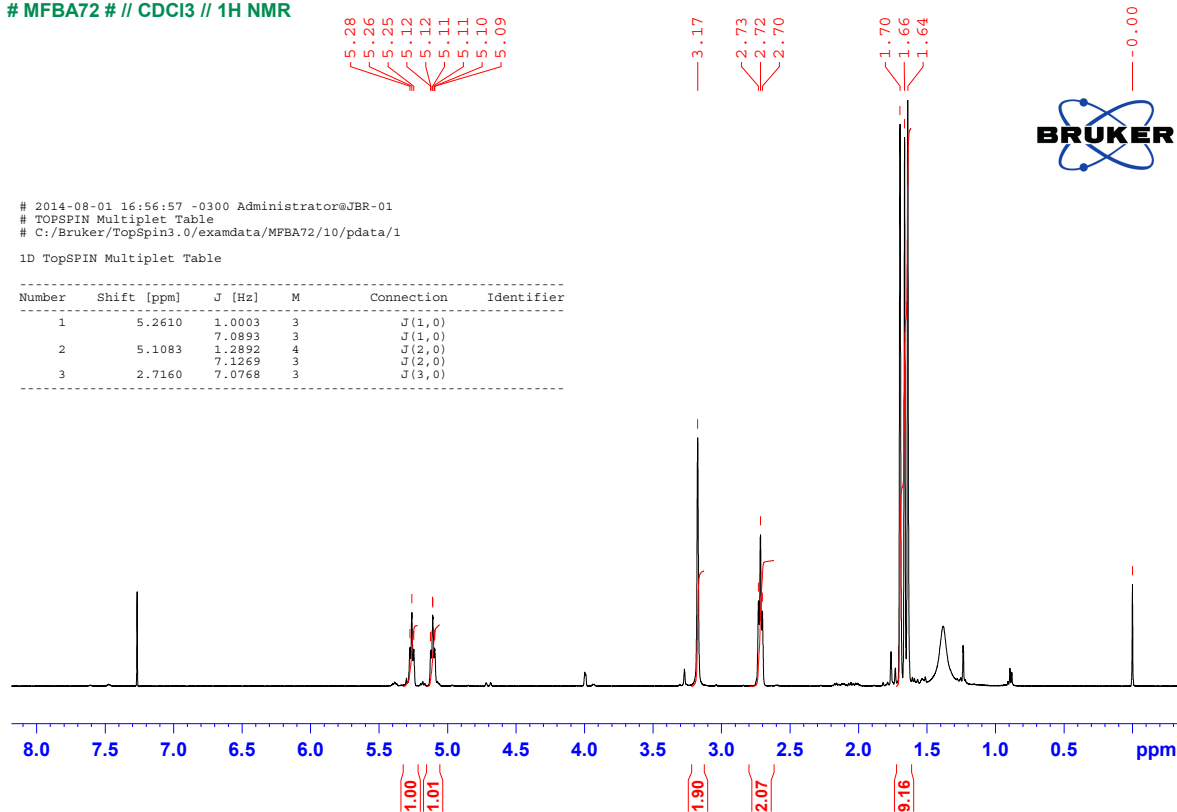
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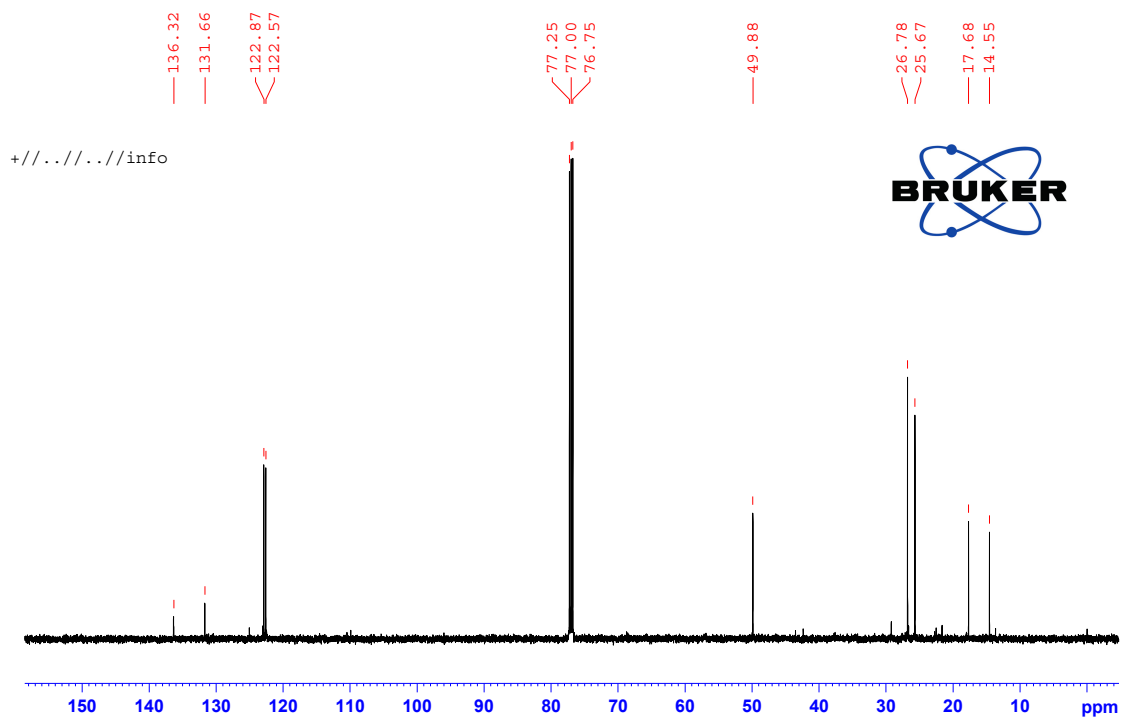
¹³C NMR spectrum of compound 30.

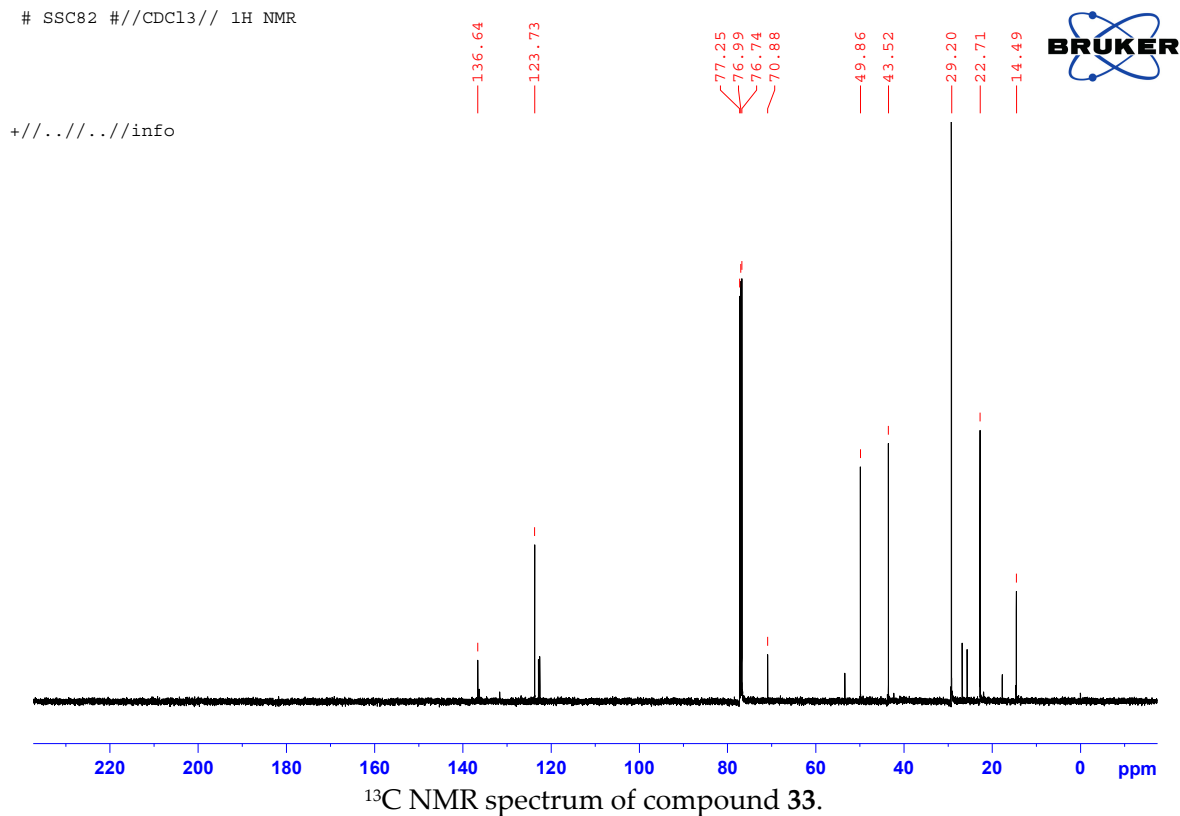
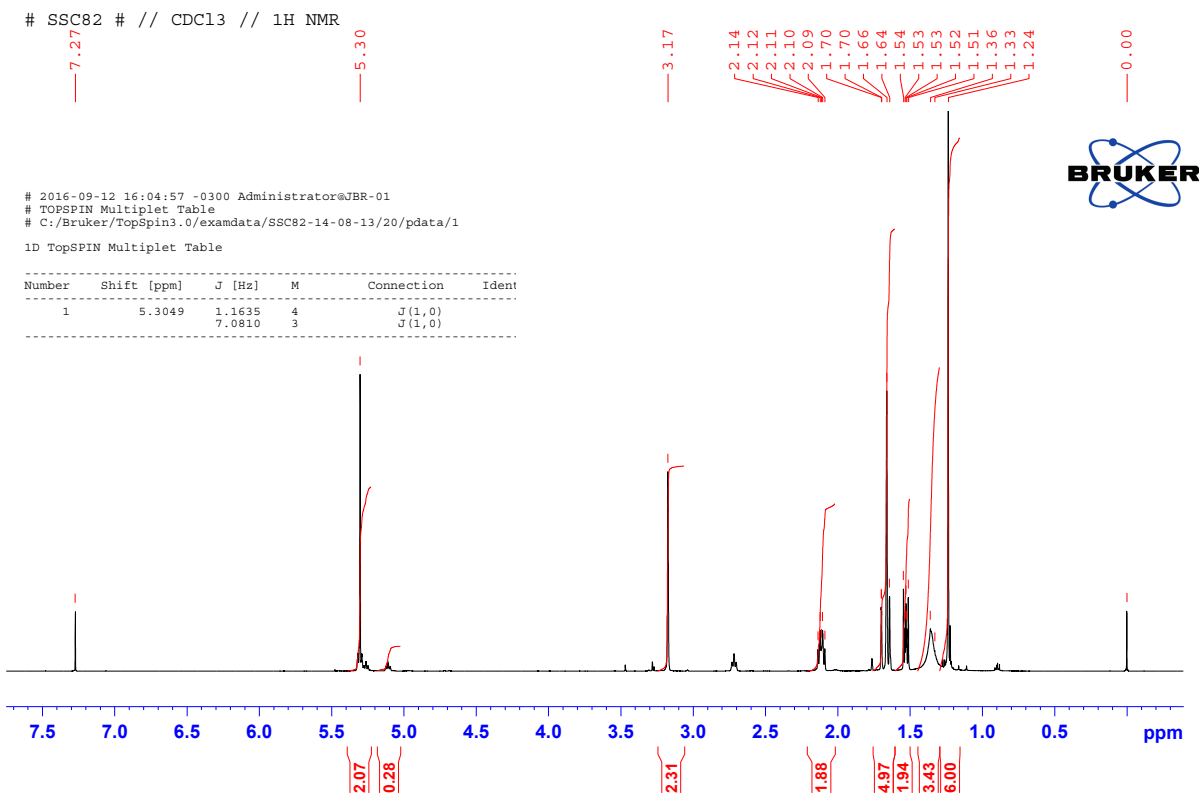


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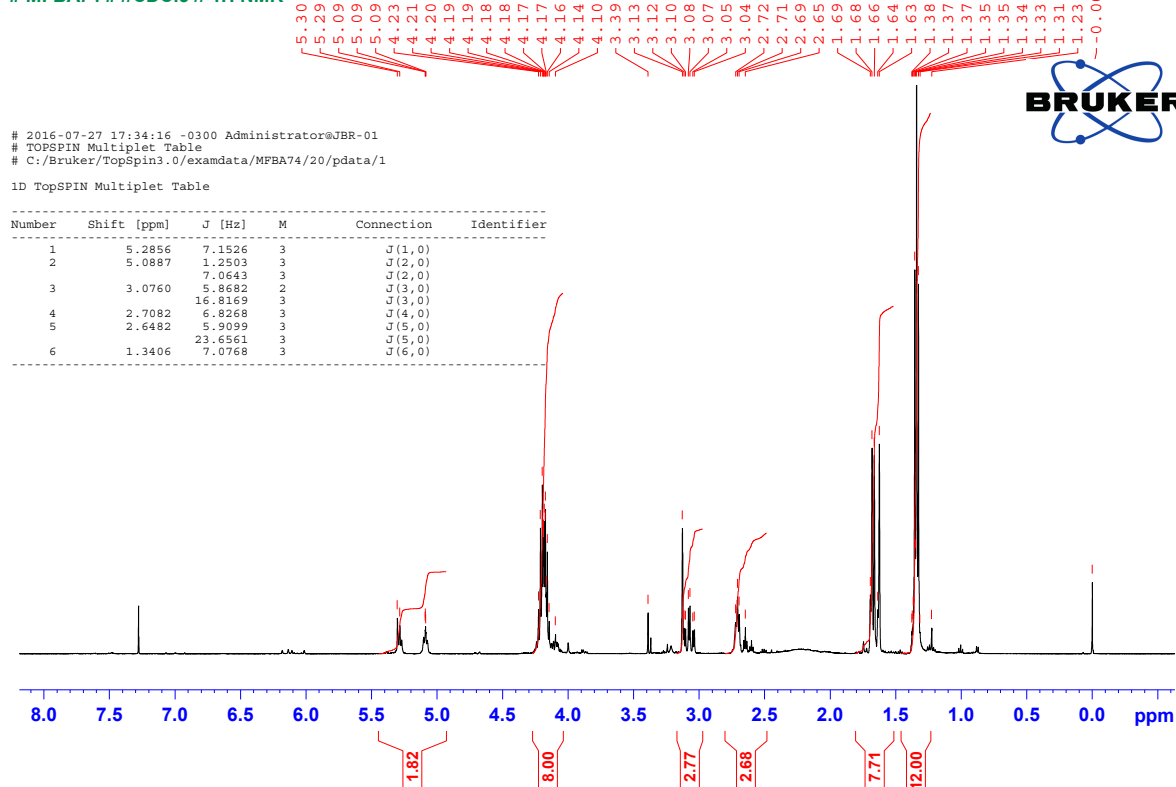
¹H NMR spectrum of compound 32.

MFBA72 # // CDCl3 // 13C NMR

¹³C NMR spectrum of compound 32.



MFBA74 # //CDCl3 // 1H NMR



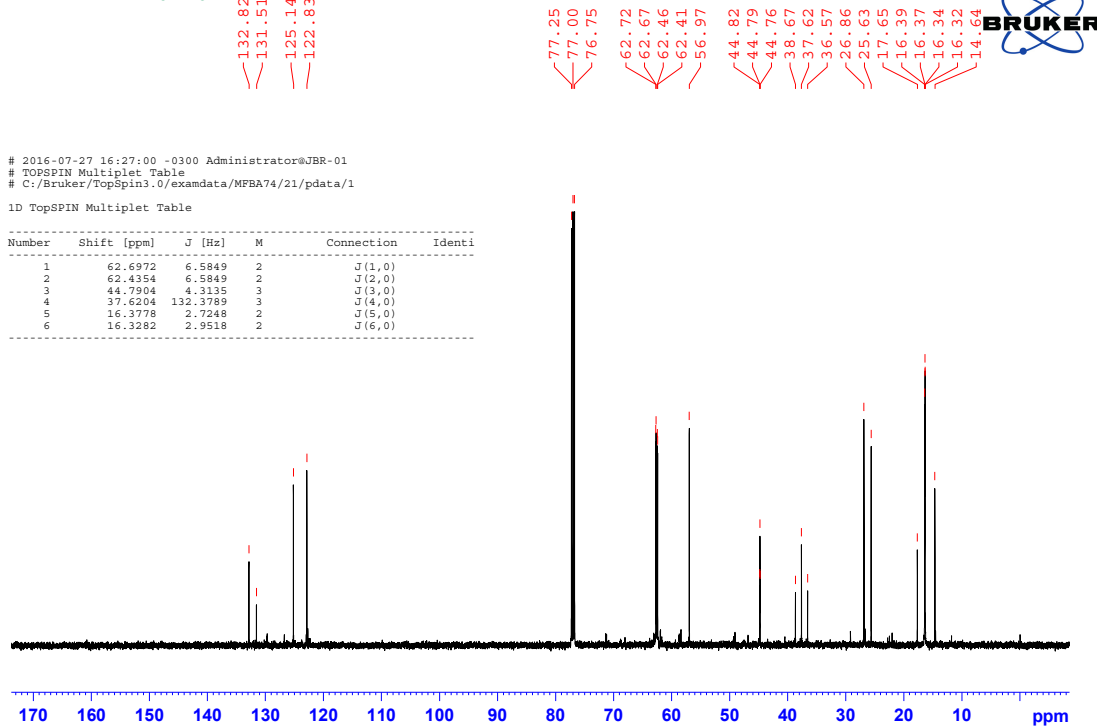
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3	3.0760	5.8682	2	J(3,0)	
4	2.7082	6.8268	3	J(4,0)	
5	2.6482	5.9099	3	J(5,0)	
6	1.3406	7.0768	3	J(6,0)	

¹H NMR spectrum of compound 34.

MFBA74 # // CDCl3 // 13C NMR



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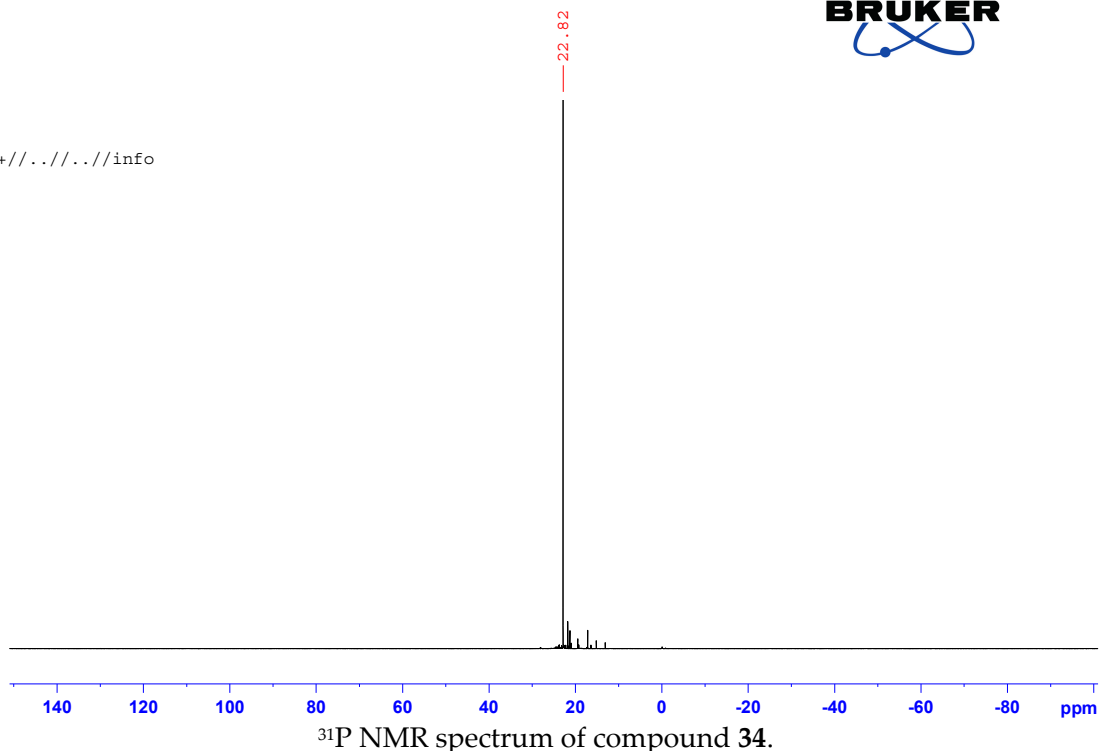
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2	62.4354	6.5849	2	J(2,0)	
3	44.7904	4.3135	3	J(3,0)	
4	37.6204	132.3789	3	J(4,0)	
5	16.3778	2.7248	2	J(5,0)	
6	16.3282	2.9518	2	J(6,0)	

¹³C NMR spectrum of compound 34.

MFBA74 # // CDCI3 // 31P NMR



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MFBA166 # // CDCI3 // 1H NMR

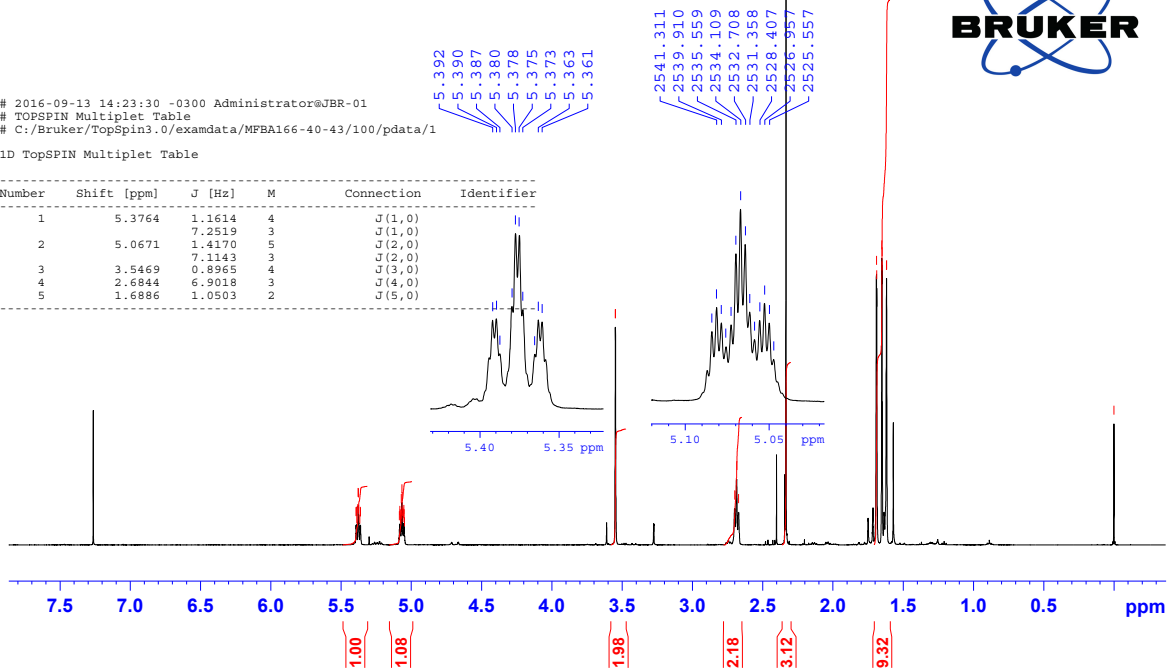
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5.06
5.06
5.05
5.05
3.55
2.70
2.67
2.33
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1.65
1.65
1.65
1.62
1.62
-0.00



2016-09-13 14:23:30 -0300 Administrator@JBR-01
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		1.4170	5	J(2,0)	
3	5.1143	7.1143	3	J(2,0)	
4	3.5469	0.8965	4	J(3,0)	
5	2.6844	6.9018	3	J(4,0)	
		1.0503	2	J(5,0)	



1H NMR spectrum of compound 36.

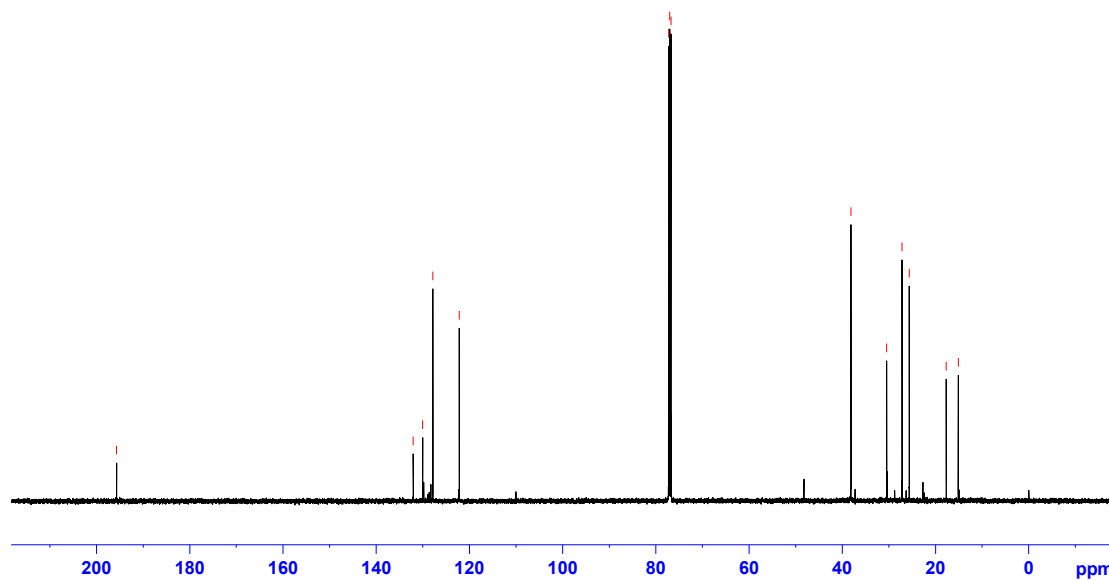
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130.04
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122.20

77.25
77.00
76.75

38.16
30.49
27.19
25.65
17.71
15.12



¹³C NMR spectrum of compound 36.

MFD3 # // CDCl3 // 1H NMR

5.333
5.311
5.311
5.291
5.288
5.133
5.113
5.111
5.111
5.110
5.099
5.088
5.088
5.077
5.066
5.066
5.055

3.24
3.14
3.11
2.75
2.72
2.69
2.67

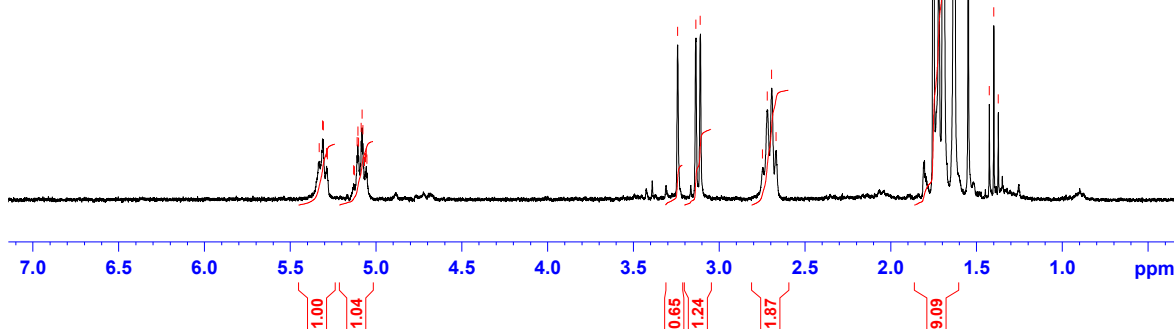
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1.72
1.69
1.63
1.55
1.43
1.40
1.37



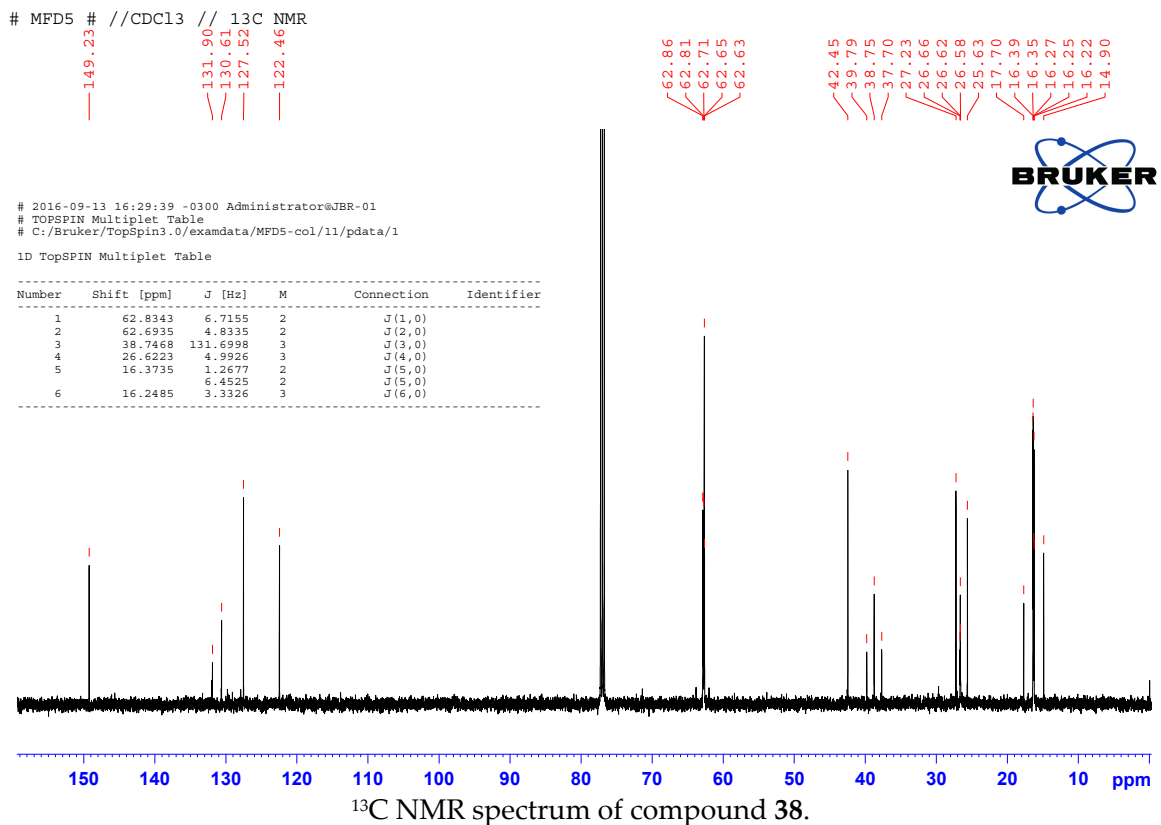
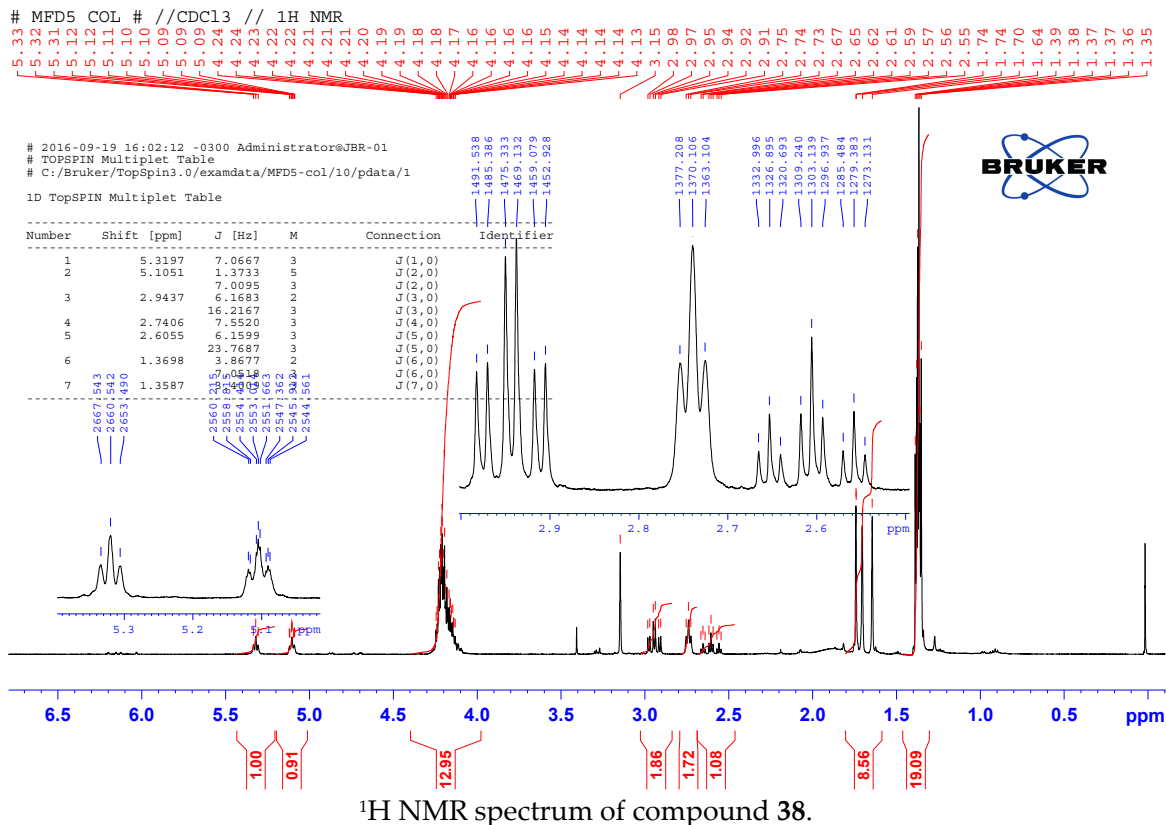
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1D TopSPIN Multiplet Table

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		7.1068	3	J(2,0)	
3	3.1228	7.8347	2	J(3,0)	
4	2.7076	7.9047	4	J(4,0)	
5	1.7518	0.9934	4	J(5,0)	
6	1.3994	7.8197	3	J(6,0)	



¹H NMR spectrum of compound 37.



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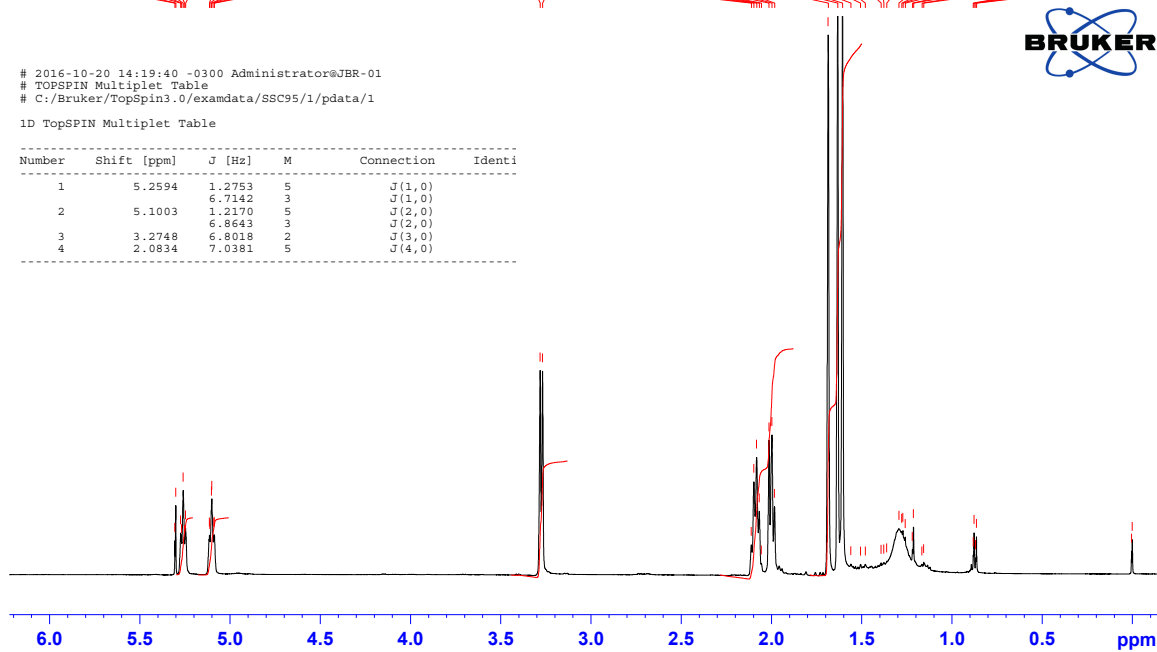
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5.10
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5.09

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3.27
2.11
2.10
2.08
2.07
2.06
2.01
2.00
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1.69
1.63
1.61
1.56
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1.39
1.38
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1.28
1.27
1.26
1.22
1.21
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1.16
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1D TopSPIN Multiplet Table

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2	5.1003	6.7142	3	J(1,0)	
3	3.2748	6.8643	3	J(2,0)	
4	2.0834	7.0381	5	J(4,0)	

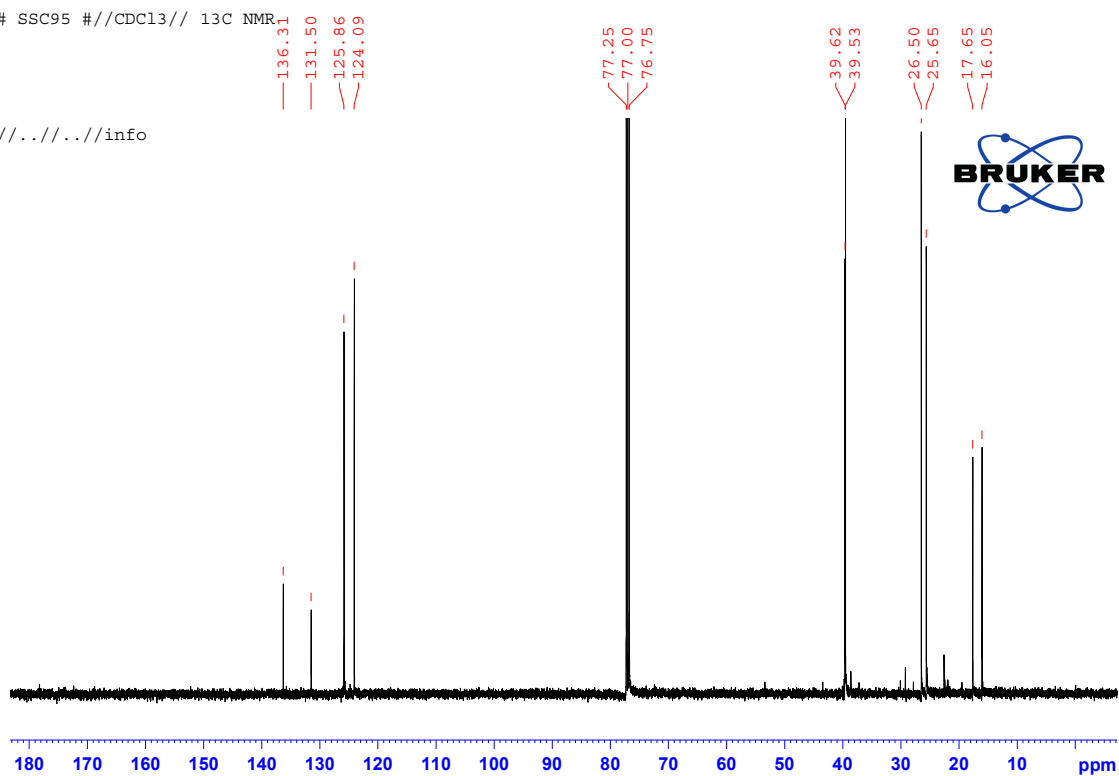
¹H NMR spectrum of compound 42.

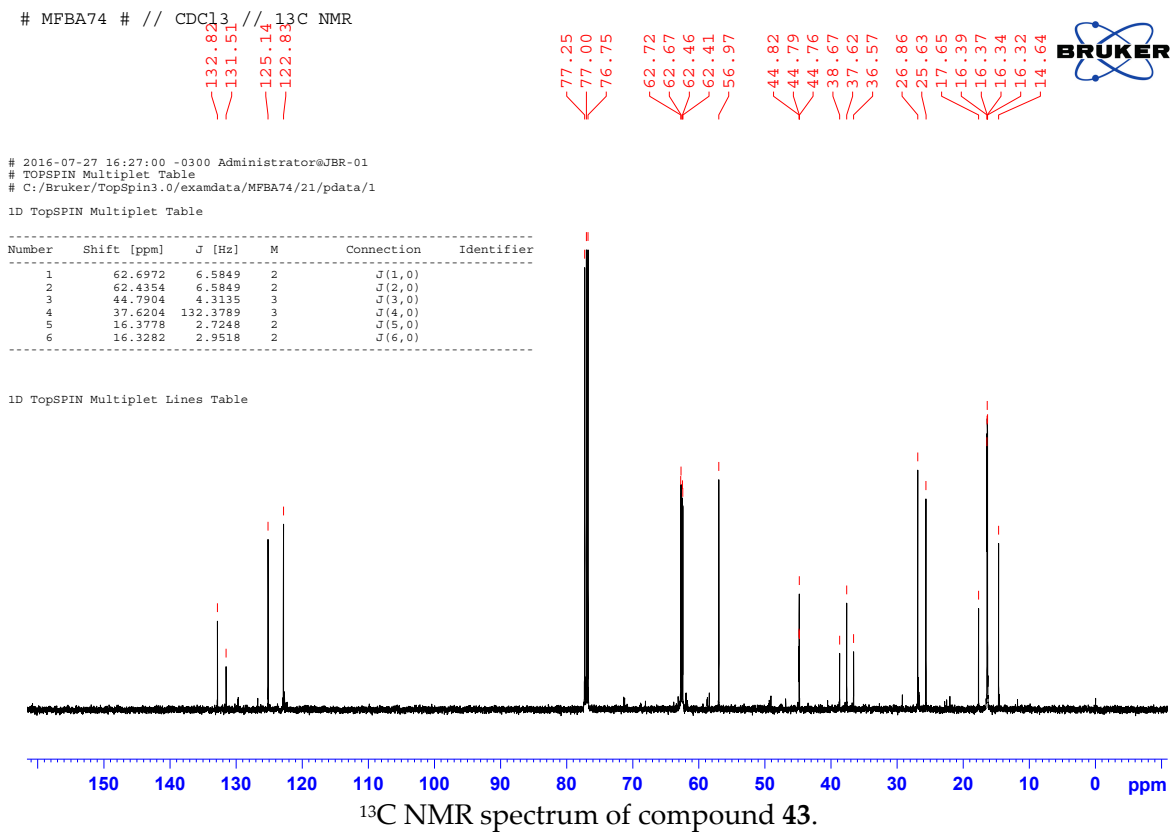
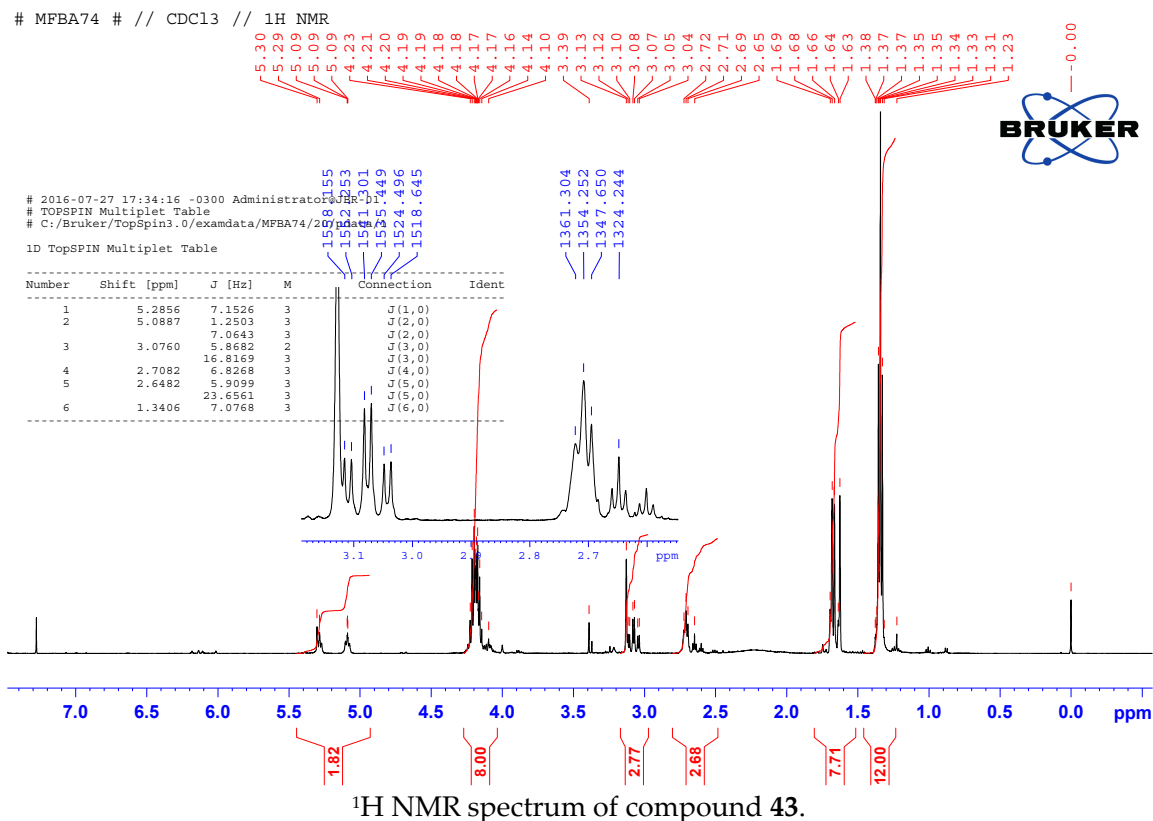
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26.50
25.65
17.65
16.05

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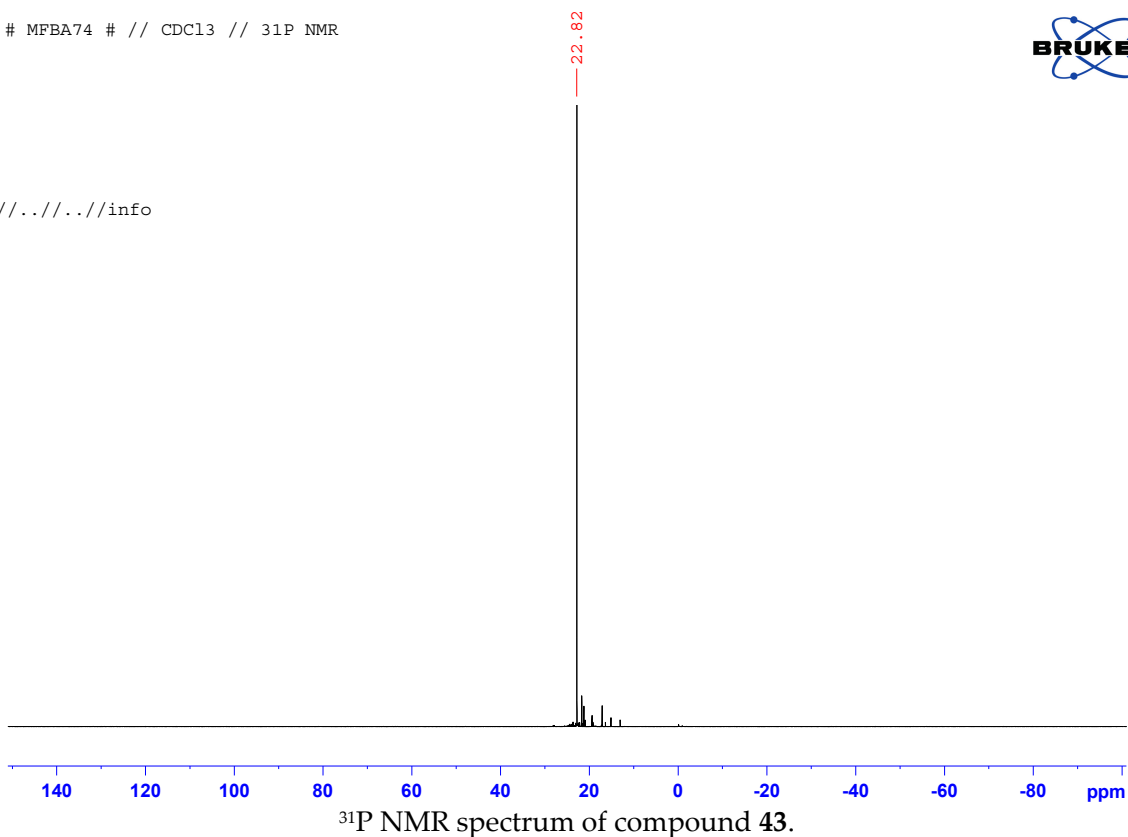
¹³C NMR spectrum of compound 42.



MFBA74 # // CDC13 // 31P NMR



+//...//...//info



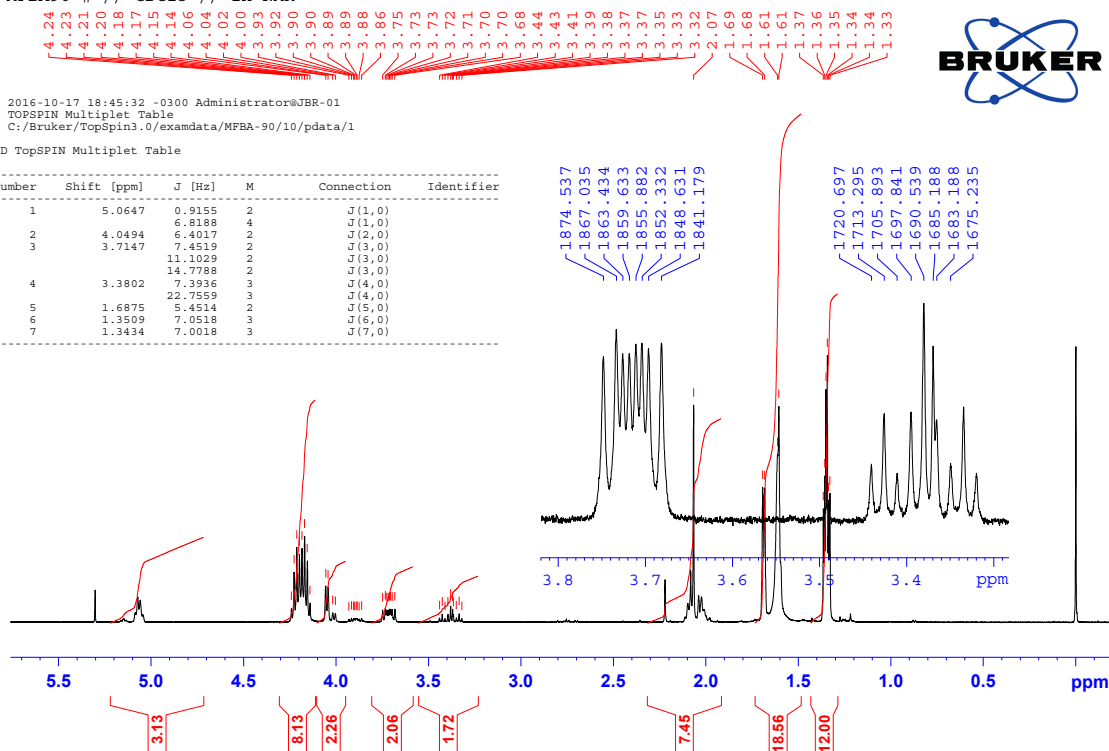
MFBA90 # // CDC13 // 1H NMR



2016-10-17 18:45:32 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/MFBA-90/10/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	5.0647	0.9155	2	J(1,0)	
2	4.0494	6.4017	4	J(1,0)	
3	3.7147	7.4519	2	J(2,0)	
		11.1029	2	J(3,0)	
		14.7788	2	J(3,0)	
4	3.3802	7.3936	3	J(4,0)	
		22.7559	3	J(4,0)	
5	1.6875	5.4514	2	J(5,0)	
6	1.3509	7.0518	3	J(6,0)	
7	1.3434	7.0018	3	J(7,0)	



MFBA90 # // CDCl3 // 13C NMR

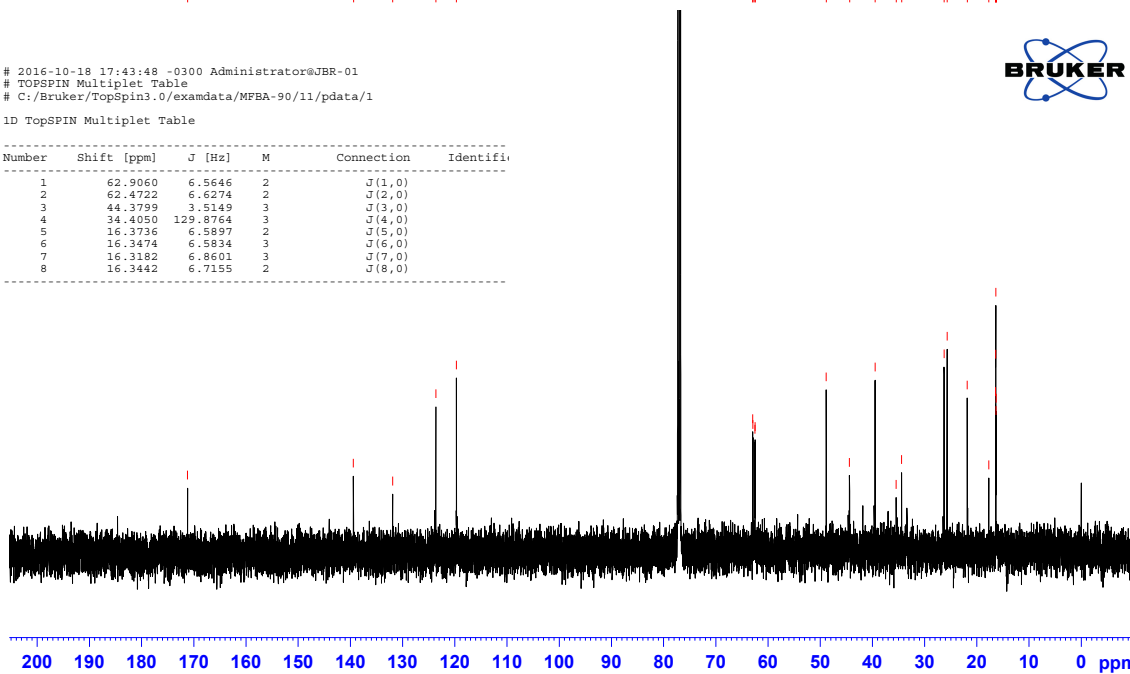
—171.10
—139.42
—131.90
—123.64
—119.68
62.93
62.88
62.50
62.45
48.85
44.38
39.47
35.44
34.40
26.26
25.68
21.83
17.69
16.40
16.37
16.35
16.32
16.26

2016-10-18 17:43:48 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/MFBA-90/11/pdata/1



1D TopSPIN Multiplet Table

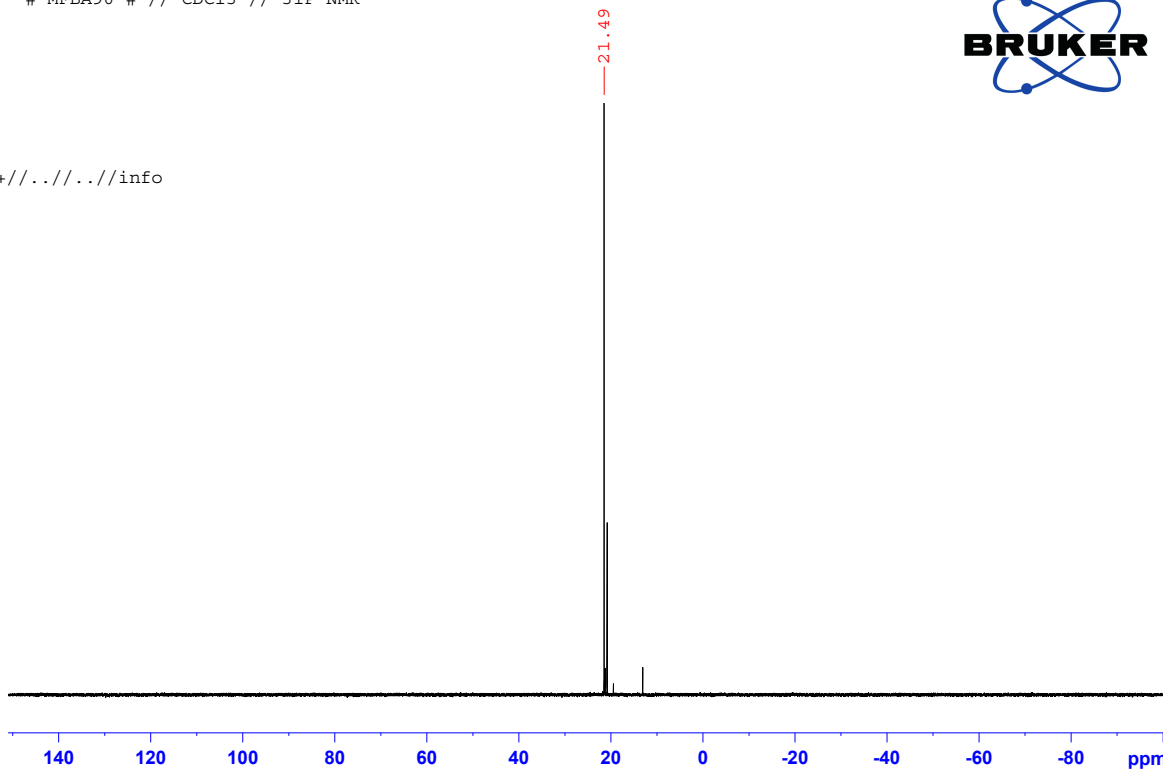
Number	Shift [ppm]	J [Hz]	M	Connection	Identifi
1	62.9060	6.5646	2	J(1,0)	
2	62.4722	6.6274	2	J(2,0)	
3	44.3799	3.5149	3	J(3,0)	
4	34.4050	129.8764	3	J(4,0)	
5	16.3736	6.5897	2	J(5,0)	
6	16.3474	6.5834	3	J(6,0)	
7	16.3182	6.8601	3	J(7,0)	
8	16.3442	6.7155	2	J(8,0)	



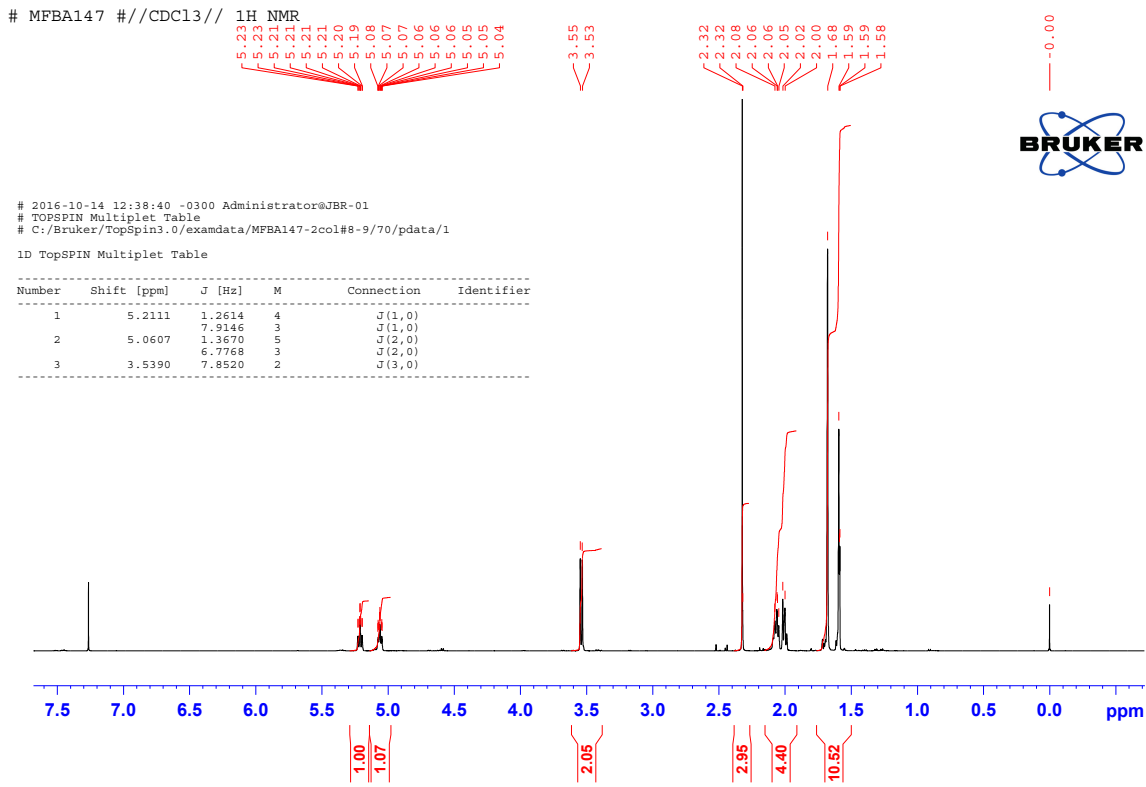
¹³C NMR spectrum of compound 46.

MFBA90 # // CDCl3 // 31P NMR

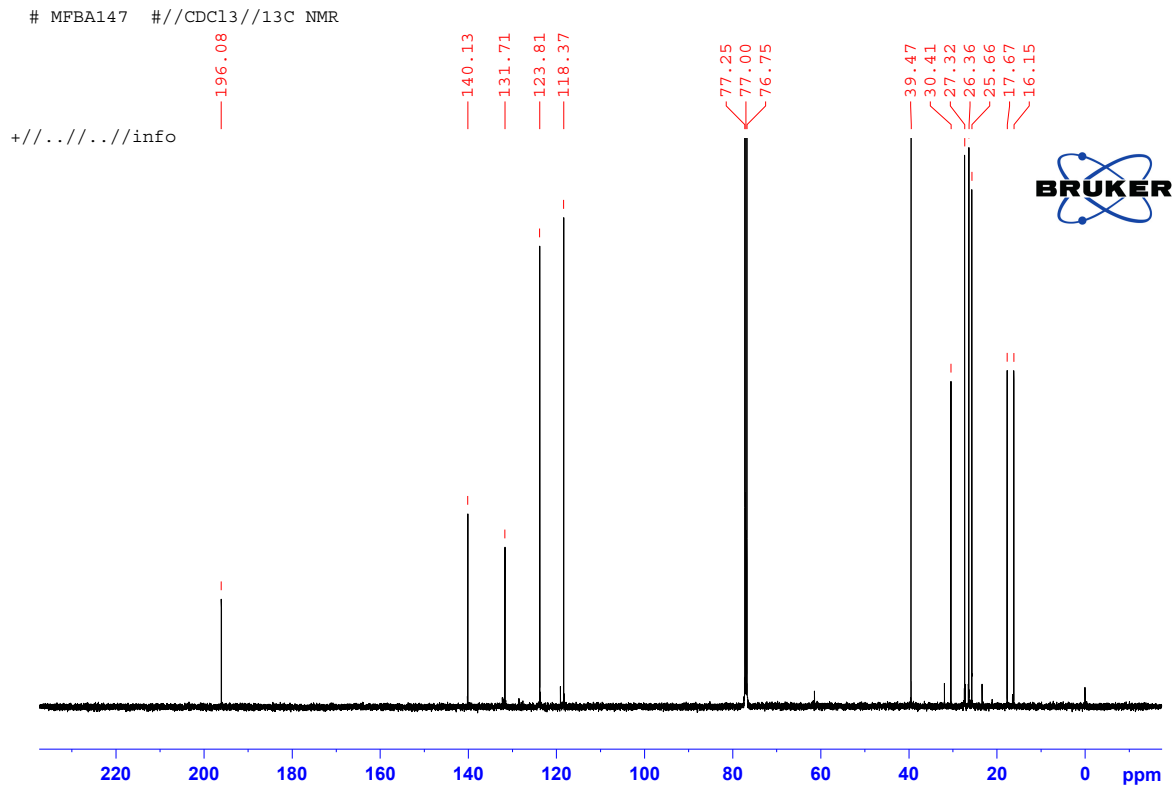
+//...//...//info



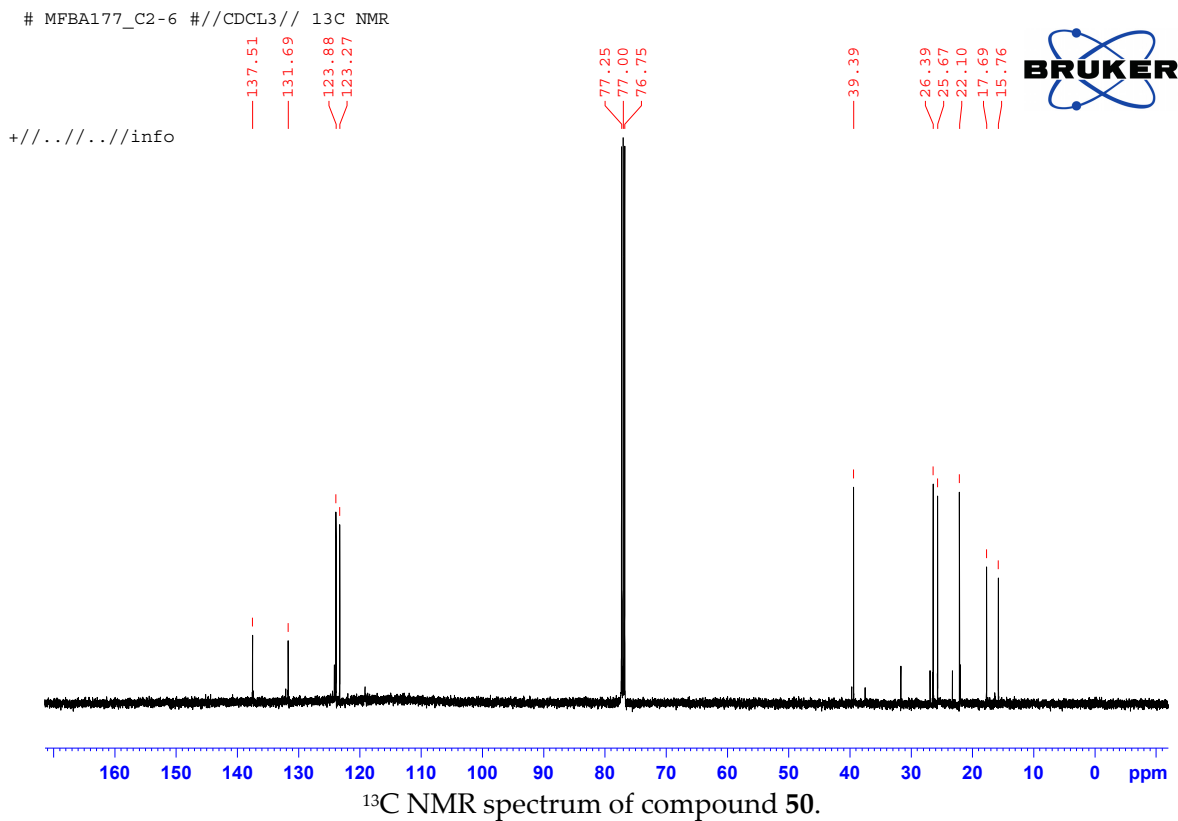
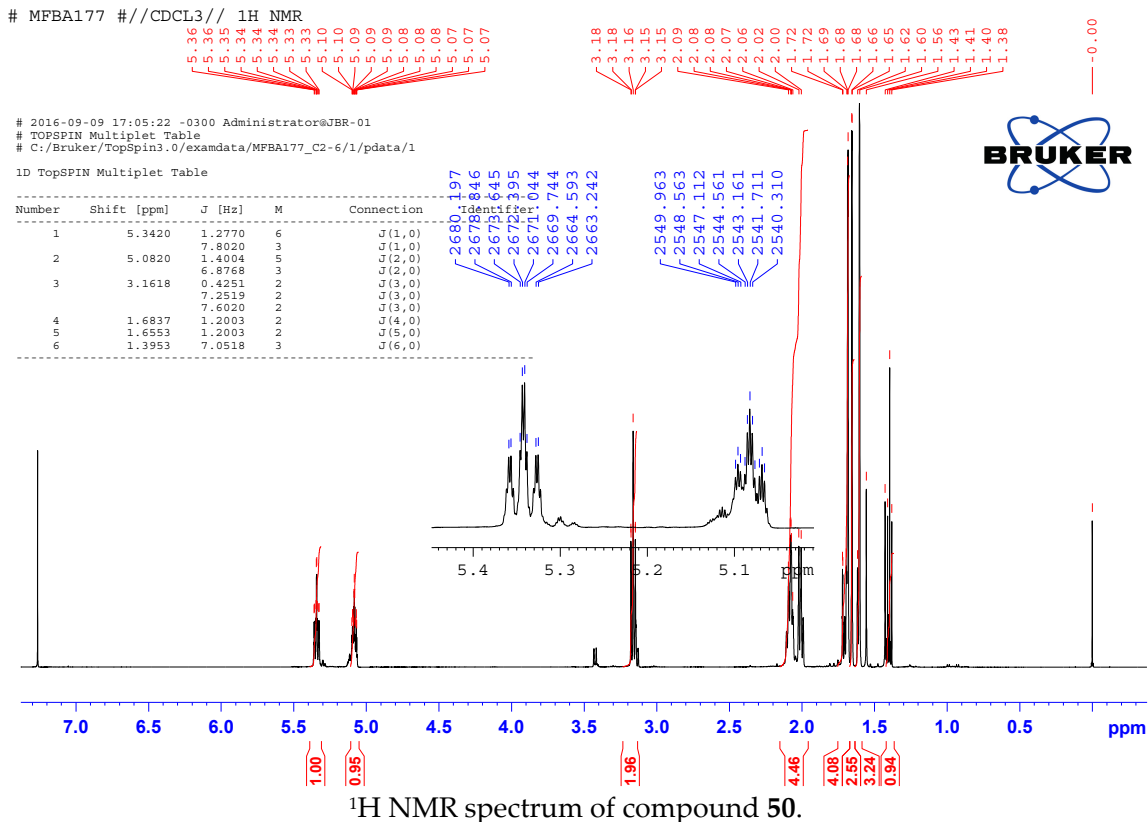
³¹P NMR spectrum of compound 46.

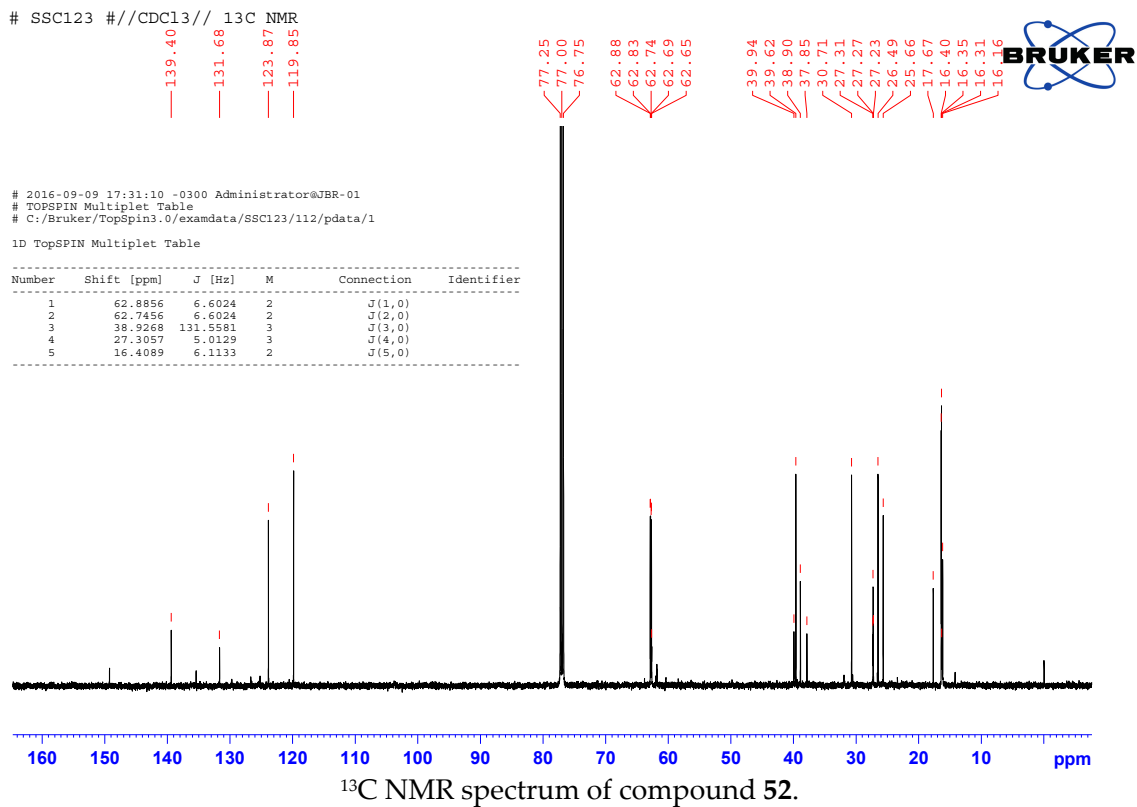
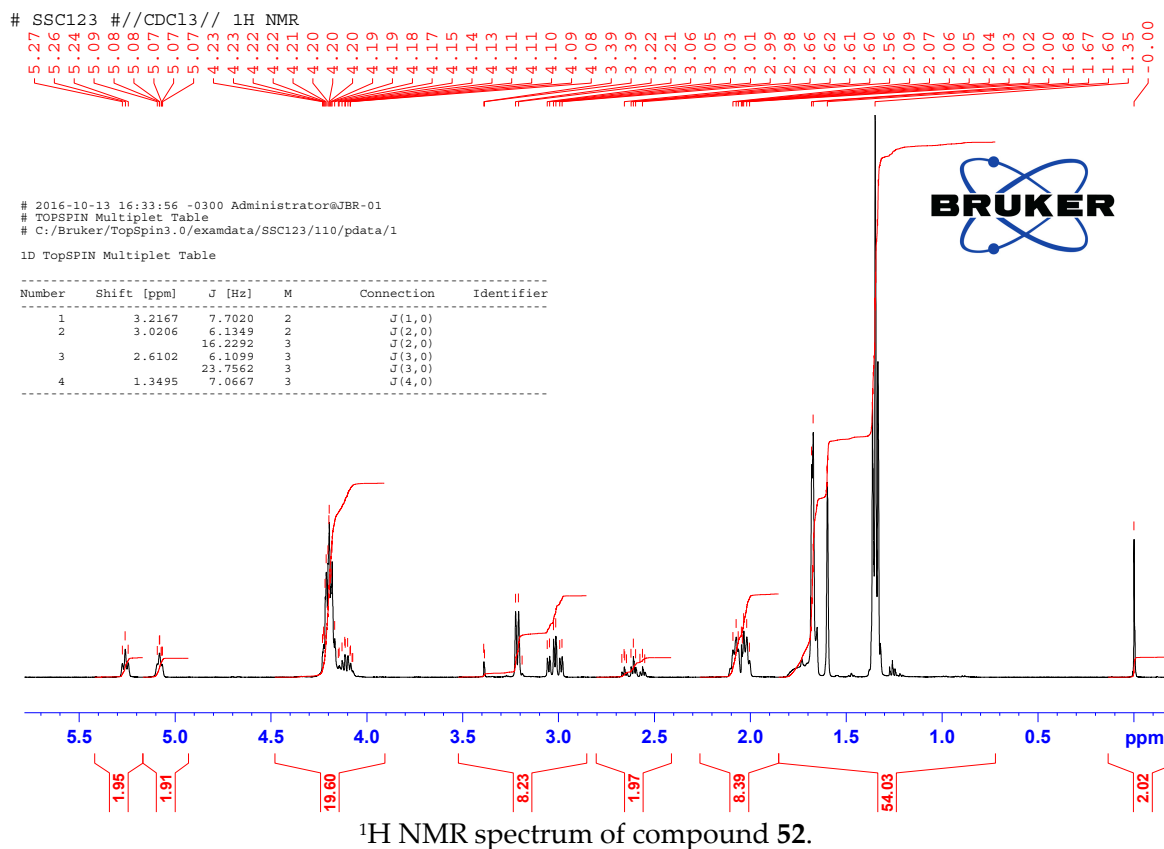


¹H NMR spectrum of compound 48.



¹³C NMR spectrum of compound 48.

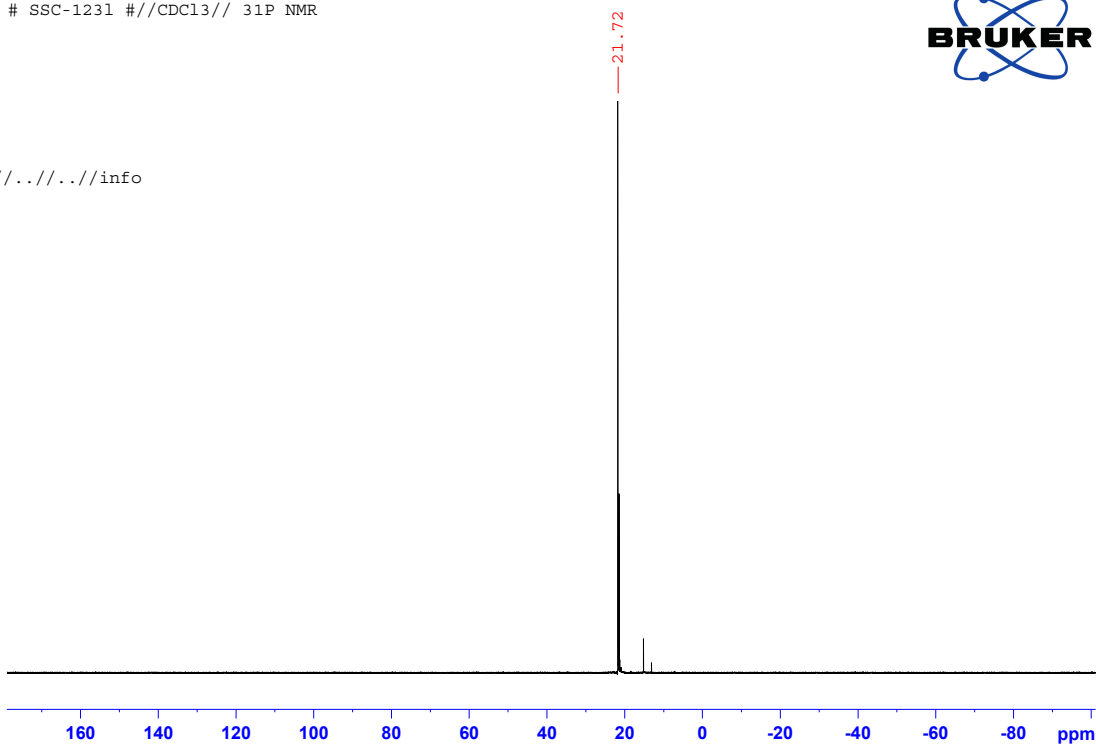




SSC-1231 #//CDC13// 31P NMR



+//...//...//info



³¹P NMR spectrum of compound 52.

MFBA181-L #//D2O// ¹H NMR

5.32
5.30
5.29
5.13
5.12
5.10

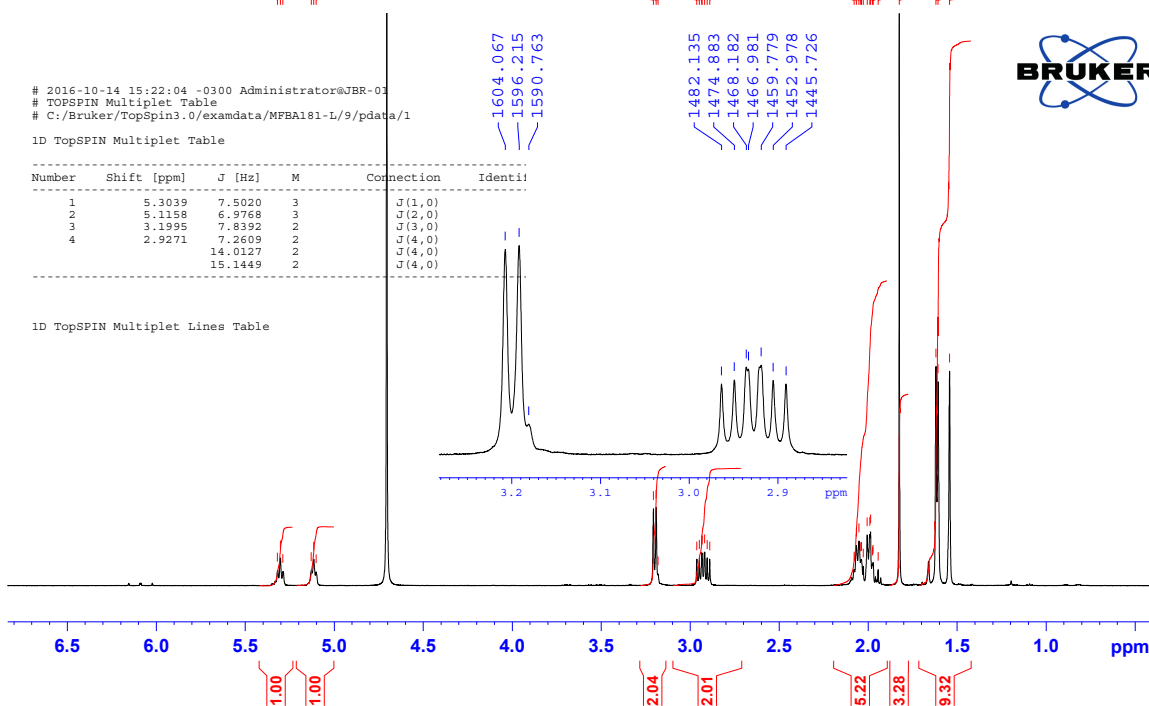
3.21
3.19
3.18
2.96
2.95
2.94
2.93
2.92
2.91
2.89
2.08
2.07
2.05
2.04
2.04
2.03
2.01
1.99
1.99
1.98
1.97
1.94
1.83
1.62
1.61
1.54

2016-10-14 15:22:04 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/MFBA181-L/9/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifi
1	5.3039	7.5020	3	J(1,0)	
2	5.1158	6.9768	3	J(2,0)	
3	3.1995	7.8392	2	J(3,0)	
4	2.9271	7.2609	2	J(4,0)	
		14.0127	2	J(4,0)	
		15.1449	2	J(4,0)	

1D TopSPIN Multiplet Lines Table



¹H NMR spectrum of compound 44.

MFBA181-L #//D2O// ¹³C NMR

— 140.16
— 133.64
— 124.24
— 119.78

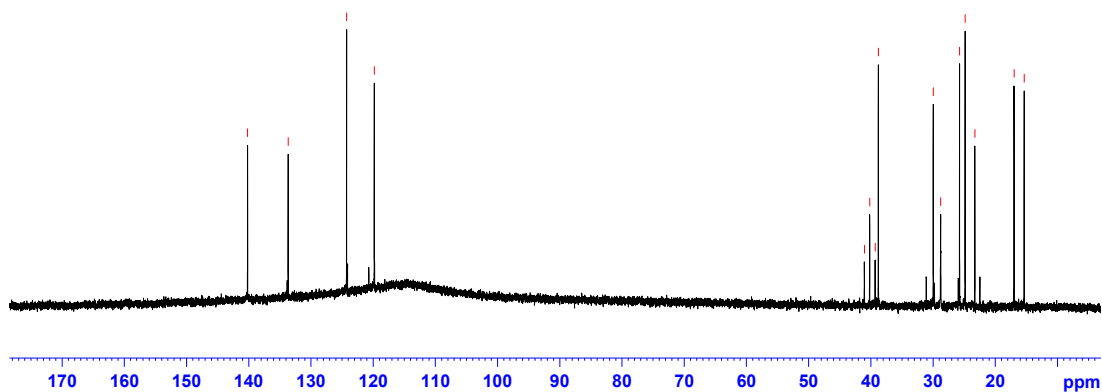


41.02
40.15
39.28
38.76
29.93
28.75
25.70
24.81
23.25
16.94
15.32

2016-10-14 14:39:49 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/MFBA181-L/4/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	40.1499	109.3057	3	J(1,0)	
2	28.7475	3.6680	3	J(2,0)	



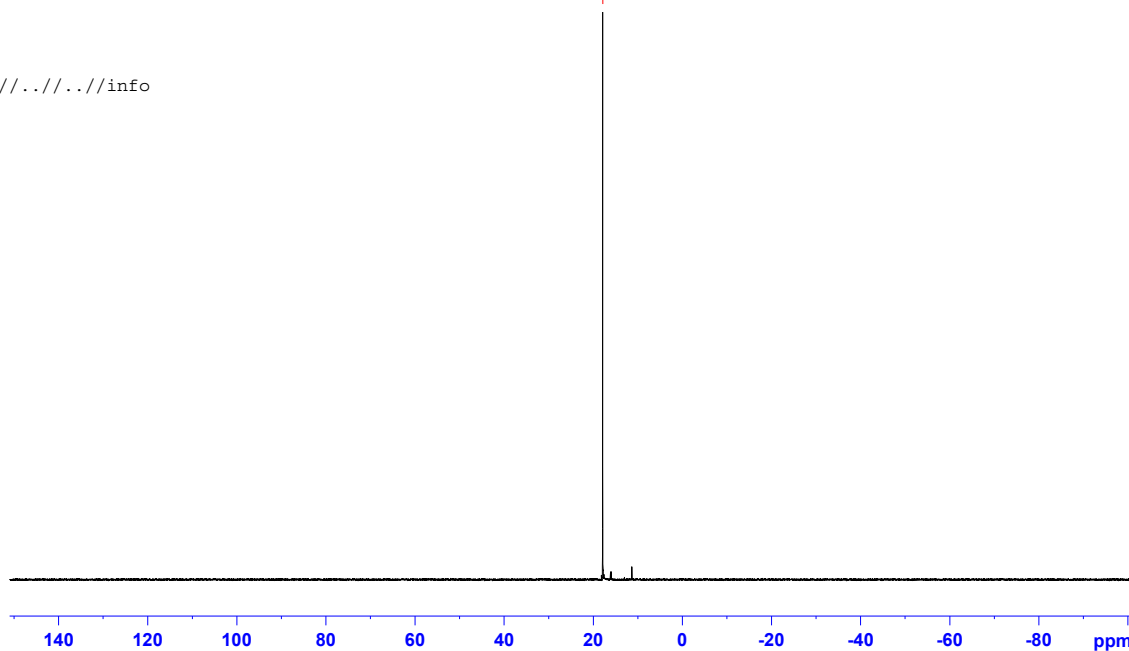
¹³C NMR spectrum of compound 44.

MFBA181-L #//D2O// ³¹P NMR

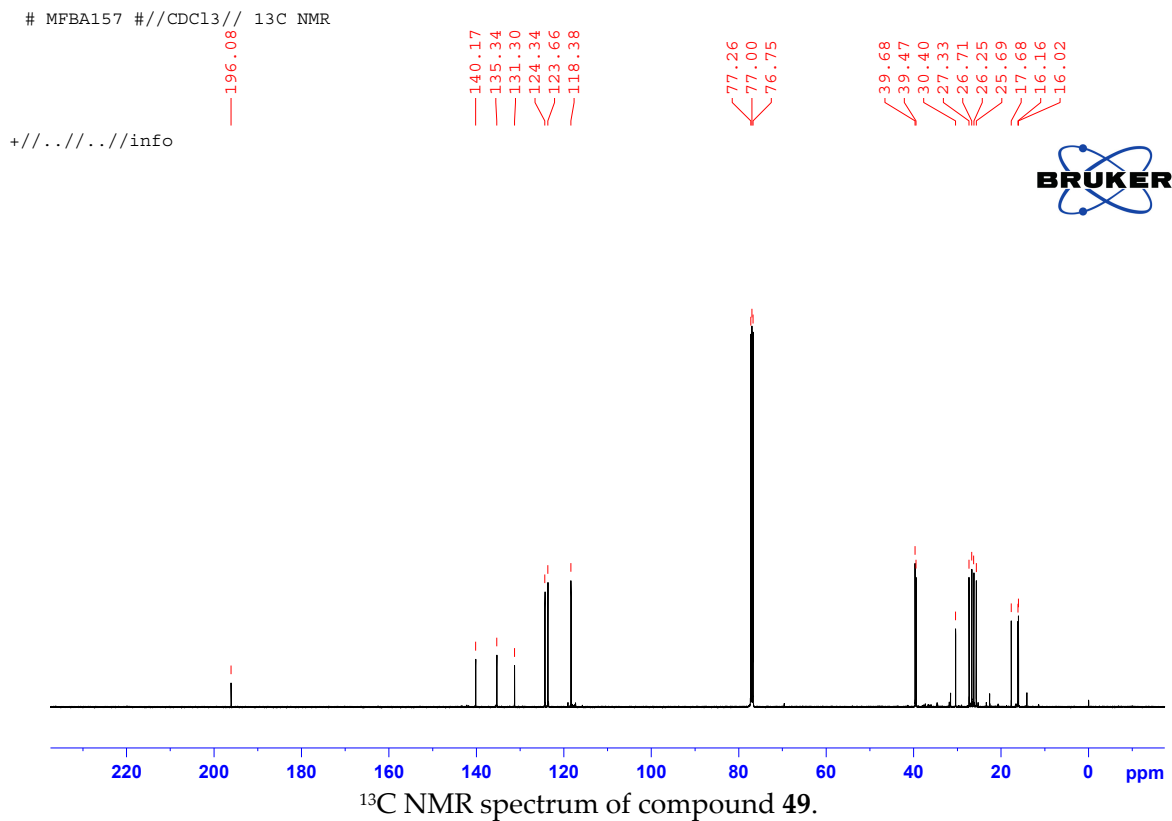
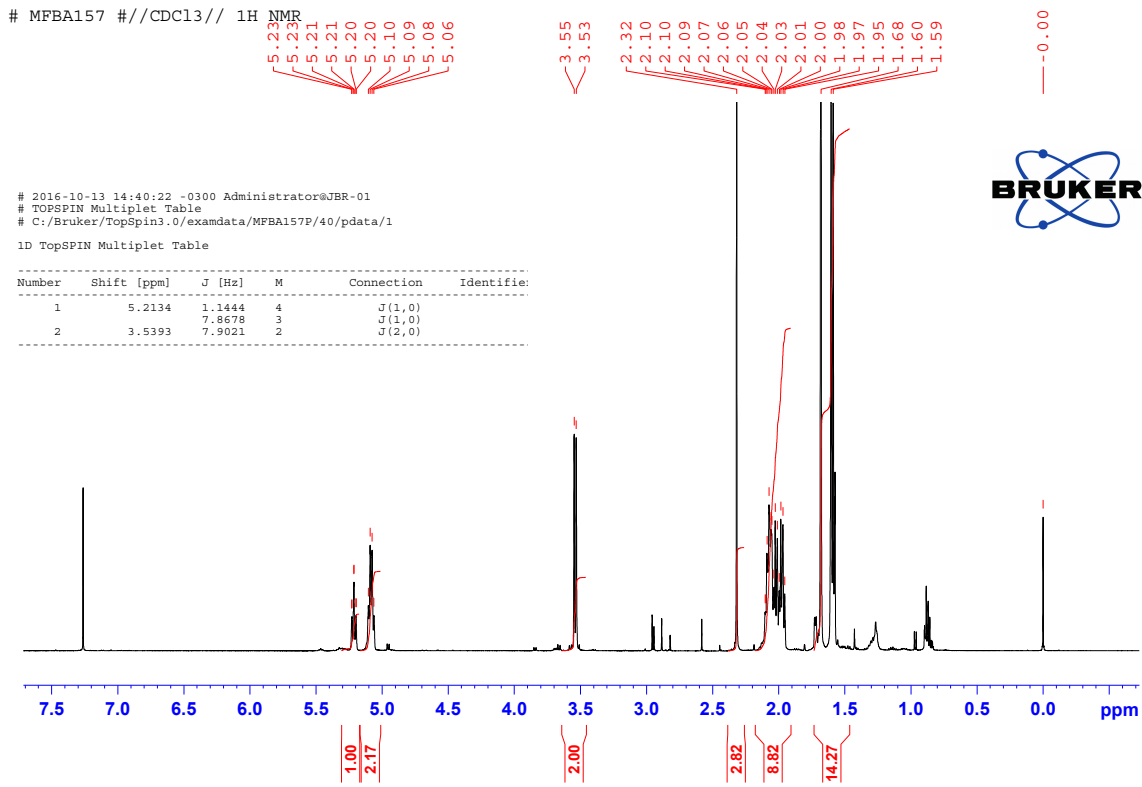
+//...//...//info



— 17.85



³¹P NMR spectrum of compound 44.



MFBA158 #//CDCl3// 1H NMR

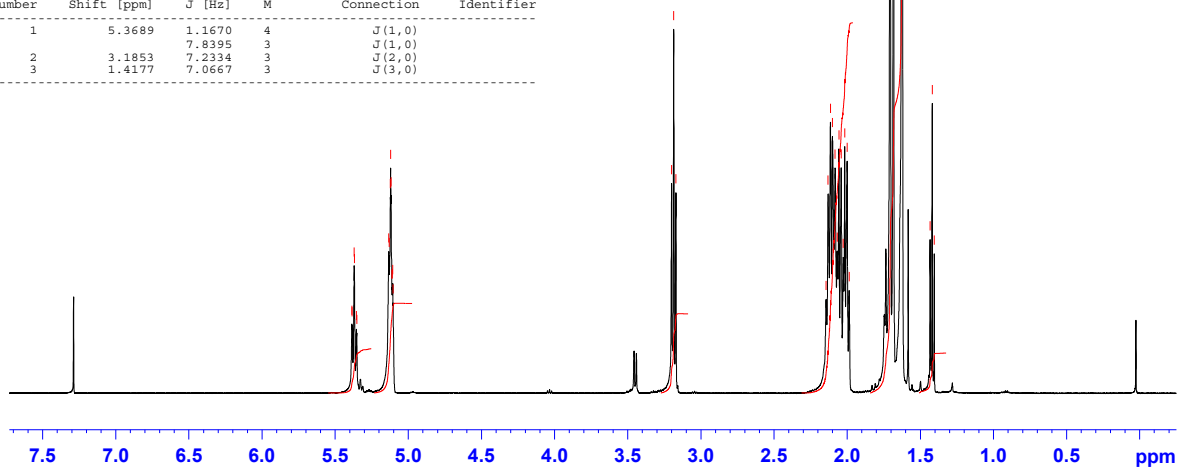
5.39
5.38
5.37
5.35
5.35
5.13
5.13
5.12
5.12
5.12
5.11
5.11
5.11
5.10

3.20
3.19
3.17
2.14
2.13
2.11
2.10
2.08
2.07
2.06
2.04
2.03
2.02
2.00
1.99
1.71
1.68
1.62
1.43
1.42
1.40

2016-10-13 13:20:09 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/MFBA158C6-34/1/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	5.3689	1.1670	4	J(1,0)	
2	3.1853	7.8395	3	J(1,0)	
3	1.4177	7.0667	3	J(2,0)	
				J(3,0)	

¹H NMR spectrum of compound 51.

MFBA158 #//CDCl3// 13C NMR

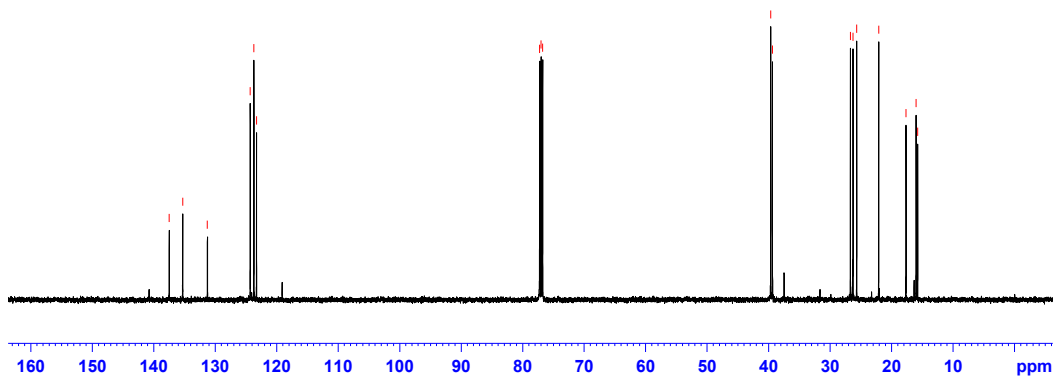
137.48
135.28
131.28
124.31
123.72
123.28

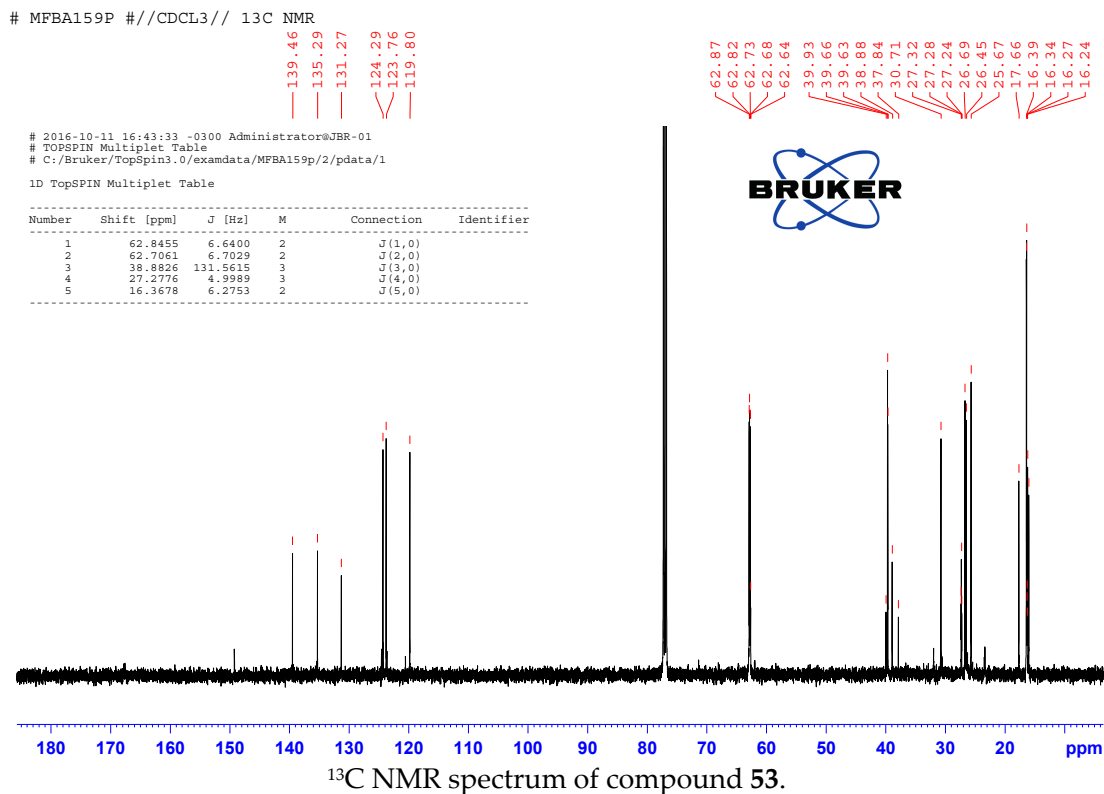
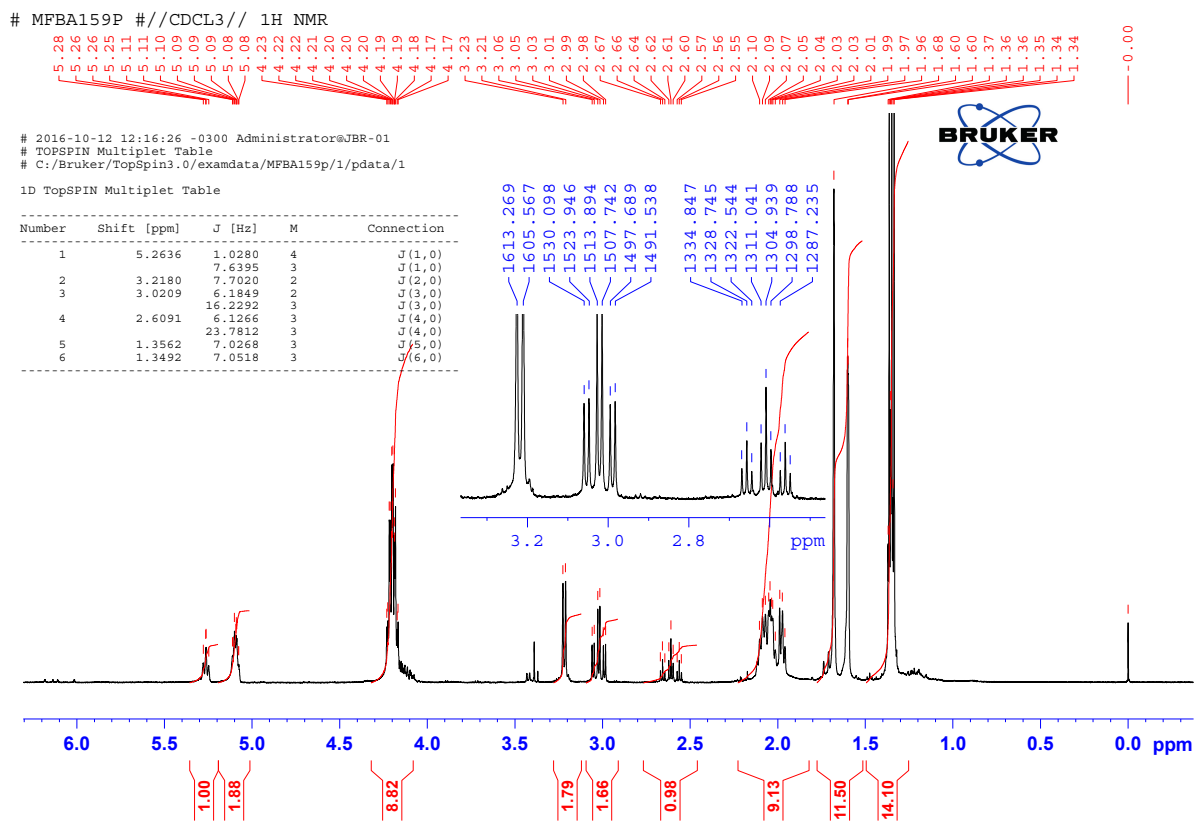
77.25
76.99
76.74

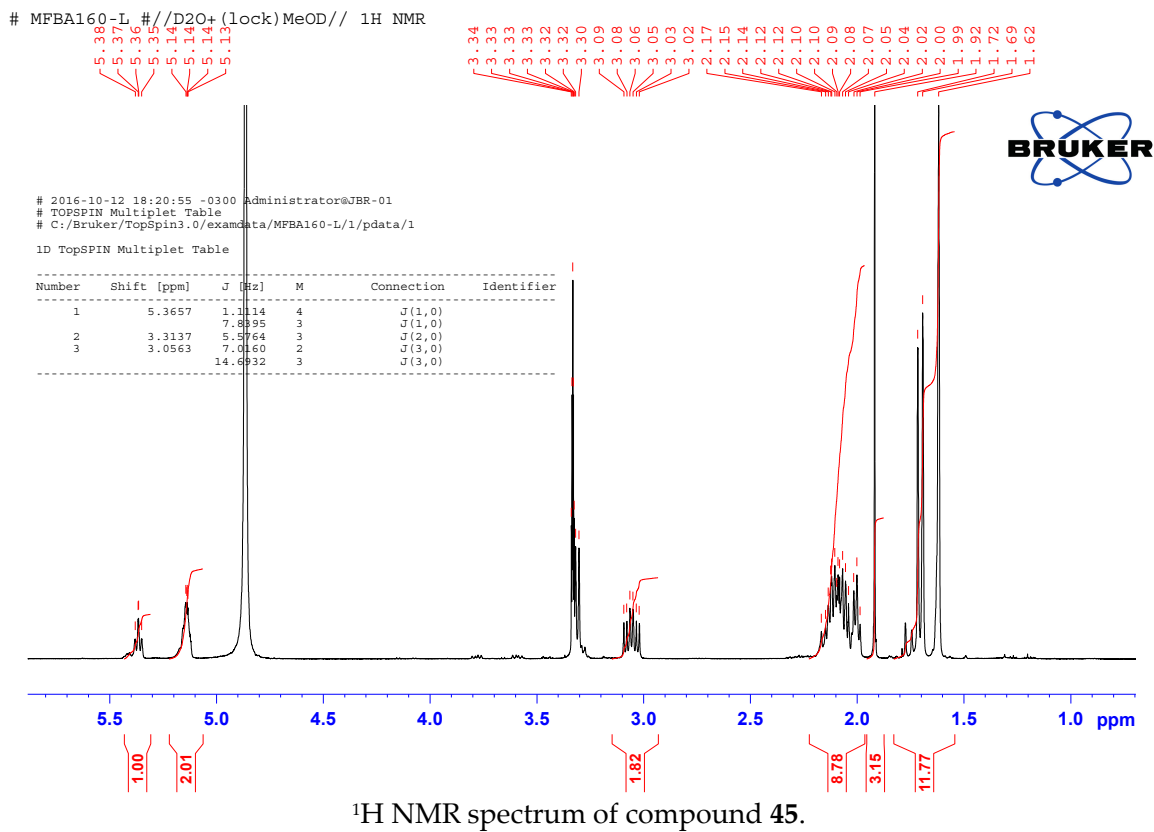
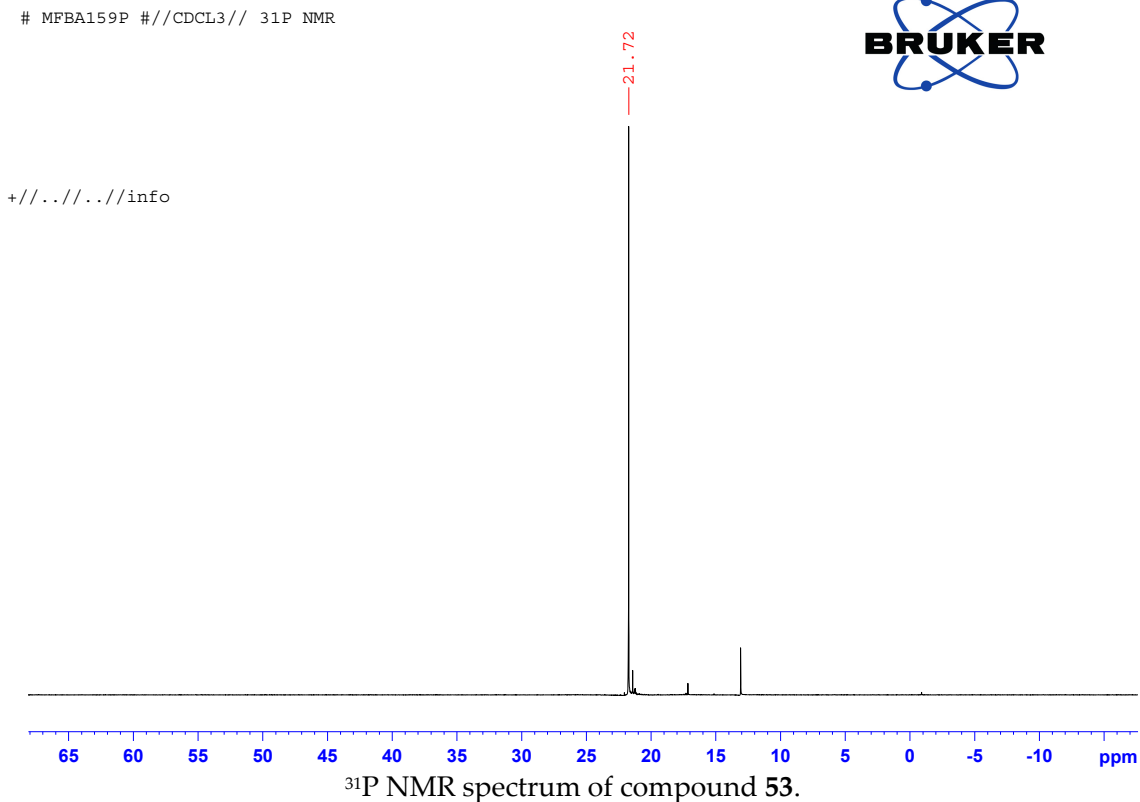
39.66
39.36

26.69
26.26
25.67
22.09
17.66
16.00
15.75

+//...//info

¹³C NMR spectrum of compound 51.





MFBA160-L #//D2O+(lock)MeOD// 13C NMR

140.59
136.70
133.41
125.93
123.82
120.95

49.52
49.34
49.17
49.00
48.83
48.66
48.48
41.47
40.60
40.11
40.09
31.36
30.16
27.01
26.93
25.85
24.29
17.85
16.29
16.11

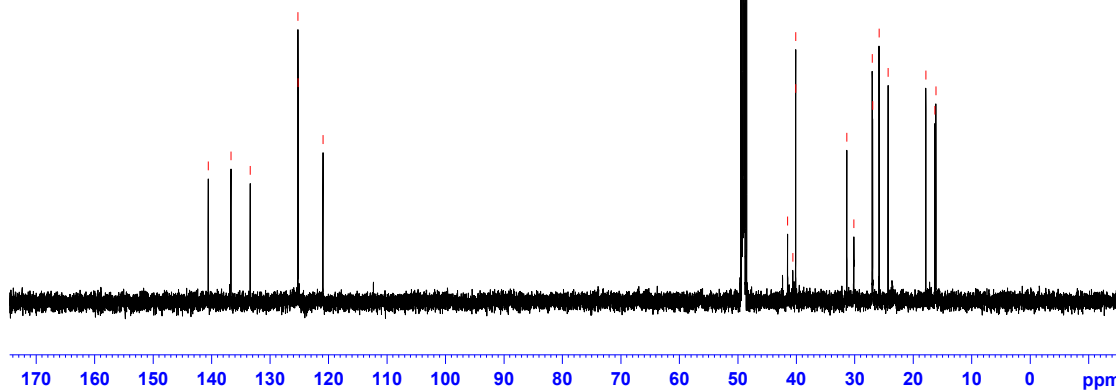


2016-10-12 14:29:07 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table

C:/Bruker/TopSpin3.0/examdata/MFBA160-L/2/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection
1	41.4742	109.4470	3	J(1,0)
2	30.1566	3.6680	3	J(2,0)



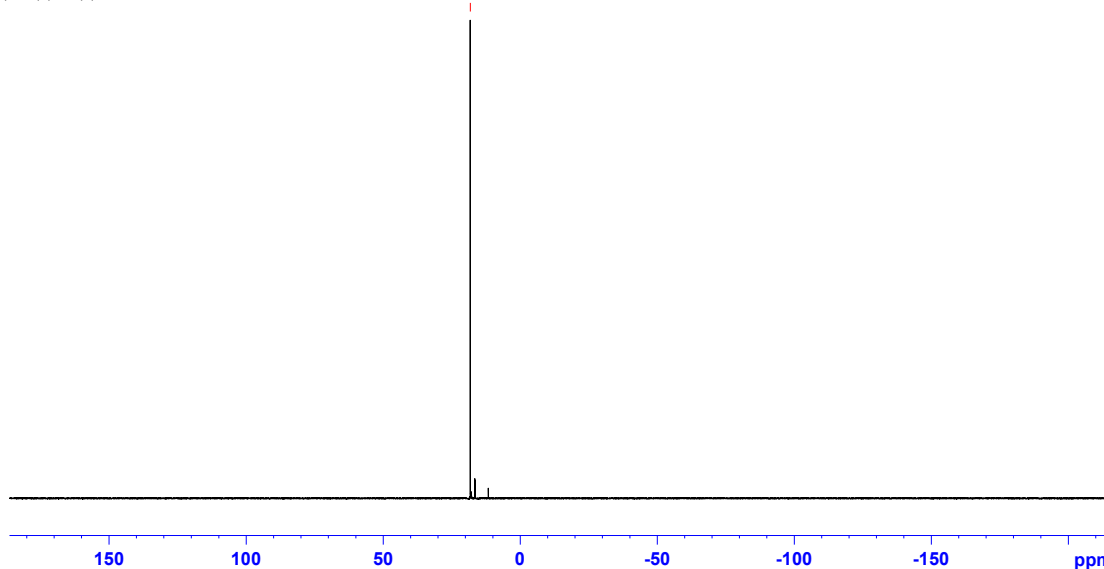
¹³C NMR spectrum of compound 45.

MFBA160-L #//D2O+(lock)MeOD// 31P NMR

-18.16

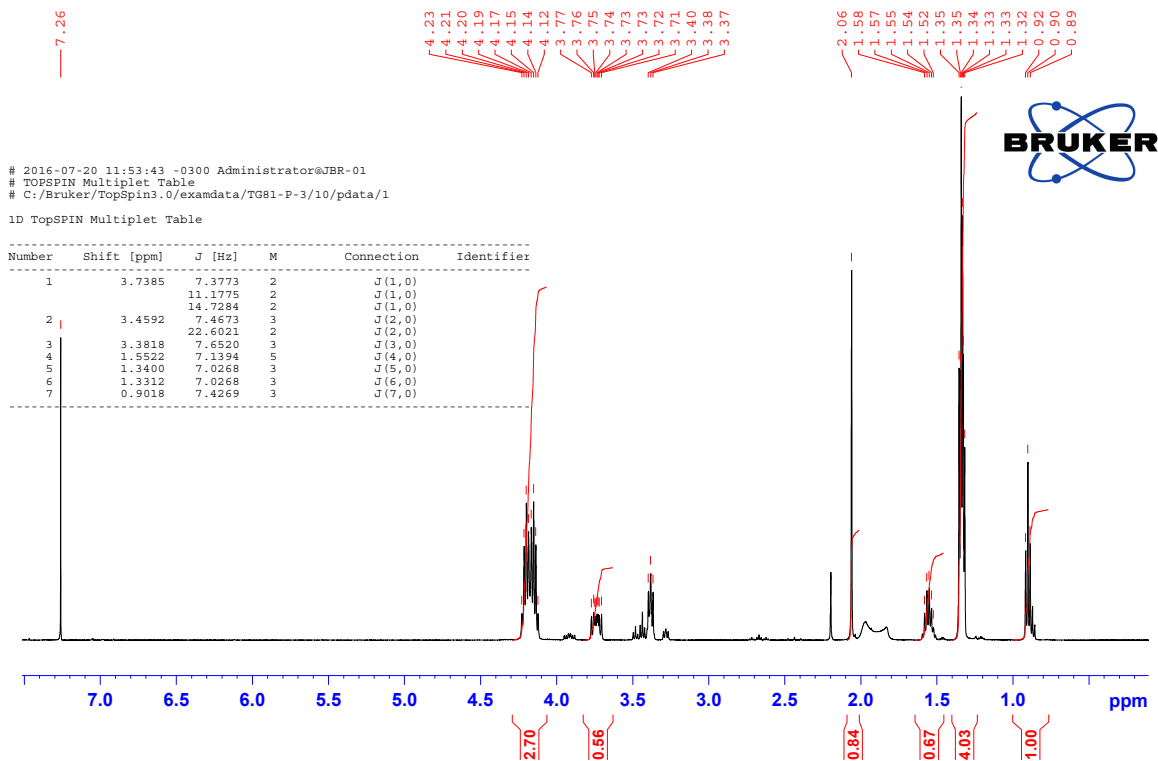


+//...//...//info

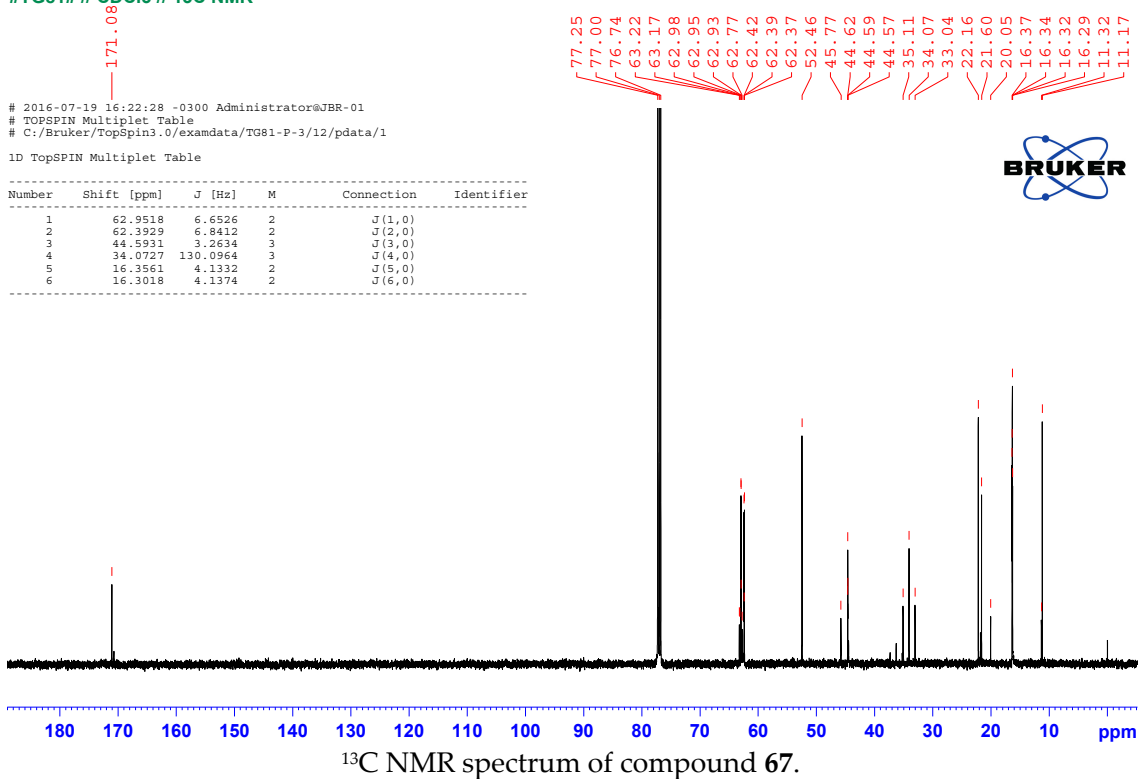


³¹P NMR spectrum of compound 45.

#TG81# // CDCl3 // 1H NMR

¹H NMR spectrum of compound 67.

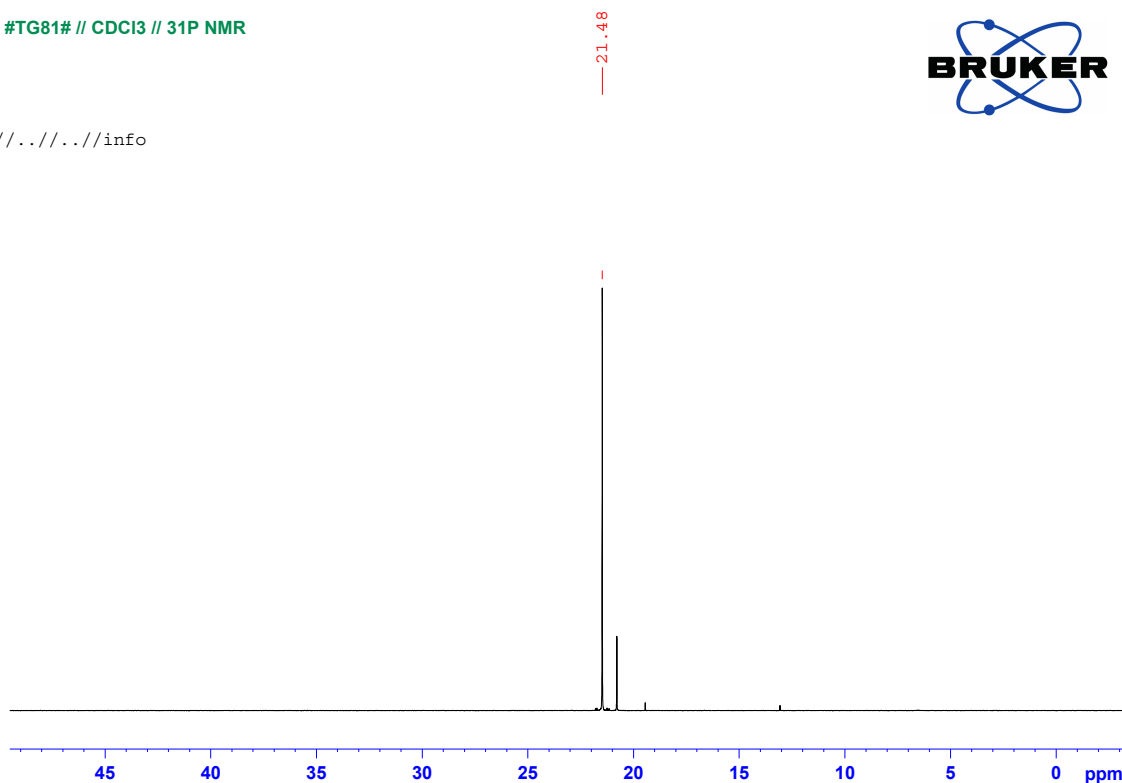
#TG81# // CDCl3 // 13C NMR

¹³C NMR spectrum of compound 67.

#TG81# // CDCI3 // 31P NMR

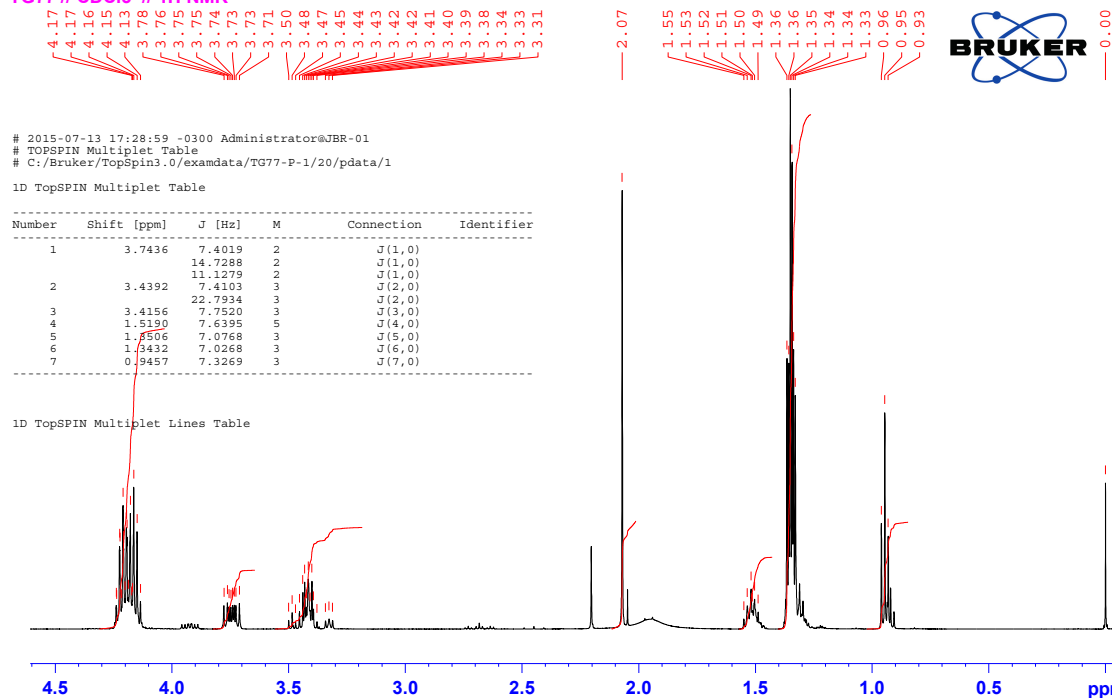


+//...//...//info

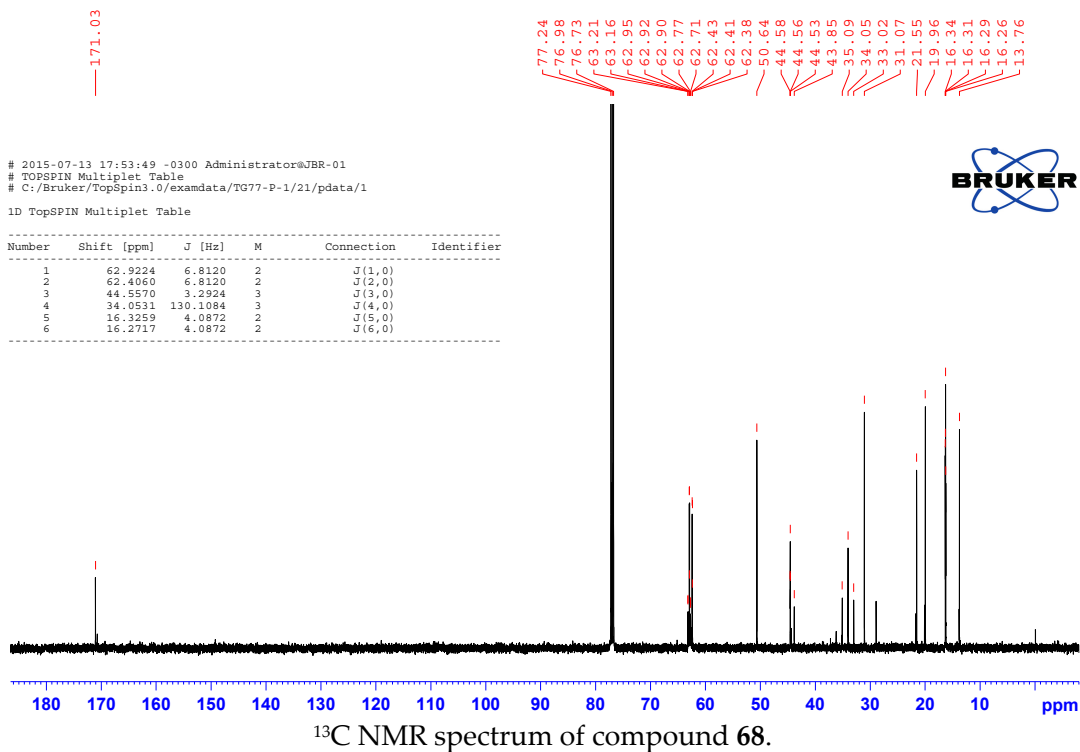
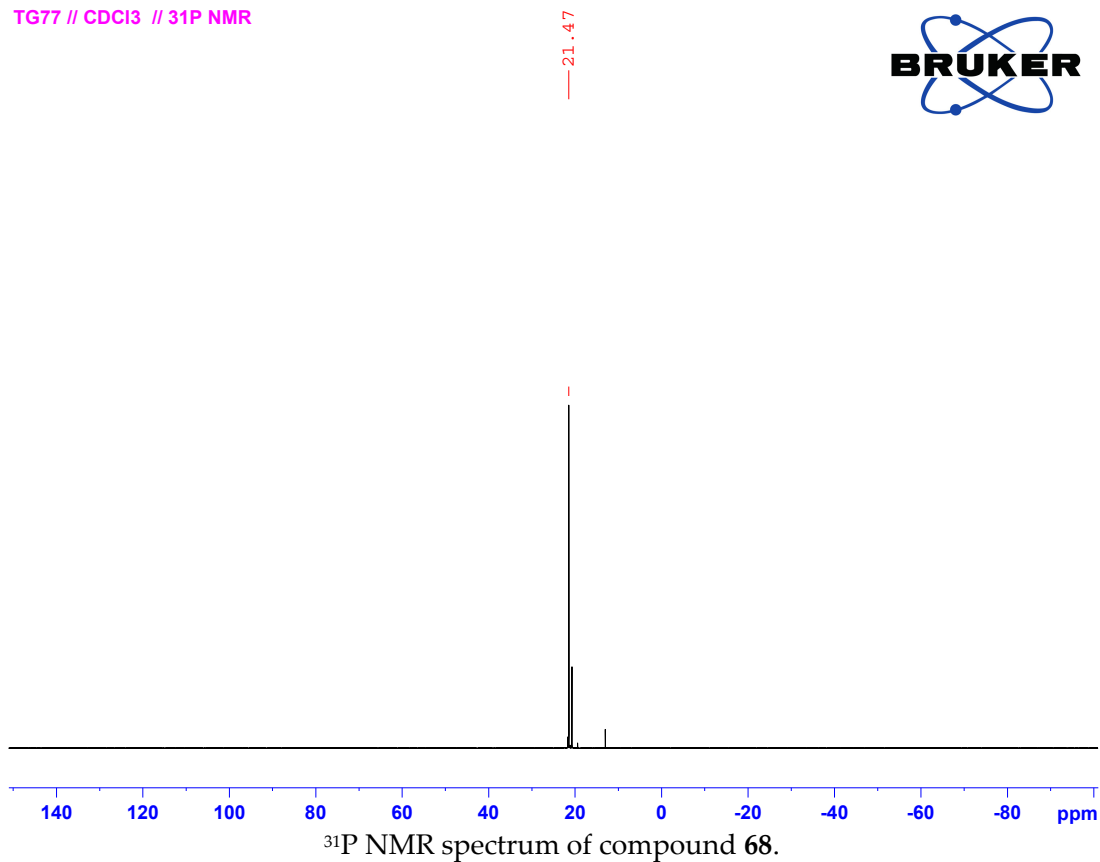


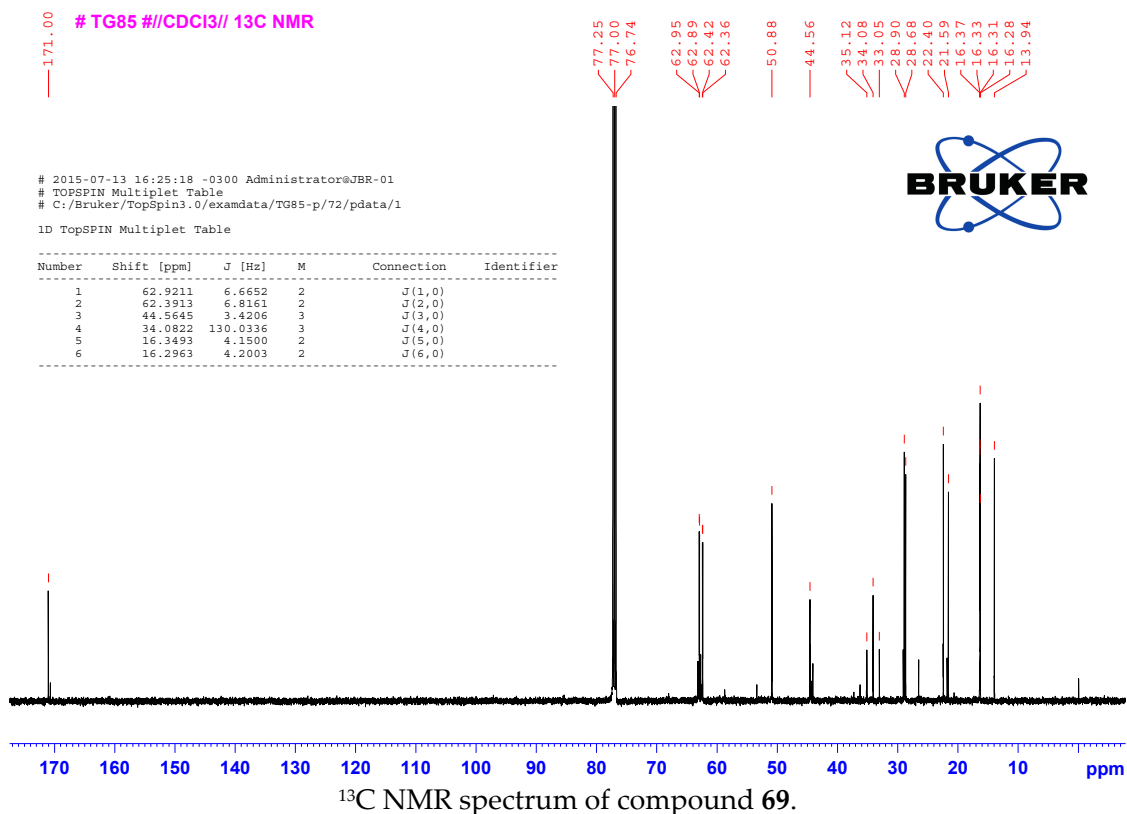
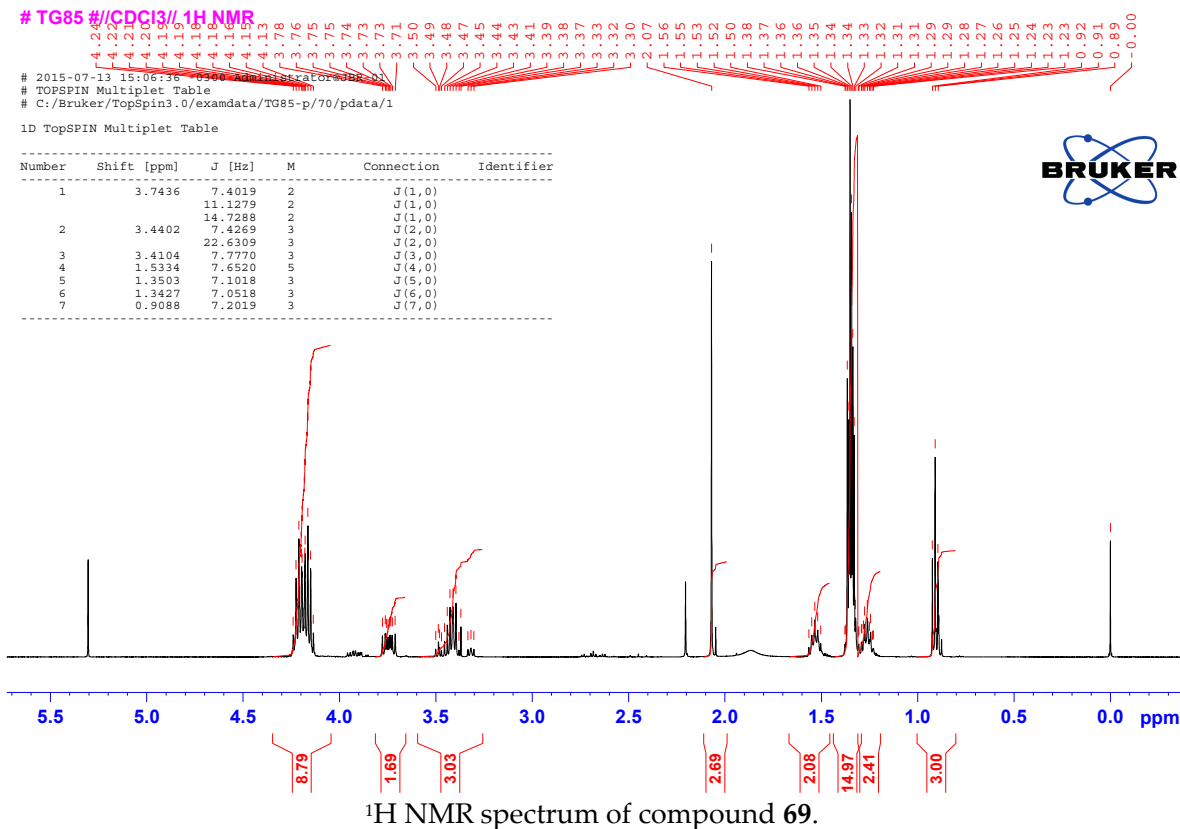
³¹P NMR spectrum of compound 67.

TG77 // CDCI3 // 1H NMR



¹H NMR spectrum of compound 68.

TG77 // CDCl₃ // ¹³C NMRTG77 // CDCl₃ // ³¹P NMR

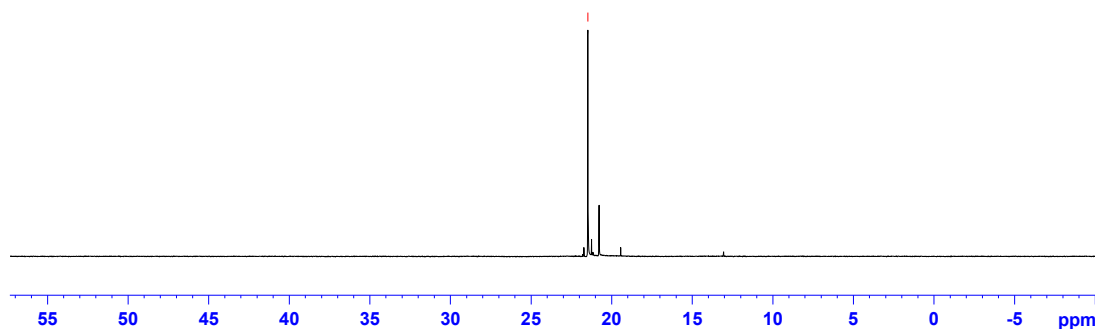


TG85-P #/CDCI3// 31P NMR

— 21.47



+//.////.//info



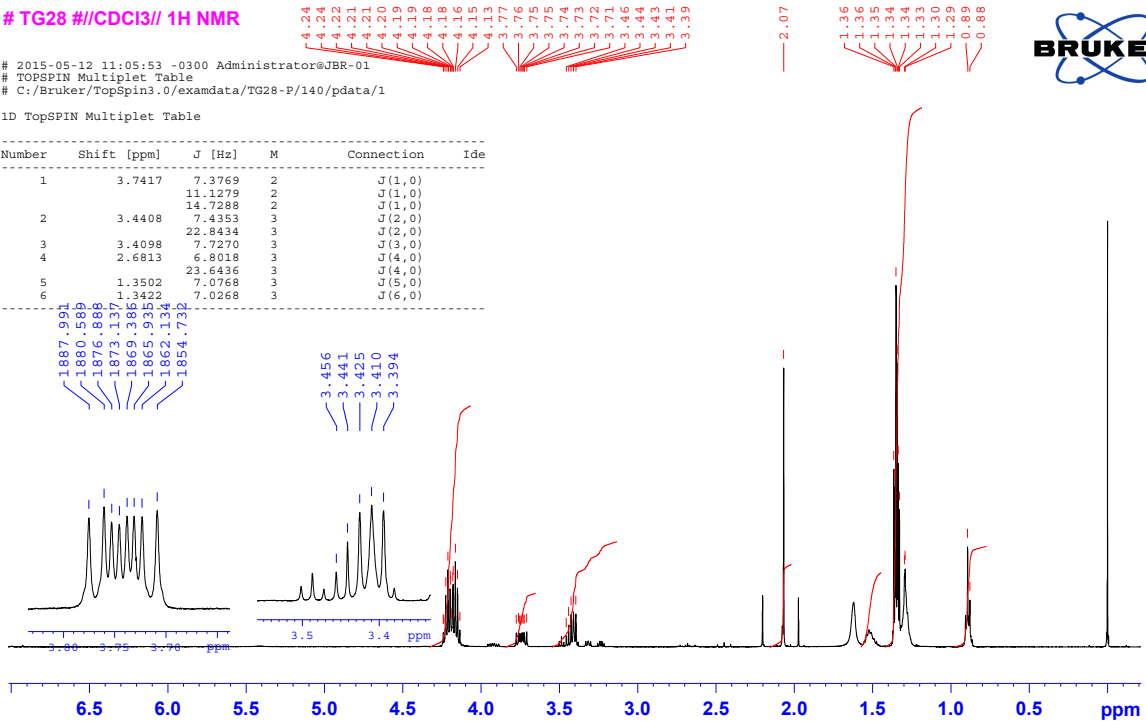
³¹P NMR spectrum of compound 69.

TG28 #/CDCI3// 1H NMR

2015-05-12 11:05:53 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG28-P/140/pdata/1

1D TopSPIN Multiplet Table

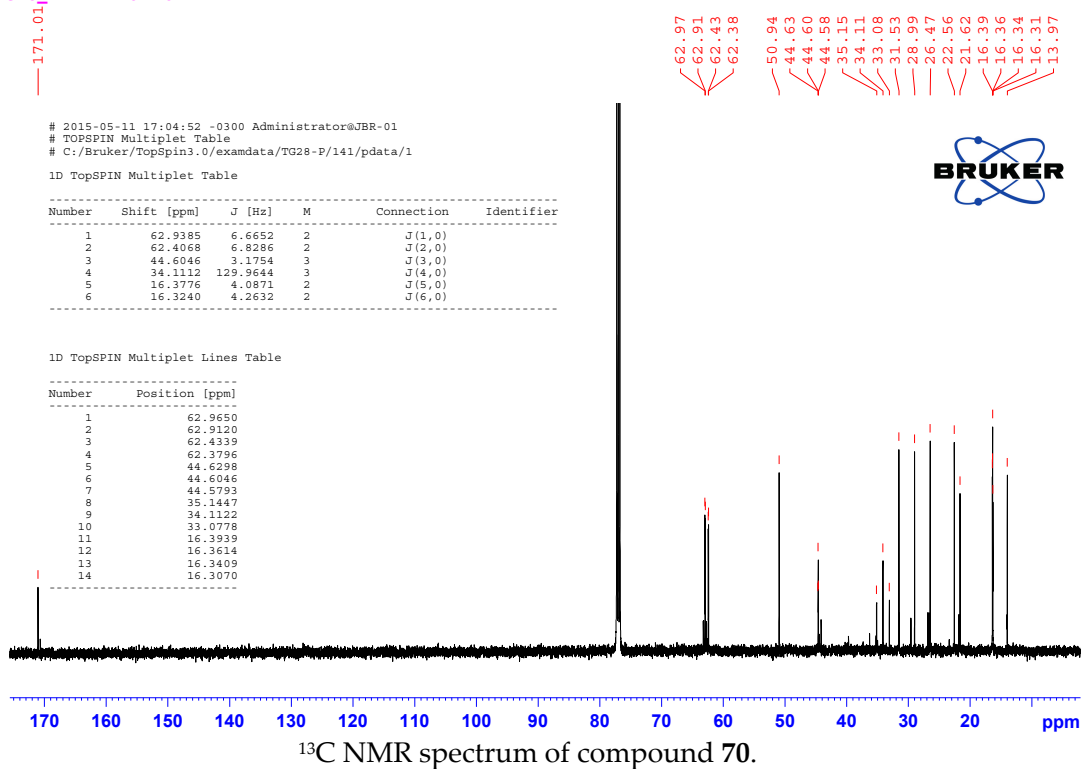
Number	Shift [ppm]	J [Hz]	M	Connection	Ide
1	3.7417	7.3769	2	J(1,0)	
		11.1279	2	J(1,0)	
		14.7288	2	J(1,0)	
2	3.4408	7.4353	3	J(2,0)	
		22.8434	3	J(2,0)	
3	3.4098	7.7270	3	J(3,0)	
4	2.6813	6.8018	3	J(4,0)	
5	1.3502	23.6436	3	J(5,0)	
		7.0768	3	J(5,0)	
6	1.3422	7.0268	3	J(6,0)	



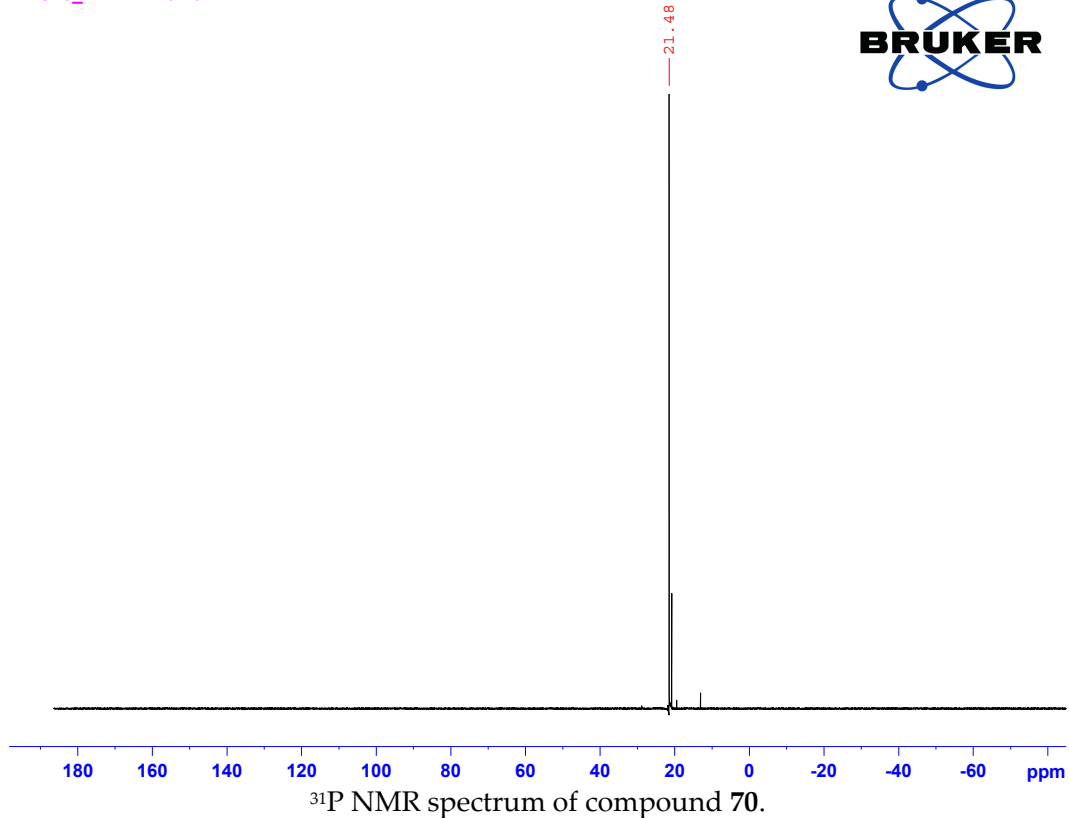
¹H NMR spectrum of compound 70.

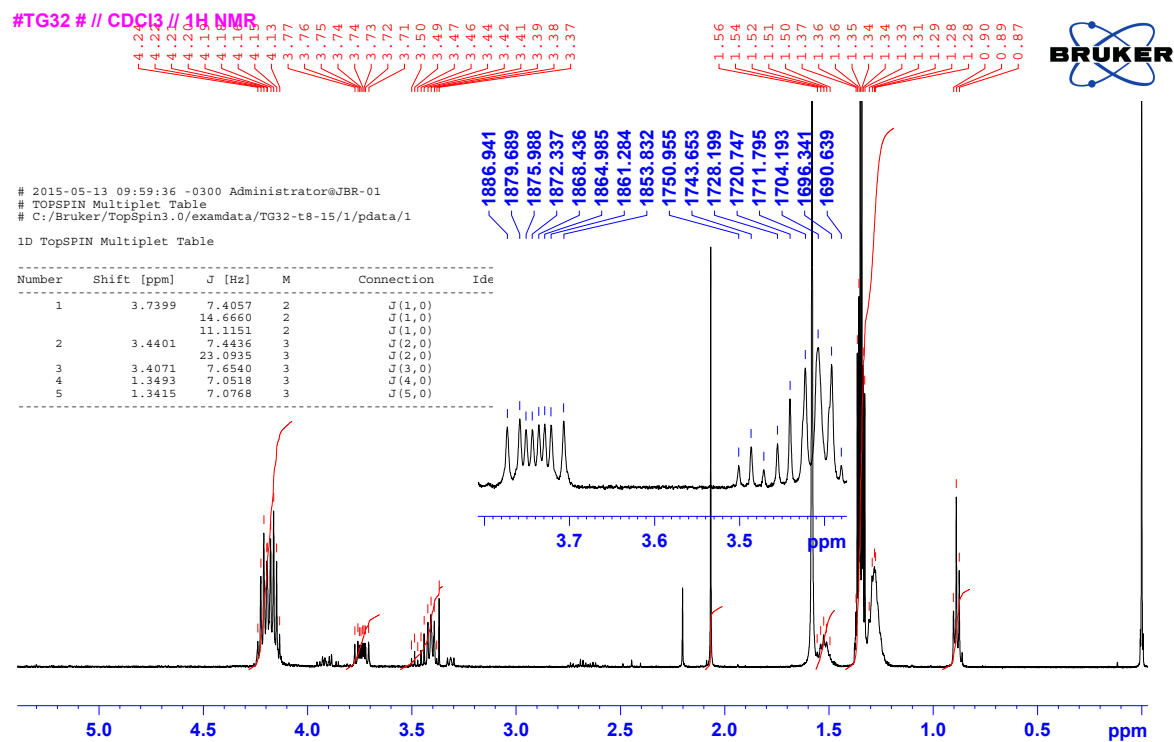
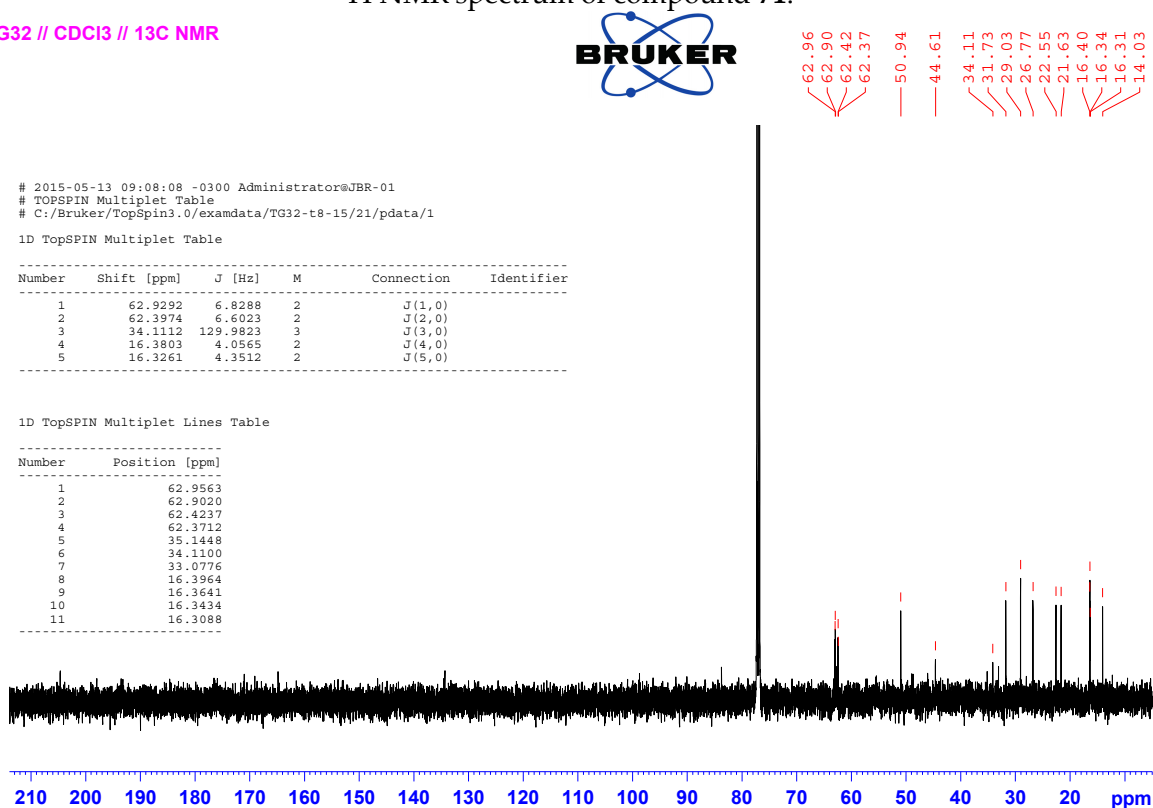


TG28_P #//CDCI3// 13C NMR

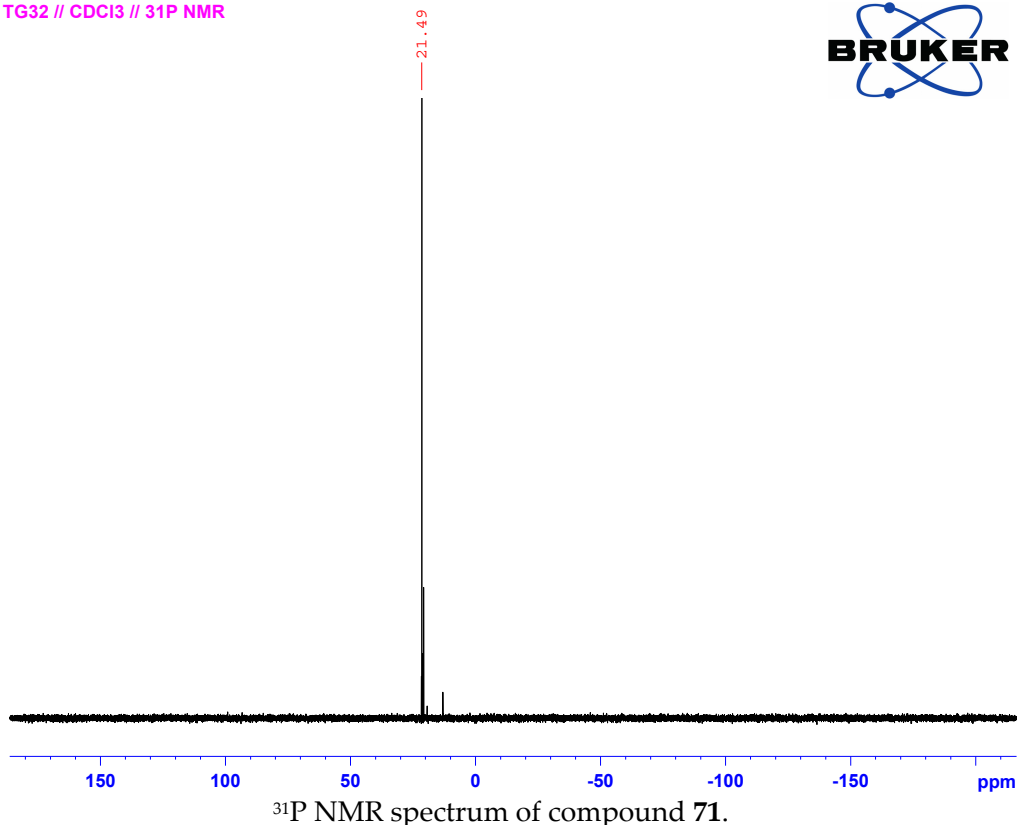


TG28_P #//CDCI3// 31P NMR

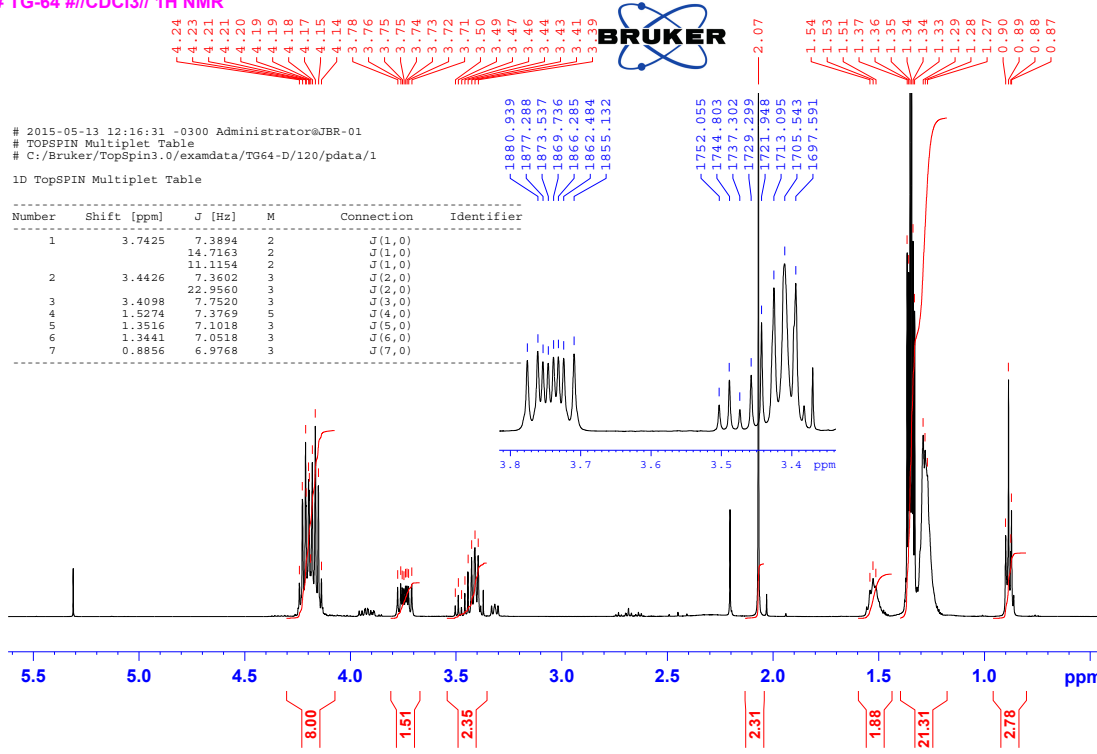


¹H NMR spectrum of compound 71.TG32 // CDCl3 // ¹³C NMR¹³C NMR spectrum of compound 71.

// TG32 // CDCl3 // 31P NMR



TG-64 #//CDCl3// 1H NMR



TG-64 #//CDCI3// 13C NMR

170.91

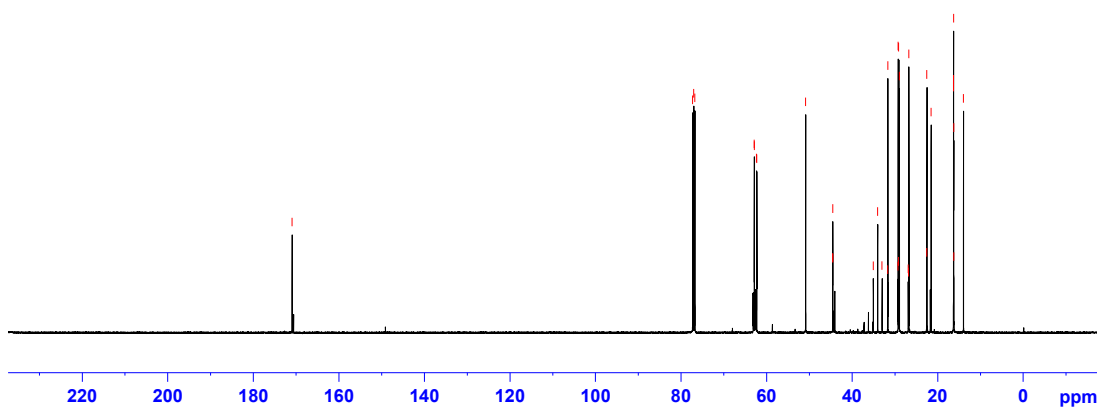
77.25
77.00
76.75
62.86
62.81
62.33
62.28
50.84
44.52
44.50
44.47
35.04
34.01
32.97
31.68
29.27
29.12
29.08
28.93
26.88
26.78
26.70
22.51
22.50
21.52
16.29
16.26
16.24

2015-05-13 10:58:24 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG64-D/121/pdata/1



1D TopSPIN Multiplet Table

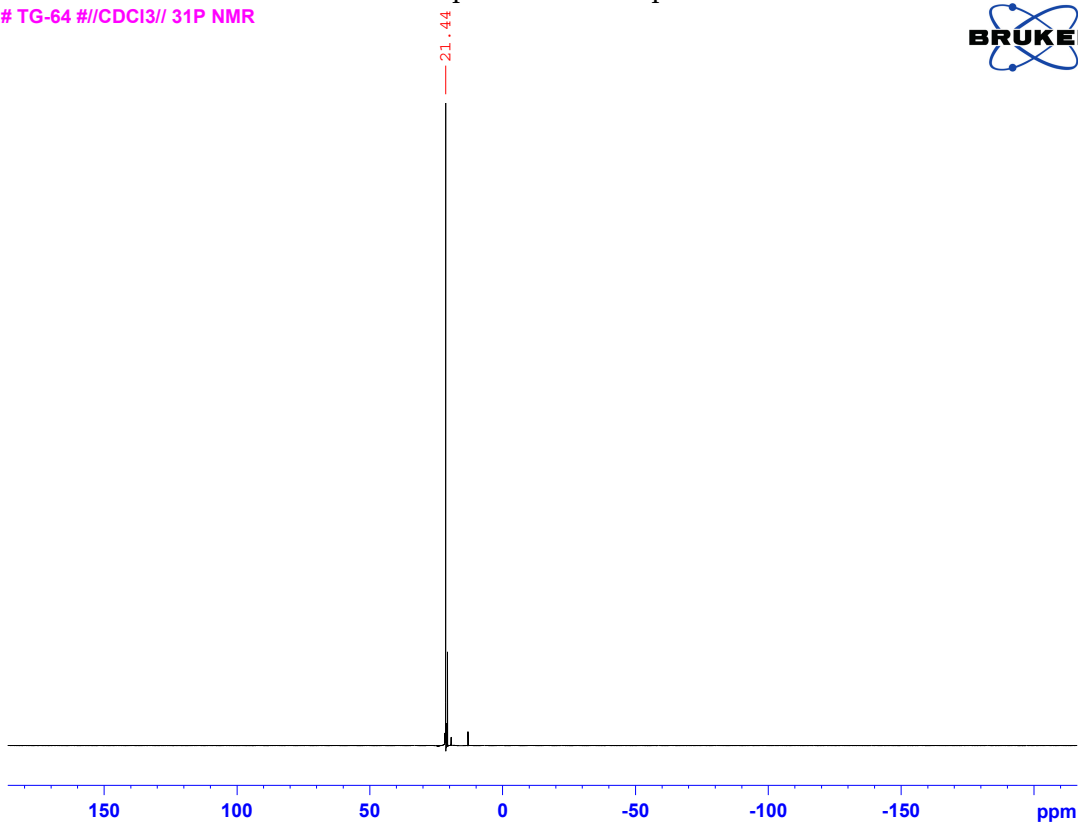
Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	62.8332	6.6023	2	J(1,0)	
2	62.3073	6.8412	2	J(2,0)	
3	44.4960	3.1754	3	J(3,0)	
4	34.0056	130.0902	3	J(4,0)	
5	16.2740	3.9125	2	J(5,0)	
6	16.2195	3.9125	2	J(6,0)	



¹³C NMR spectrum of compound 72.

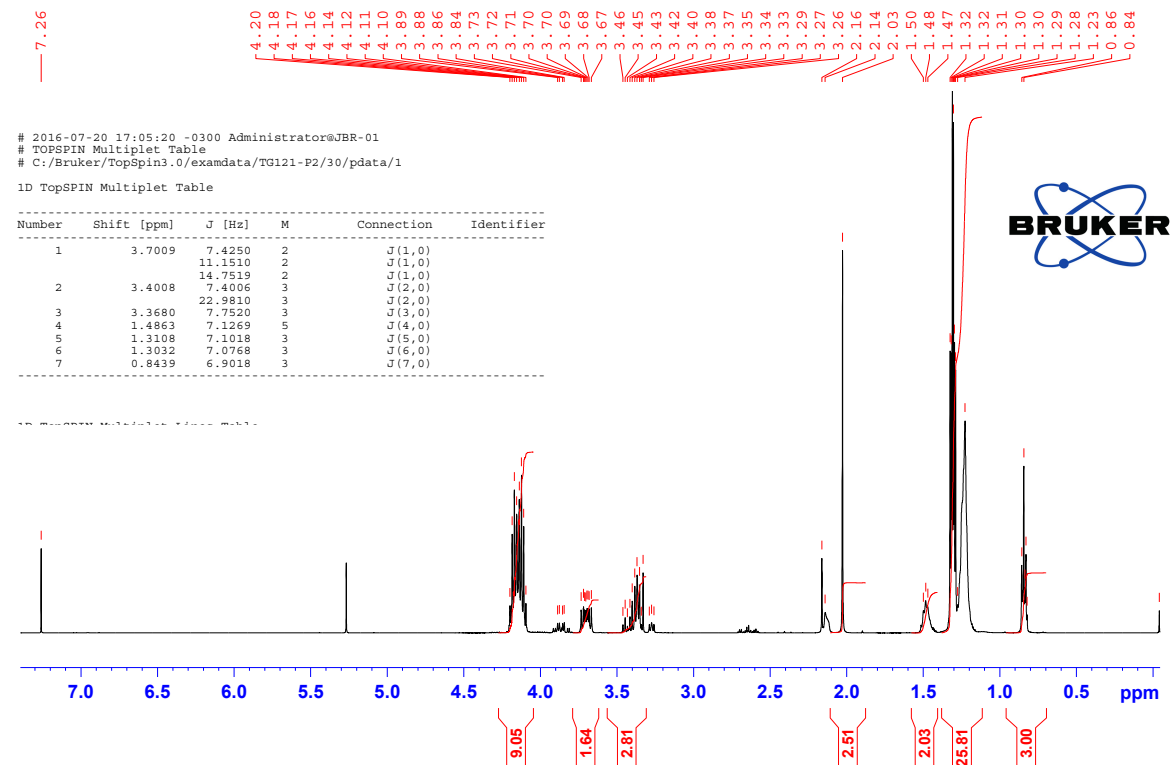
TG-64 #//CDCI3// 31P NMR

21.44

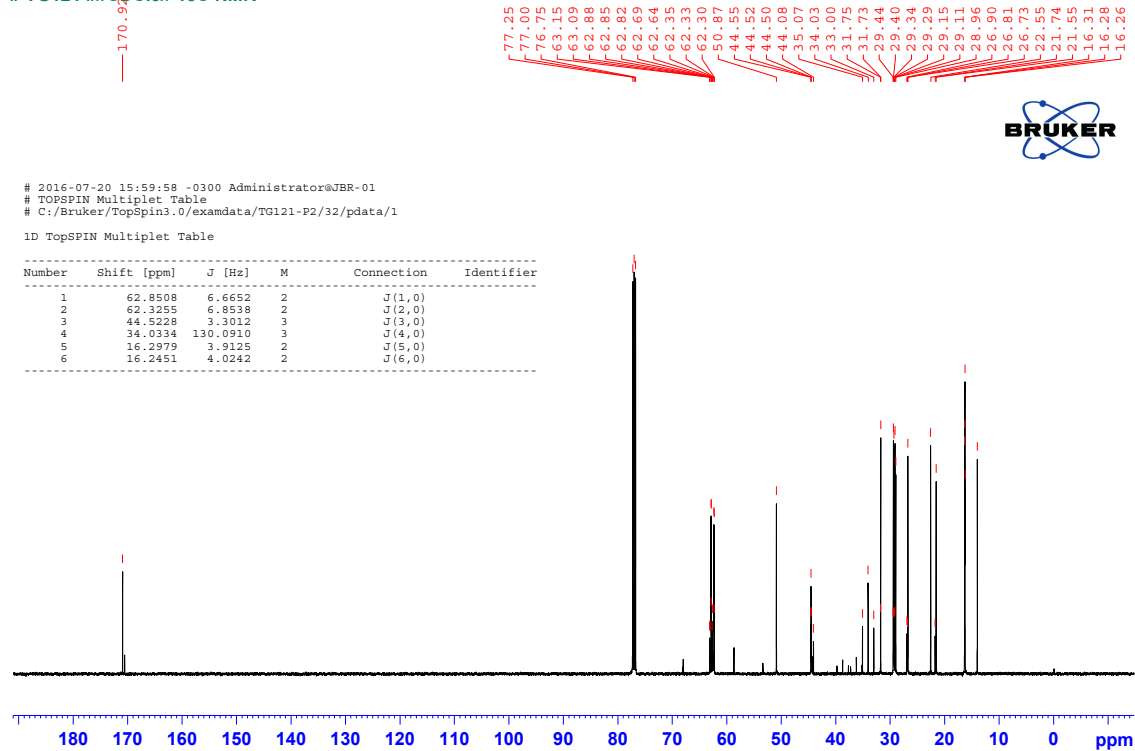


³¹P NMR spectrum of compound 72.

TG121 #//CDCl3// 1H NMR

¹H NMR spectrum of compound 73.

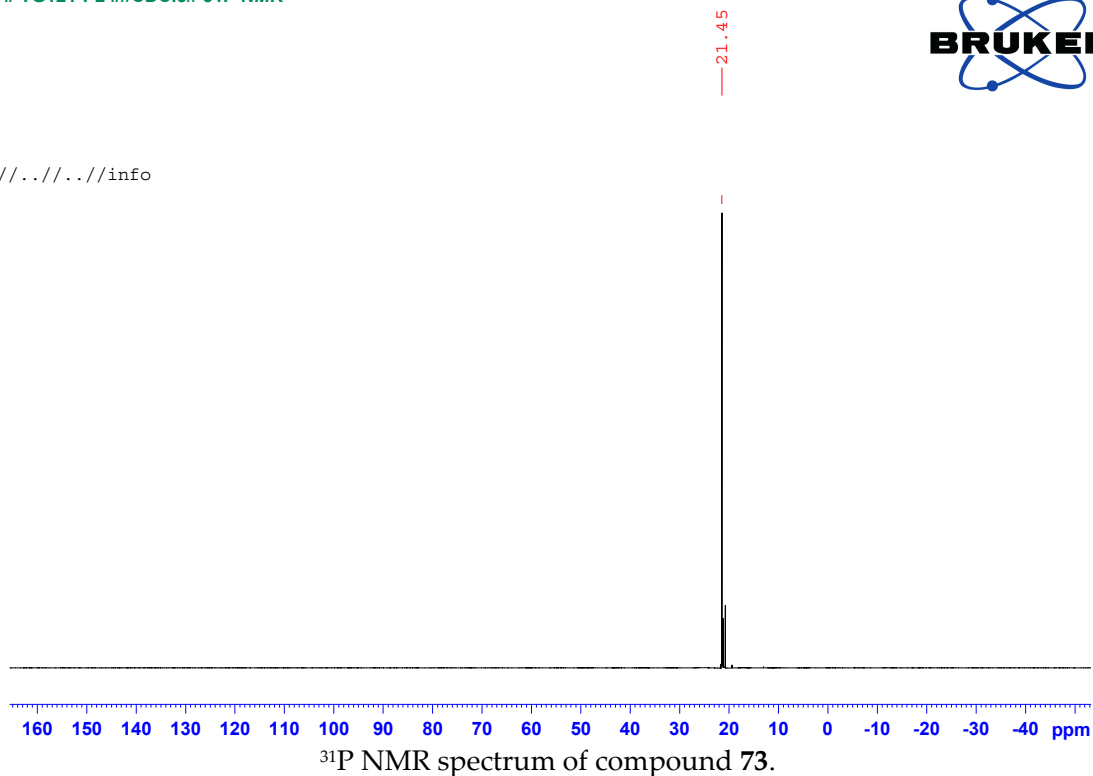
TG121 #//CDCl3// 13C NMR

¹³C NMR spectrum of compound 73.

TG121-P2 #//CDCI3// 31P NMR



+//...//...//info



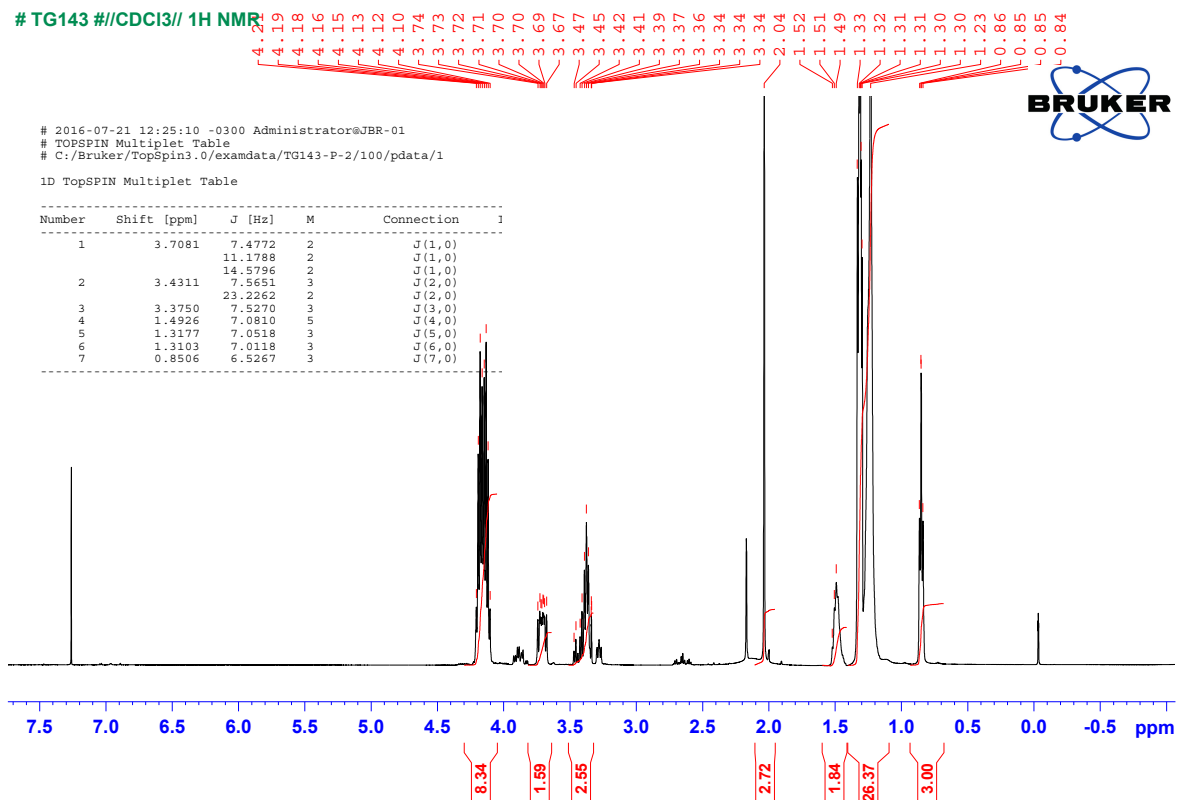
TG143 #//CDCI3// 1H NMR



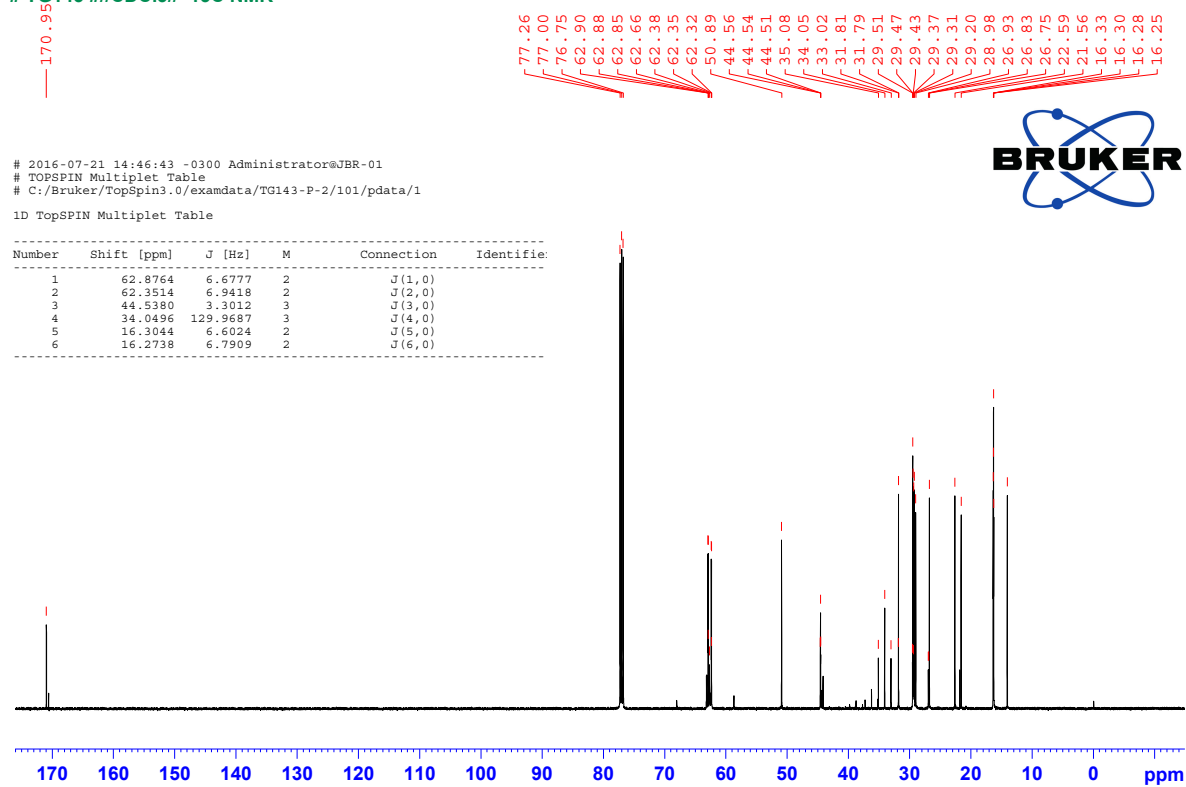
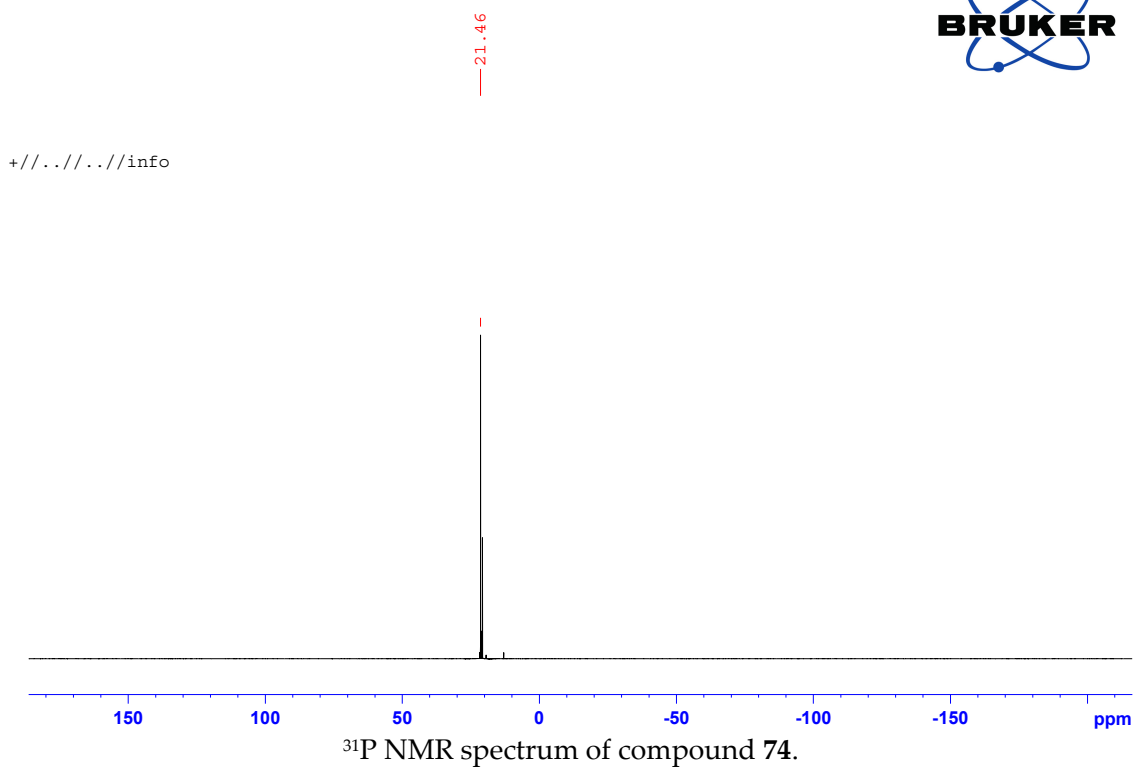
2016-07-21 12:25:10 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG143-P-2/100/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	I
1	3.7081	7.4772	2	J(1,0)	
		11.1788	2	J(1,0)	
		14.5796	2	J(1,0)	
2	3.4311	7.5651	3	J(2,0)	
		23.2262	2	J(2,0)	
3	3.3750	7.5270	3	J(3,0)	
4	1.4926	7.0810	5	J(4,0)	
5	1.3177	7.0518	3	J(5,0)	
6	1.3103	7.0118	3	J(6,0)	
7	0.8506	6.5267	3	J(7,0)	



1H NMR spectrum of compound 74.

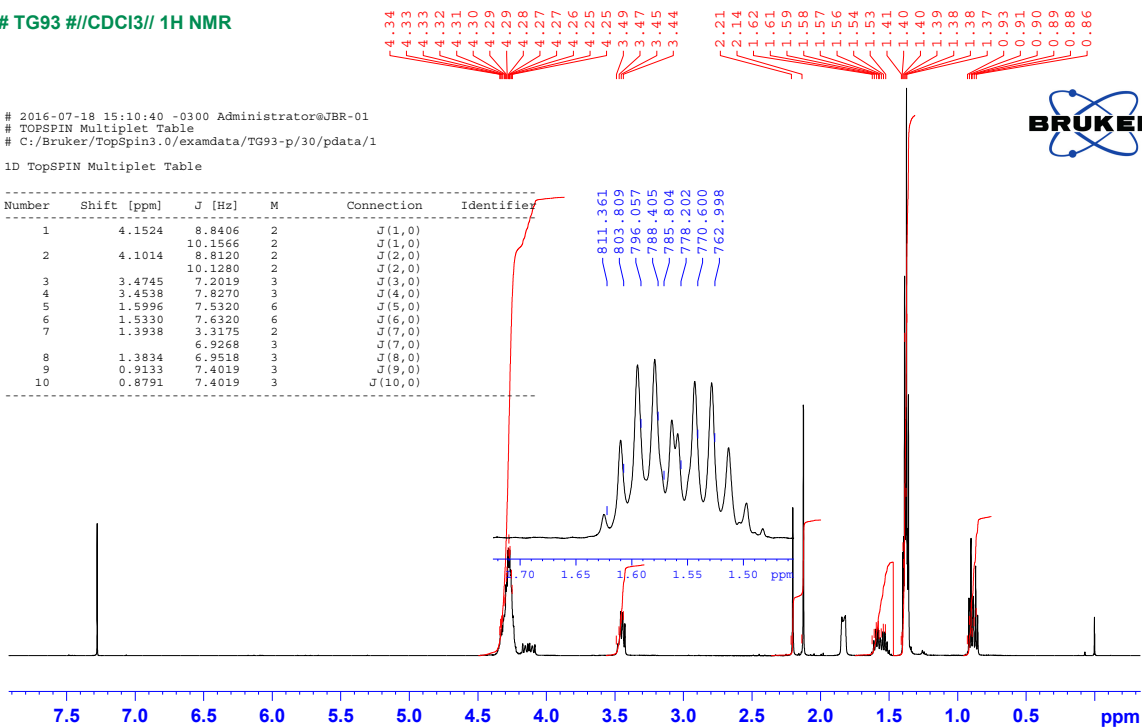
TG143 #//CDCI3// ¹³C NMR# TG143 #//CDCI3// ¹H RMN

TG93 #//CDCl3// 1H NMR

2016-07-18 15:10:40 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG93-p/30/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	4.1524	8.8406	2	J(1,0)	
2	4.1014	10.1566	2	J(1,0)	
		8.8120	2	J(2,0)	
		10.1280	2	J(2,0)	
3	3.4745	7.2019	3	J(3,0)	
4	3.4538	7.8270	3	J(4,0)	
5	1.5996	7.5320	6	J(5,0)	
6	1.5330	7.6320	6	J(6,0)	
7	1.3938	3.3175	2	J(7,0)	
		6.9268	3	J(7,0)	
8	1.3834	6.9518	3	J(8,0)	
9	0.9133	7.4019	3	J(9,0)	
10	0.8791	7.4019	3	J(10,0)	

¹H NMR spectrum of compound 75.

TG93 #//CDCl3// 13C NMR

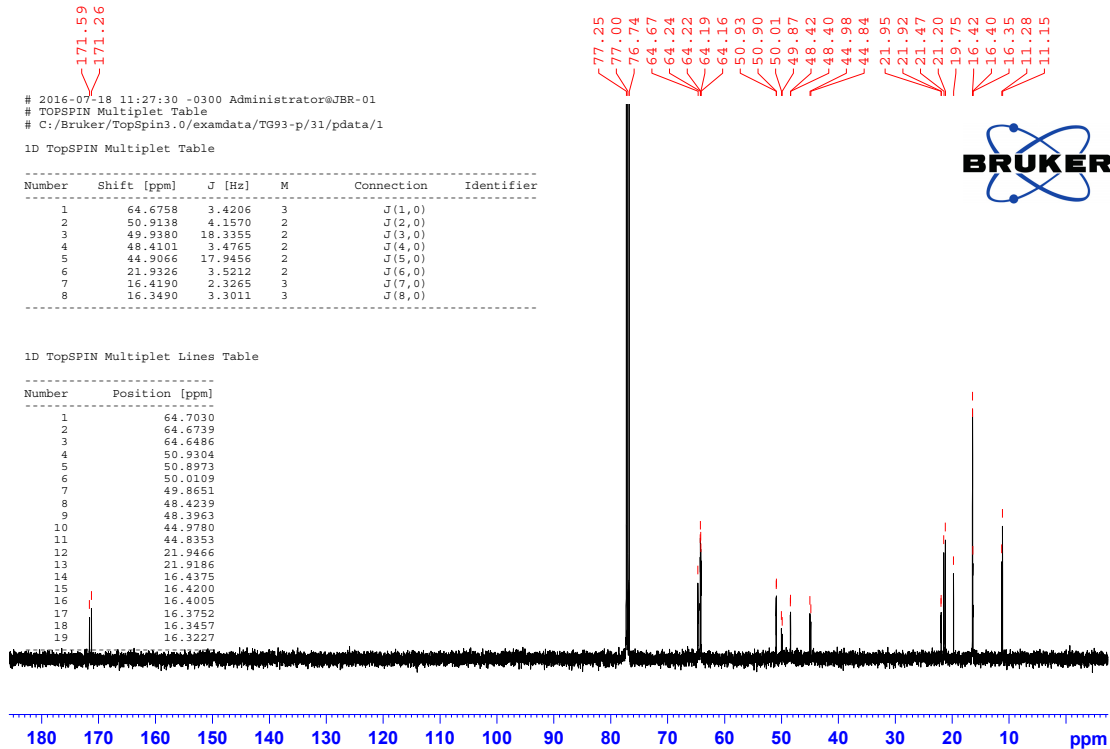
2016-07-18 11:27:30 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG93-p/31/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	64.6758	3.4206	3	J(1,0)	
2	50.9138	4.1570	2	J(2,0)	
3	49.9380	18.3355	2	J(3,0)	
4	48.4101	3.4765	2	J(4,0)	
5	44.9066	17.9456	2	J(5,0)	
6	21.9326	3.5212	2	J(6,0)	
7	16.4190	2.3265	3	J(7,0)	
8	16.3490	3.3011	3	J(8,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	64.7030
2	64.6739
3	64.6486
4	50.9304
5	50.8973
6	50.0109
7	49.8651
8	48.4239
9	48.3963
10	44.9780
11	44.8353
12	21.9466
13	21.9186
14	16.4375
15	16.4200
16	16.4005
17	16.3752
18	16.3457
19	16.3227

¹³C NMR spectrum of compound 75.

TG93 #//CDCI3// 31P NMR



--12.09
--11.87
--11.71
--11.51

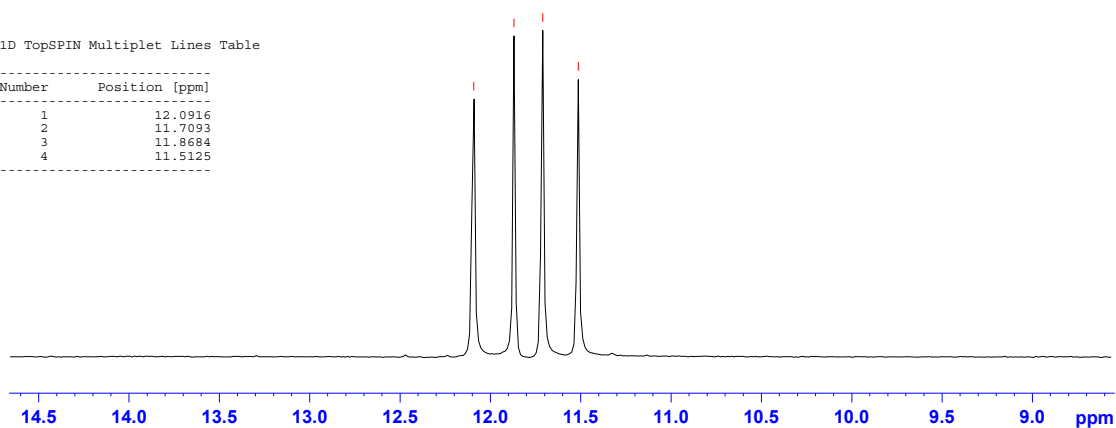
2016-07-14 17:41:40 -0300 Administrator@JBR-01
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1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	11.9004	77.3991	2	J(1,0)	
2	11.6904	72.0542	2	J(2,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	12.0916
2	11.7093
3	11.8684
4	11.5125



³¹P NMR spectrum of compound 75.

TG93 #//CDCI3// 19F NMR



--192.38
--192.55
--192.65
--192.71
--192.80
--192.95

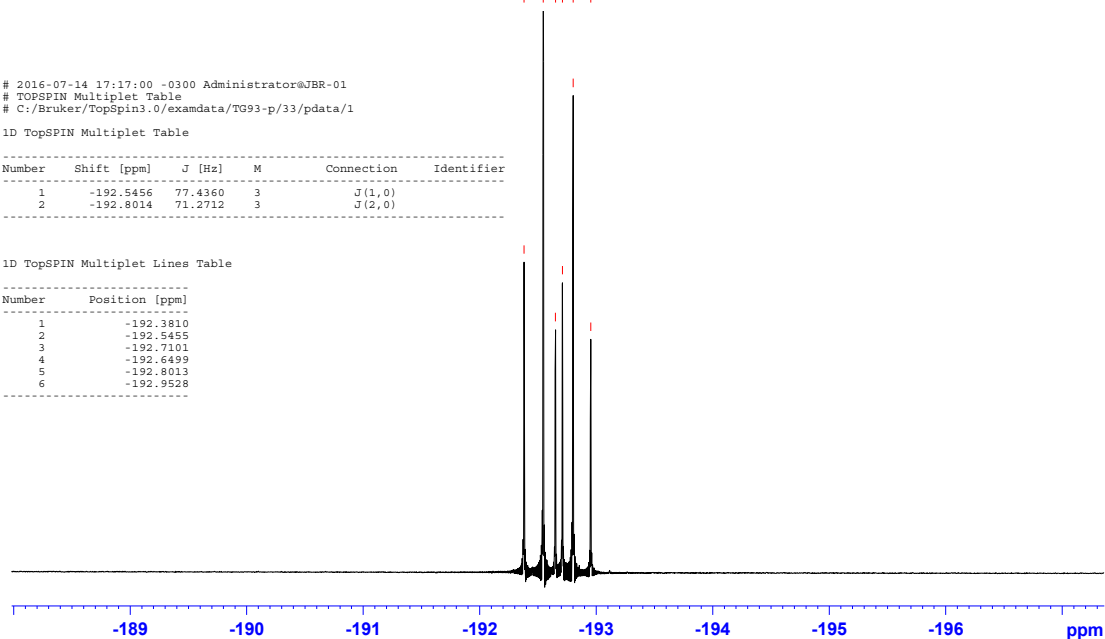
2016-07-14 17:17:00 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG93-p/33/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	-192.5456	77.4360	3	J(1,0)	
2	-192.8014	71.2712	3	J(2,0)	

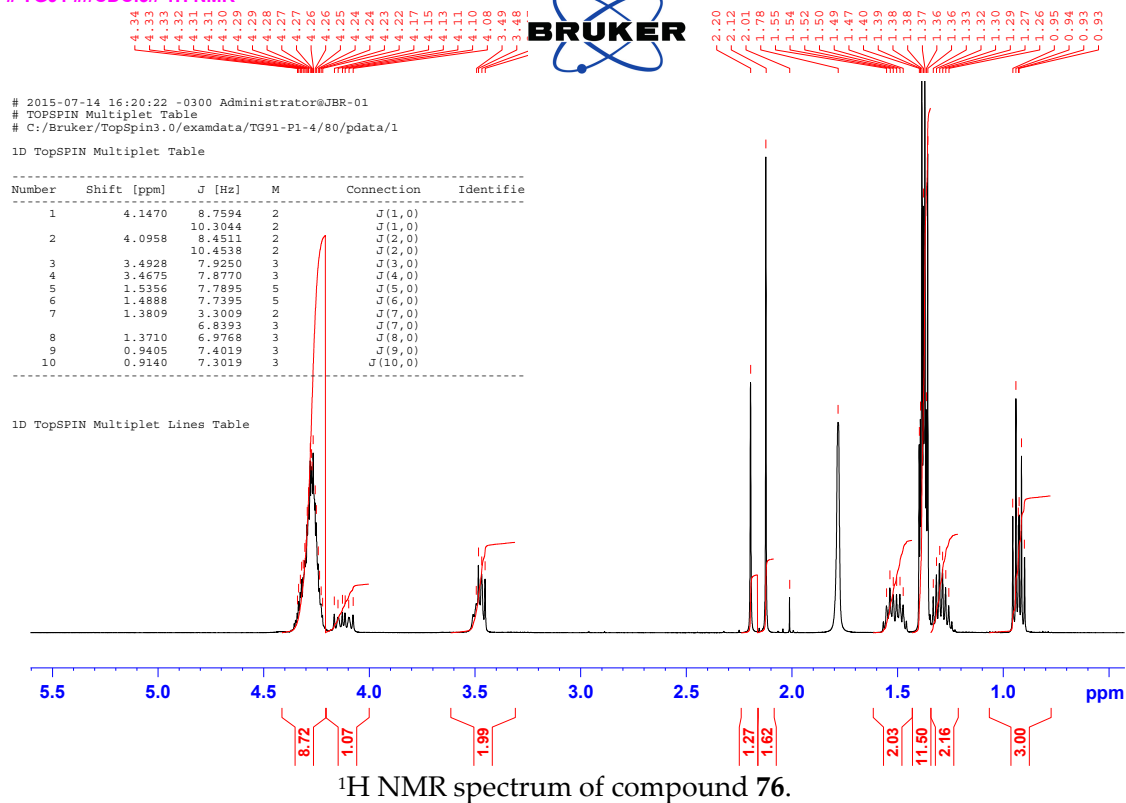
1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	-192.3810
2	-192.5455
3	-192.7101
4	-192.6499
5	-192.8013
6	-192.9528

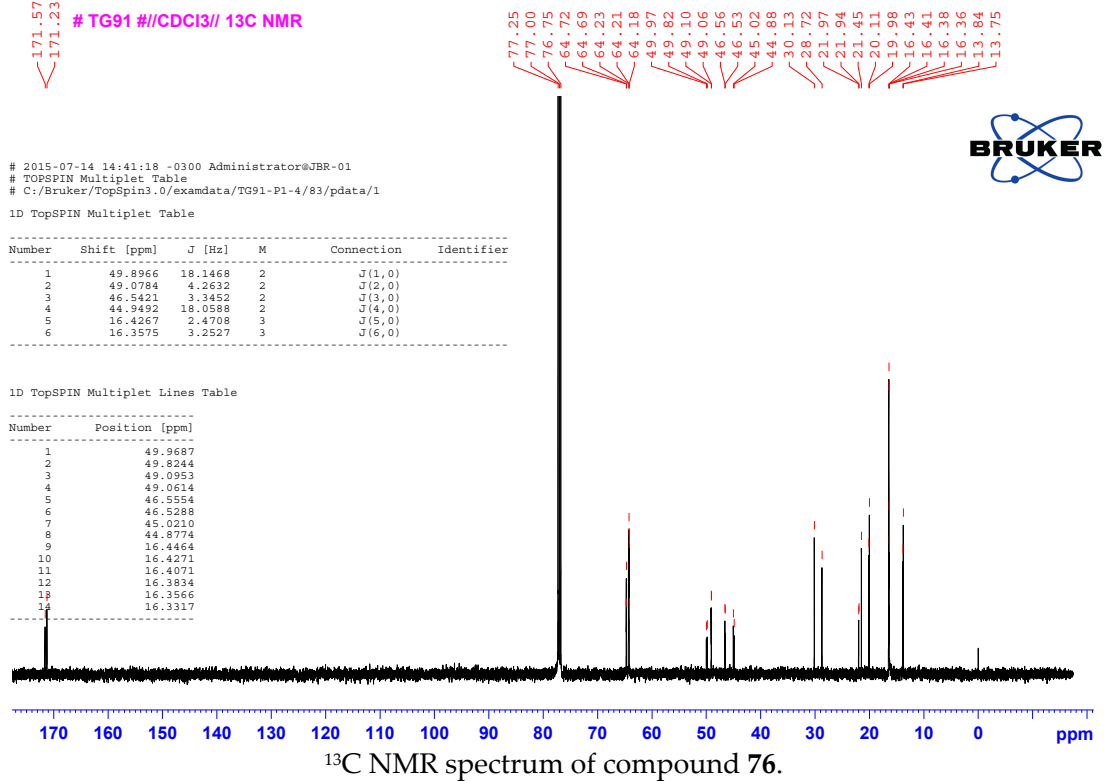


¹⁹F NMR spectrum of compound 75.

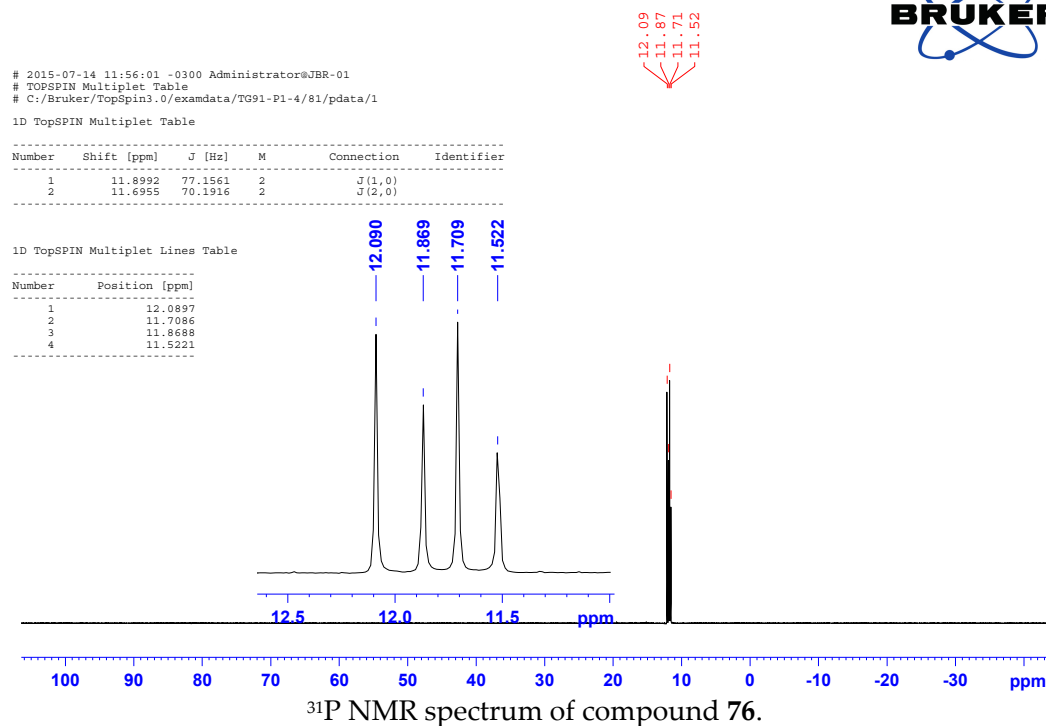
TG91 #//CDCI3// 1H NMR



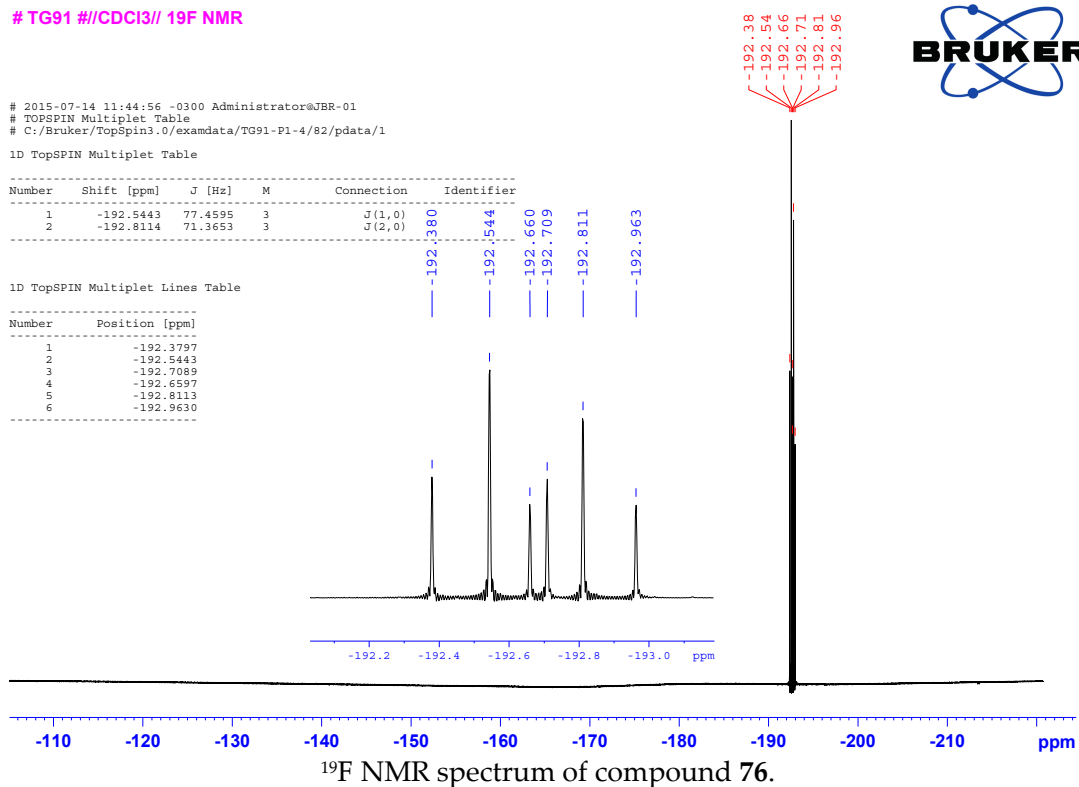
TG91 #//CDCI3// 13C NMR

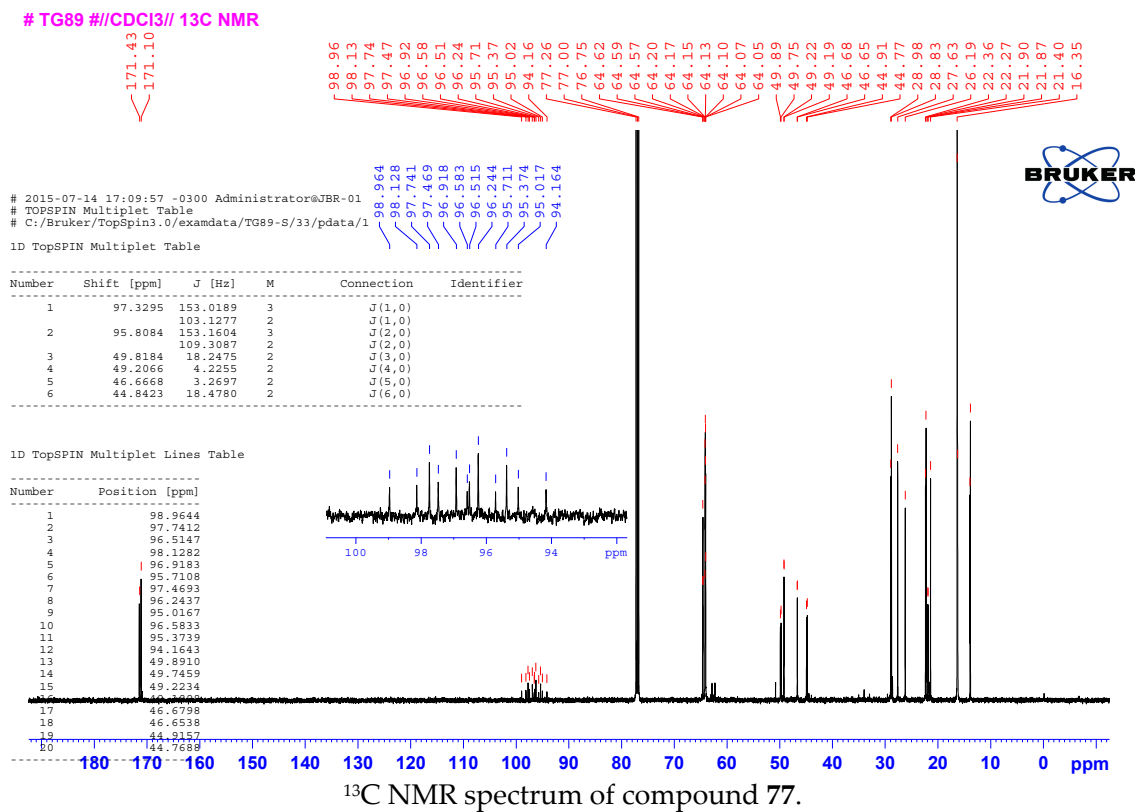
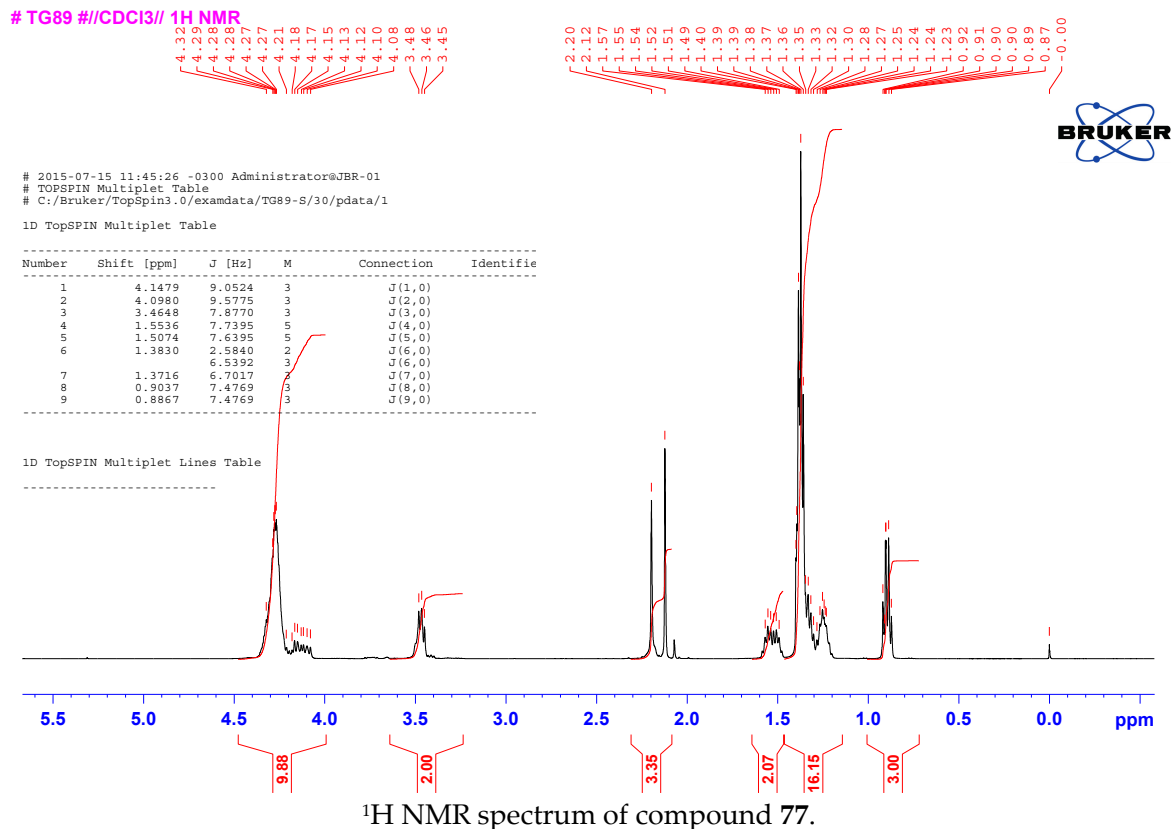


TG91 #/CDCl3// 31P NMR



TG91 #/CDCl3// 19F NMR





TG89 #//CDCI3// ³¹P NMR

12.06
11.84
11.68
11.49



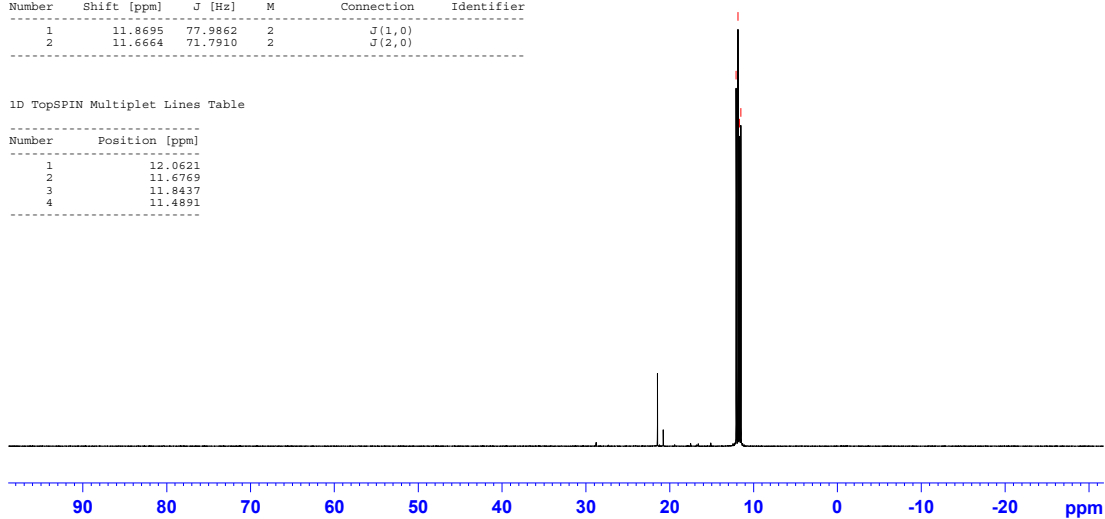
2015-07-14 16:54:42 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG89-S/31/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	11.8695	77.9862	2	J(1,0)	
2	11.6664	71.7910	2	J(2,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	12.0621
2	11.6769
3	11.8437
4	11.4891



³¹P NMR spectrum of compound 77.

TG89 #//CDCI3// ¹⁹F NMR

-192.40
-192.56
-192.68
-192.73
-192.83
-192.98



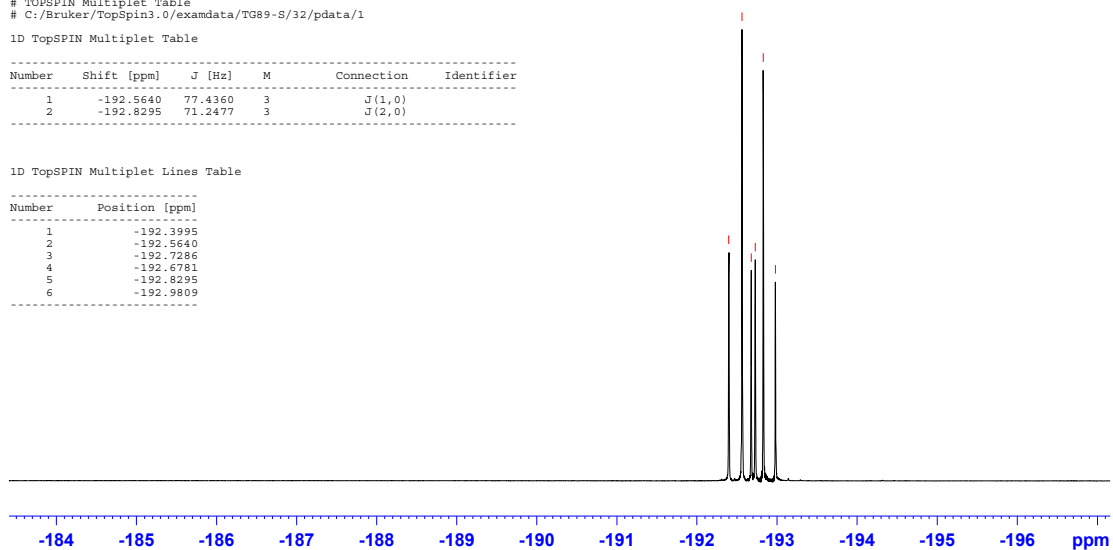
2015-07-14 16:45:19 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
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1D TopSPIN Multiplet Table

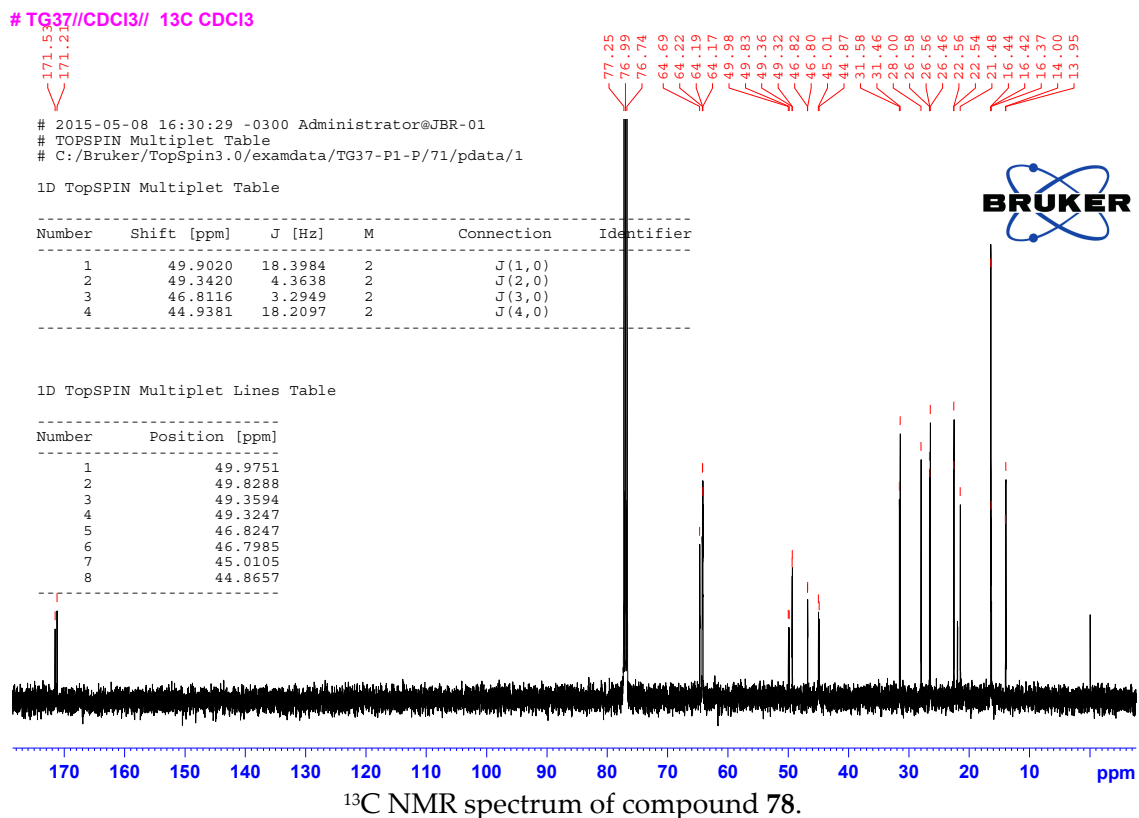
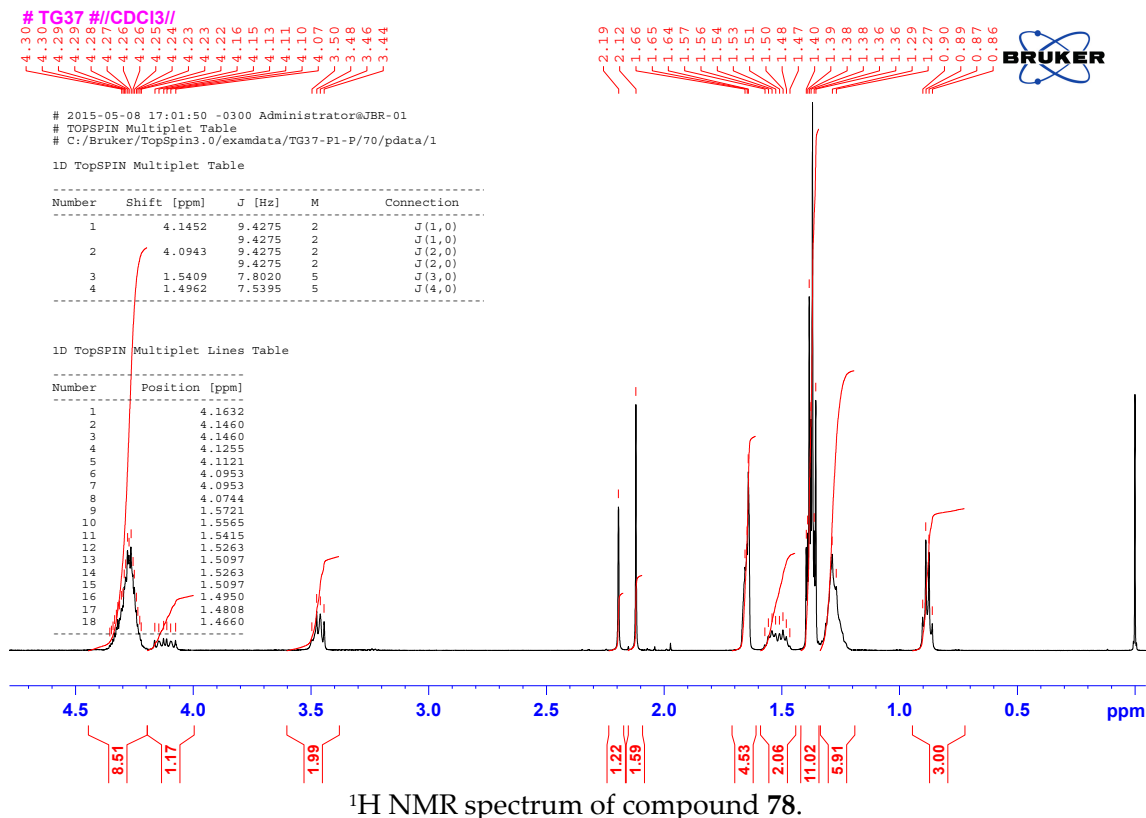
Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	-192.5640	77.4360	3	J(1,0)	
2	-192.8295	71.2477	3	J(2,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	-192.3995
2	-192.5640
3	-192.7286
4	-192.6781
5	-192.8295
6	-192.9809



¹⁹F NMR spectrum of compound 77.



TG37 #/CDCl3// 31P NMR

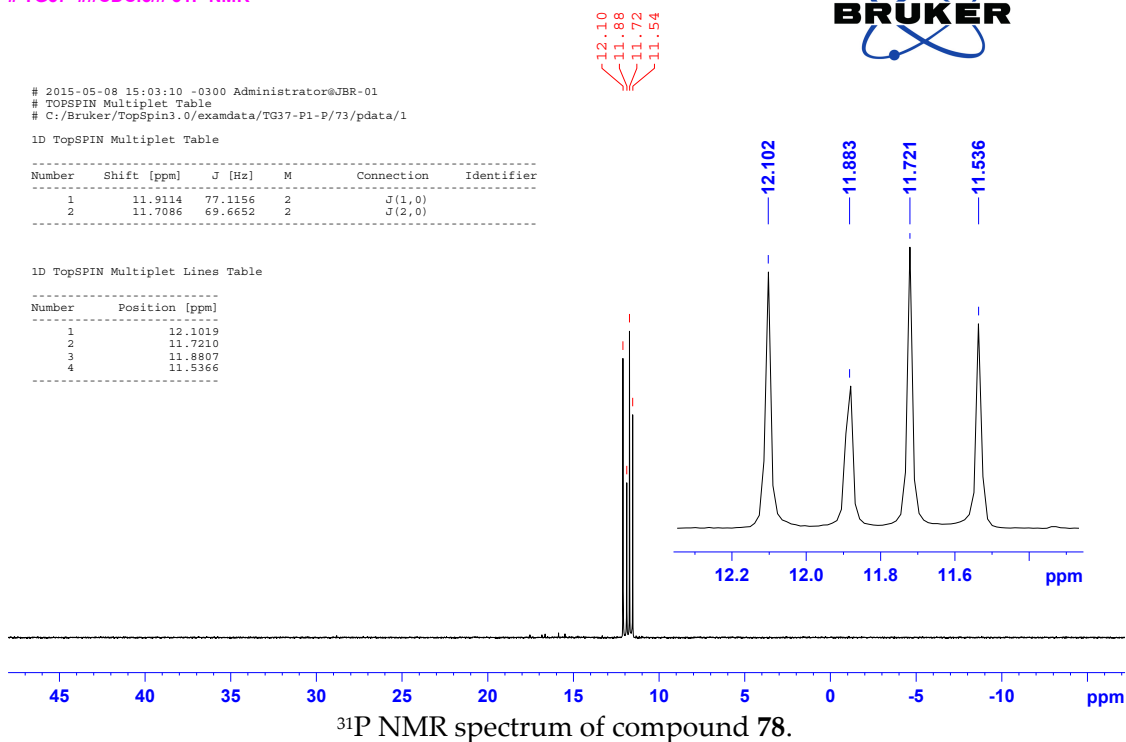
2015-05-08 15:03:10 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG37-P1-P/73/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	11.9114	77.1156	2	J(1,0)	
2	11.7086	69.6652	2	J(2,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	12.1019
2	11.7210
3	11.8807
4	11.5366



TG37 #/CDCl3// 19F NMR

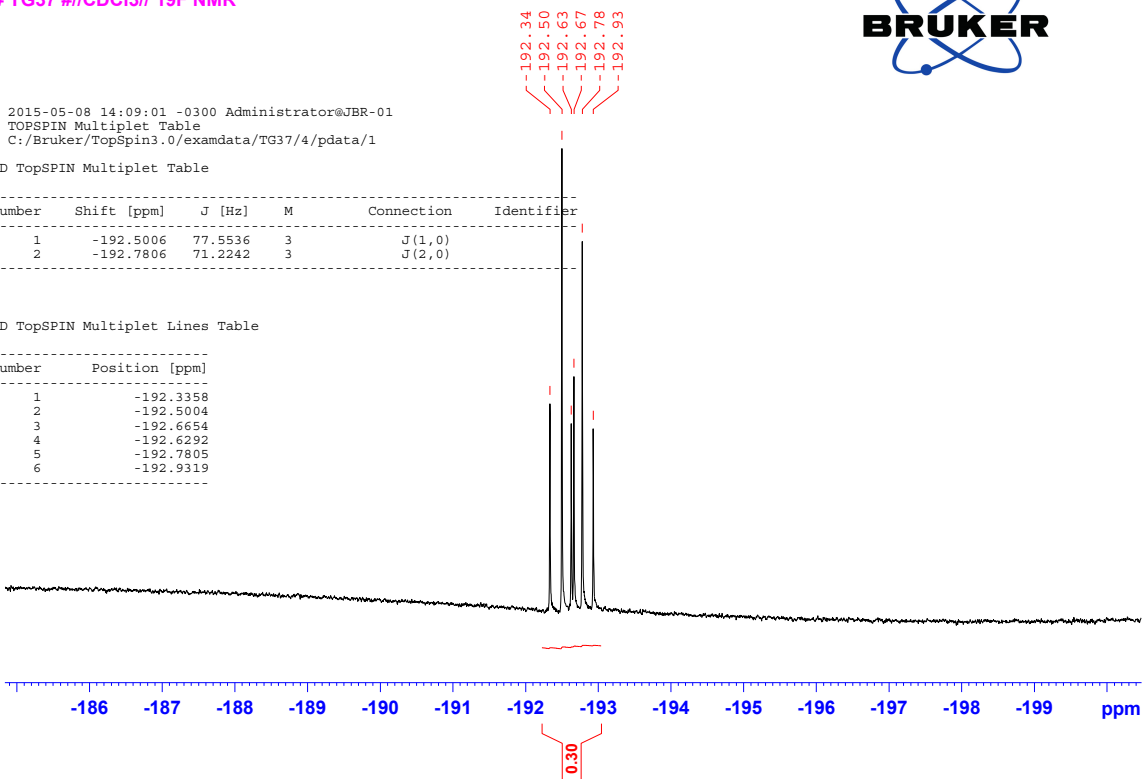
2015-05-08 14:09:01 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG37/4/pdata/1

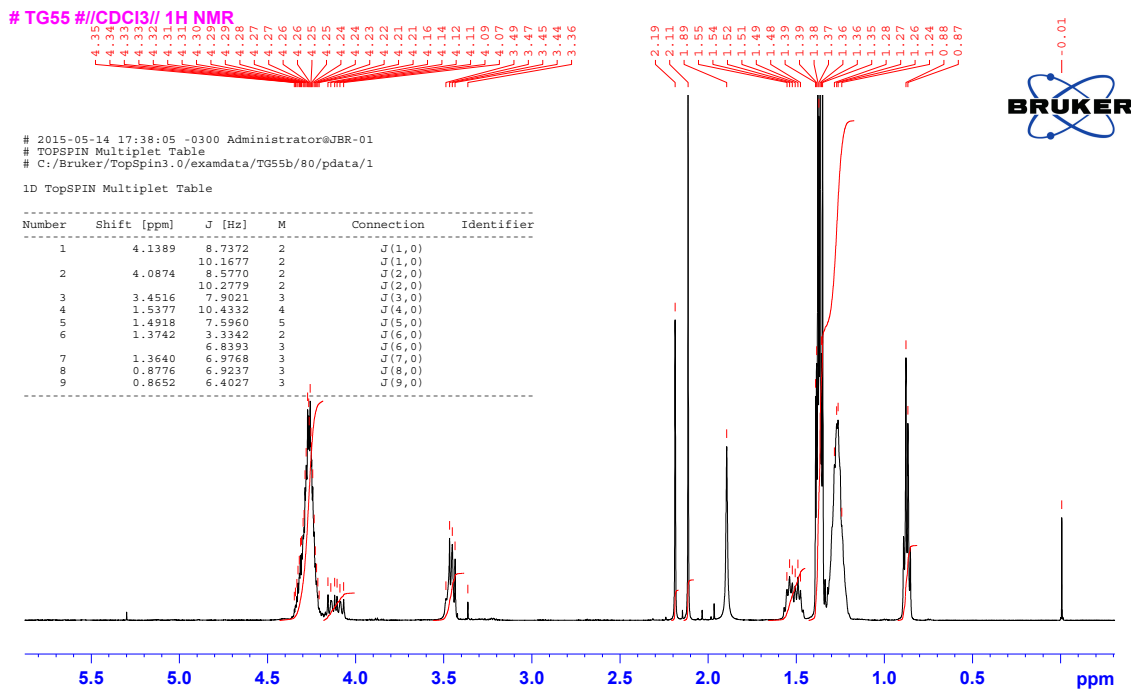
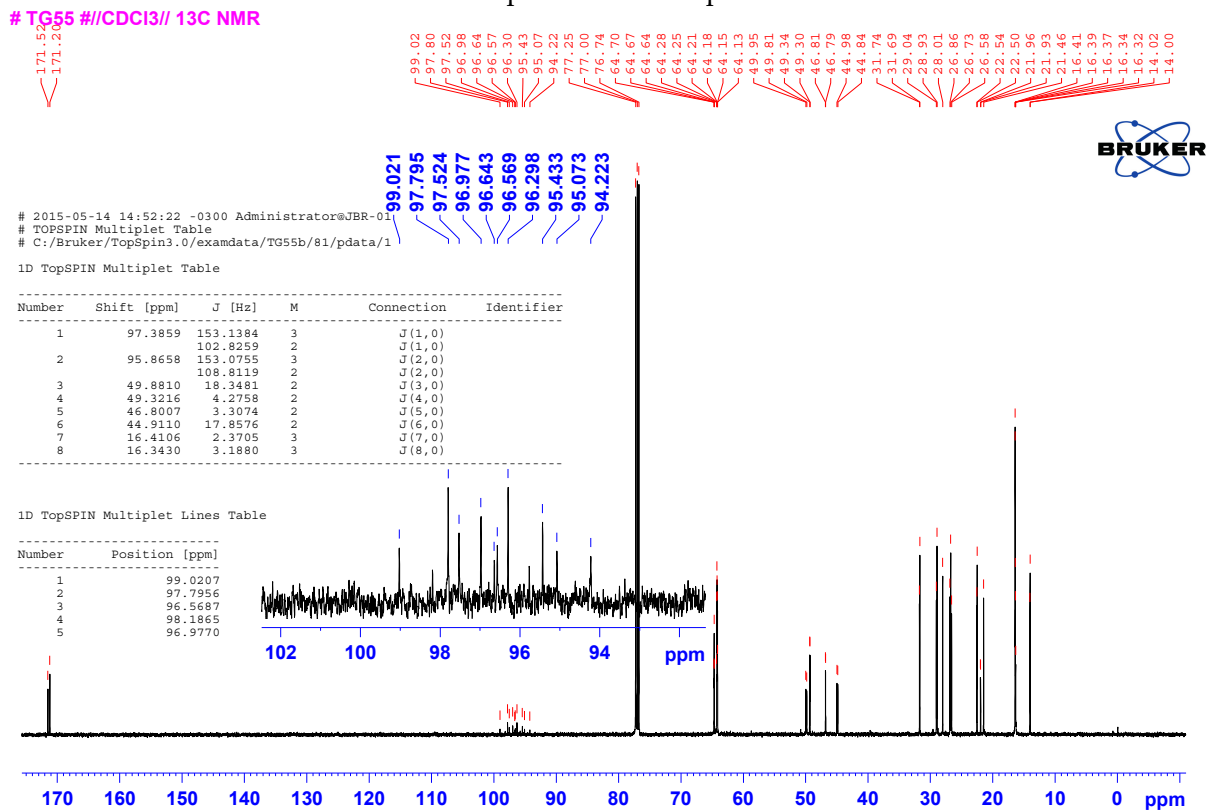
1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	-192.5006	77.5536	3	J(1,0)	
2	-192.7806	71.2242	3	J(2,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	-192.3358
2	-192.5004
3	-192.6654
4	-192.6292
5	-192.7805
6	-192.9319



¹H NMR spectrum of compound 79.¹³C NMR spectrum of compound 79.

TG55 #/CDCl3// 31P NMR

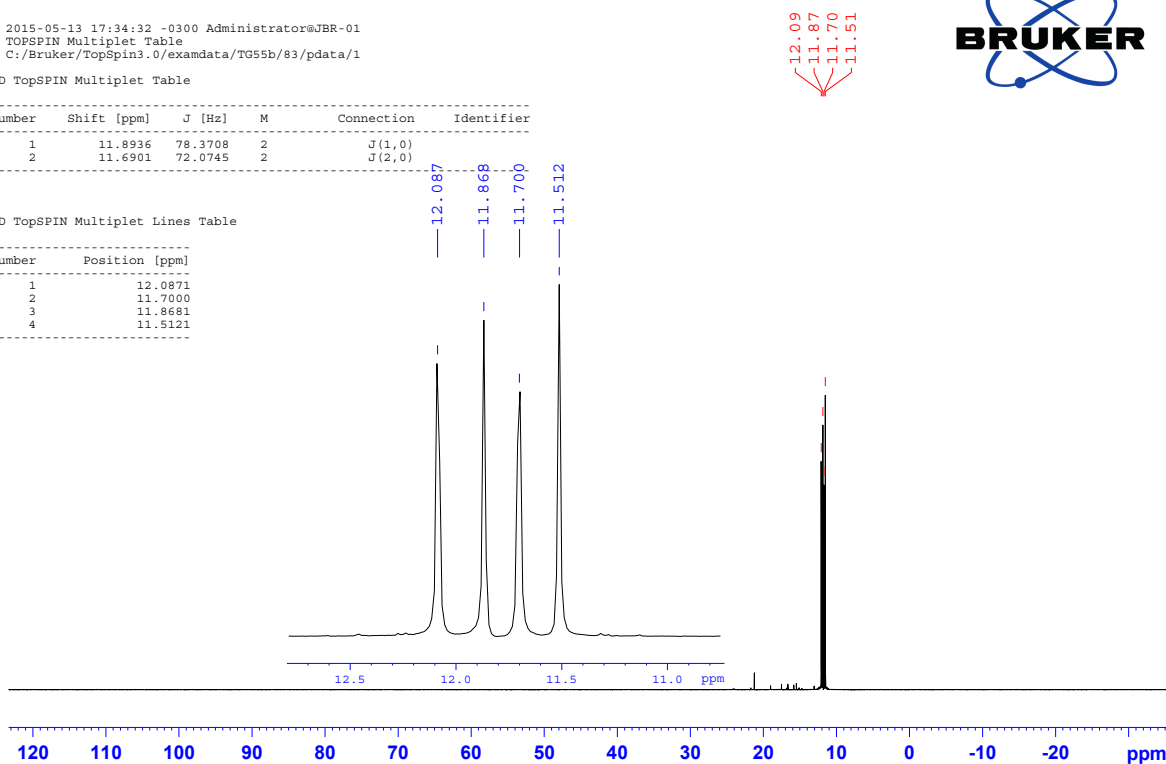
2015-05-13 17:34:32 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG55b/83/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	11.8936	78.3708	2	J(1,0)	
2	11.6901	72.0745	2	J(2,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	12.0871
2	11.7000
3	11.8681
4	11.5121



31P NMR spectrum of compound 79.

TG55 #/CDCl3// 19F NMR

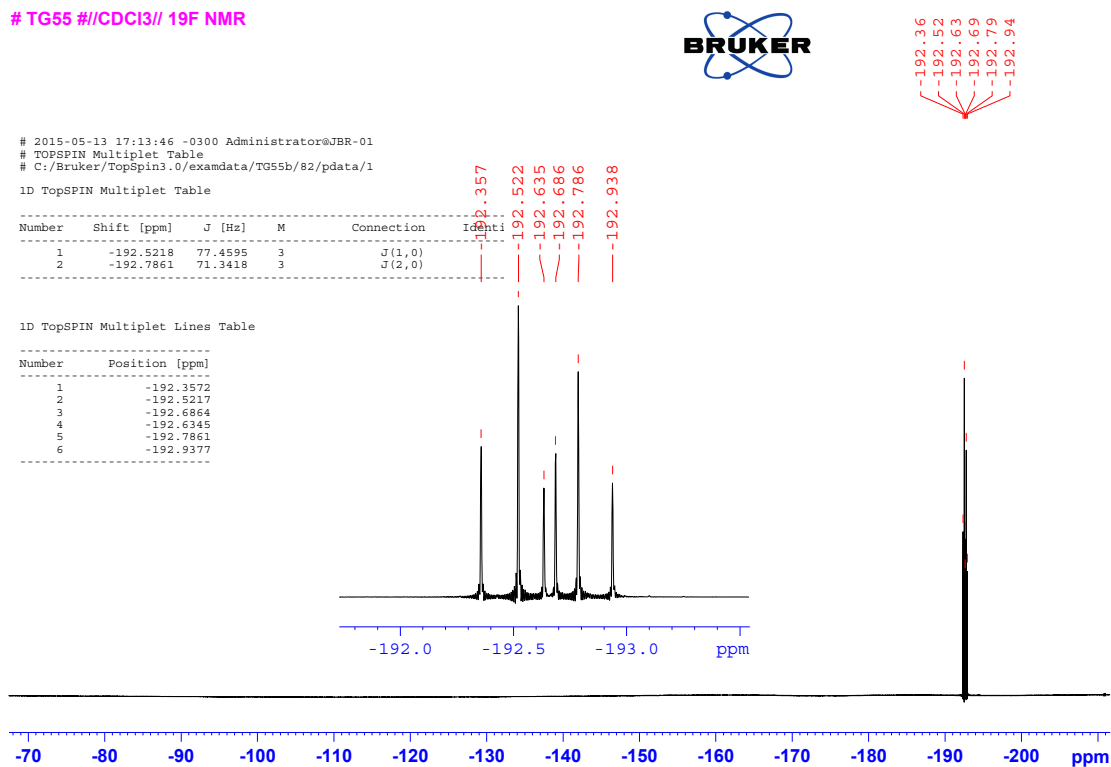
2015-05-13 17:13:46 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG55b/82/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	-192.5218	77.4595	3	J(1,0)	
2	-192.7861	71.3418	3	J(2,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	-192.3572
2	-192.5217
3	-192.6864
4	-192.6345
5	-192.7861
6	-192.9377



19F NMR spectrum of compound 79.

TG71-#//CDCl3// 31P NMR

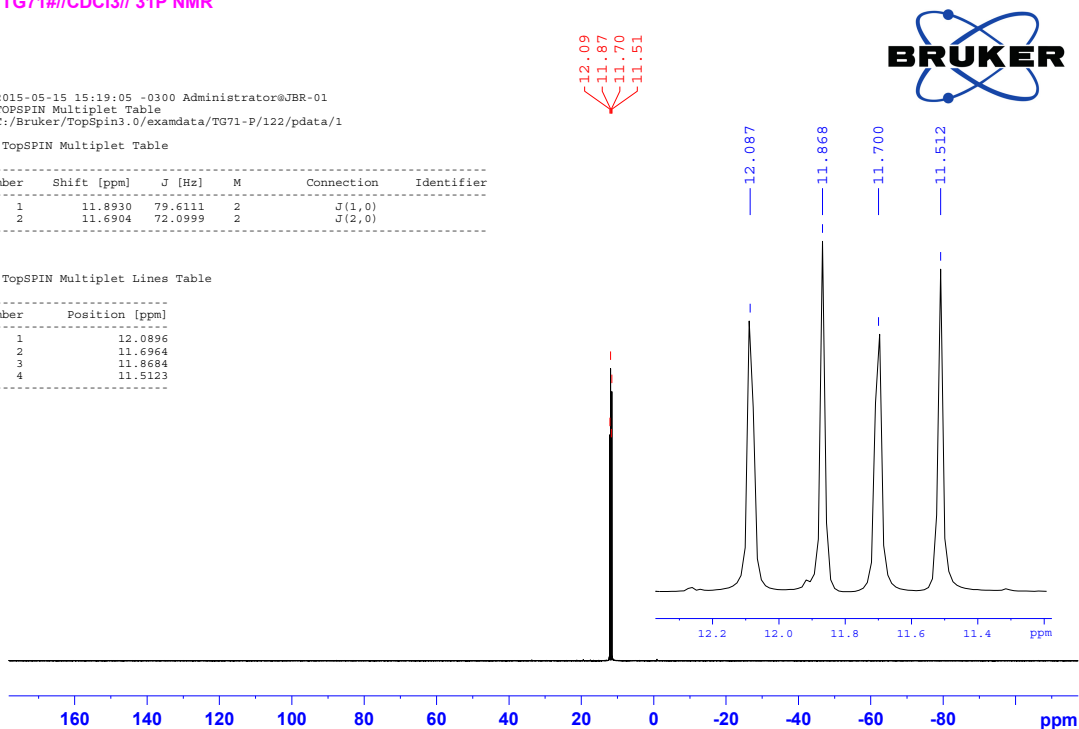
2015-05-15 15:19:05 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG71-P/122/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	11.8930	79.6111	2	J(1,0)	
2	11.6904	72.0999	2	J(2,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	12.0896
2	11.6964
3	11.8684
4	11.5123



31P NMR spectrum of compound 80.

TG71-P #//CDCl3// 19F NMR

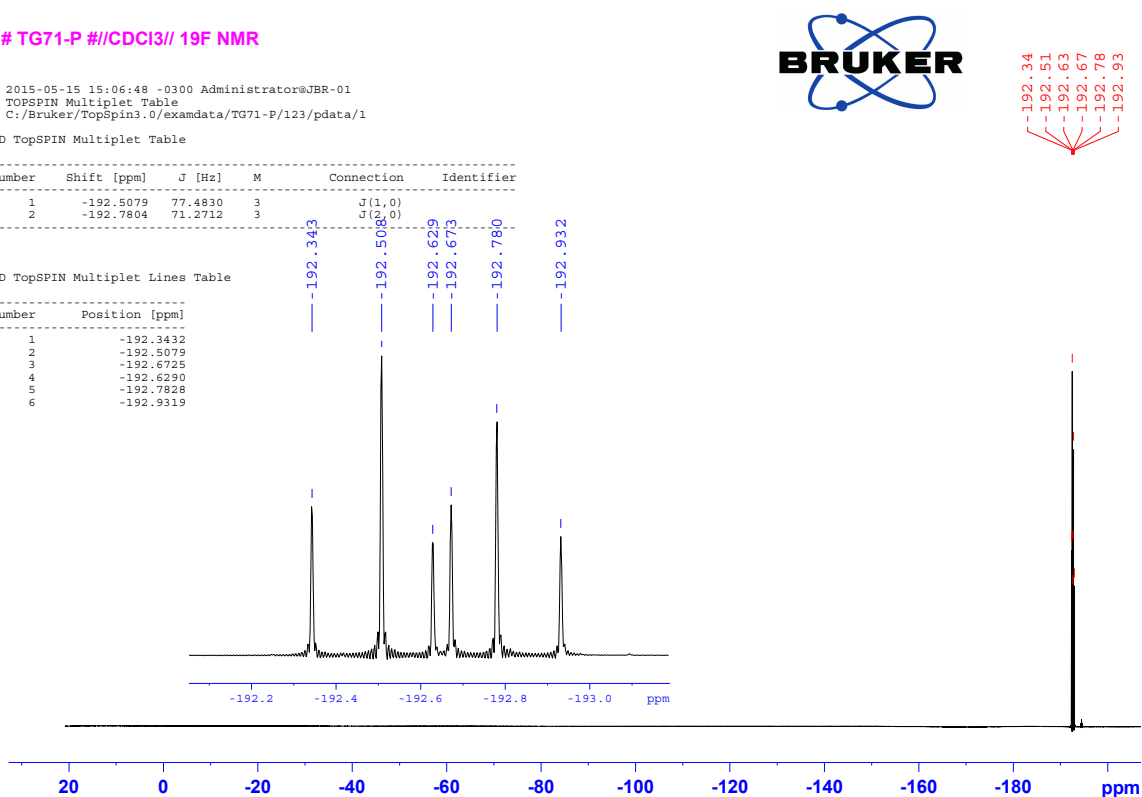
2015-05-15 15:06:48 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG71-P/123/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	-192.5079	77.4830	3	J(1,0)	
2	-192.7804	71.2712	3	J(2,0)	

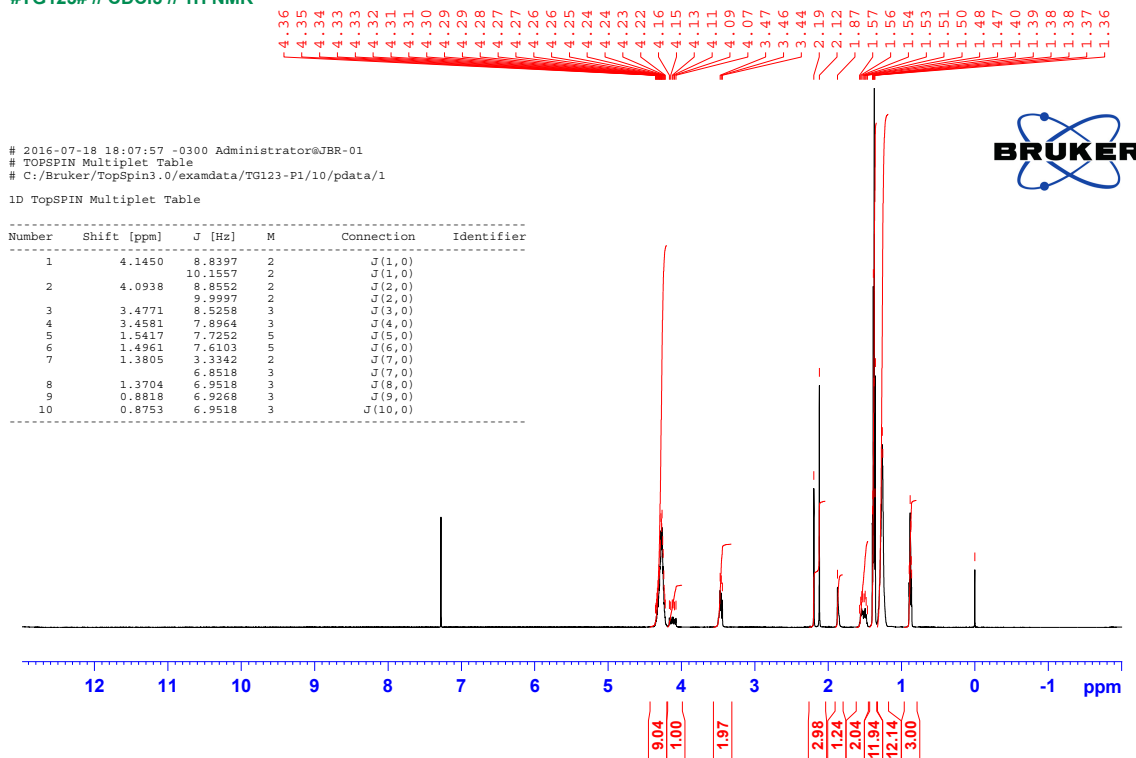
1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	-192.3432
2	-192.5079
3	-192.6725
4	-192.6290
5	-192.7828
6	-192.9319

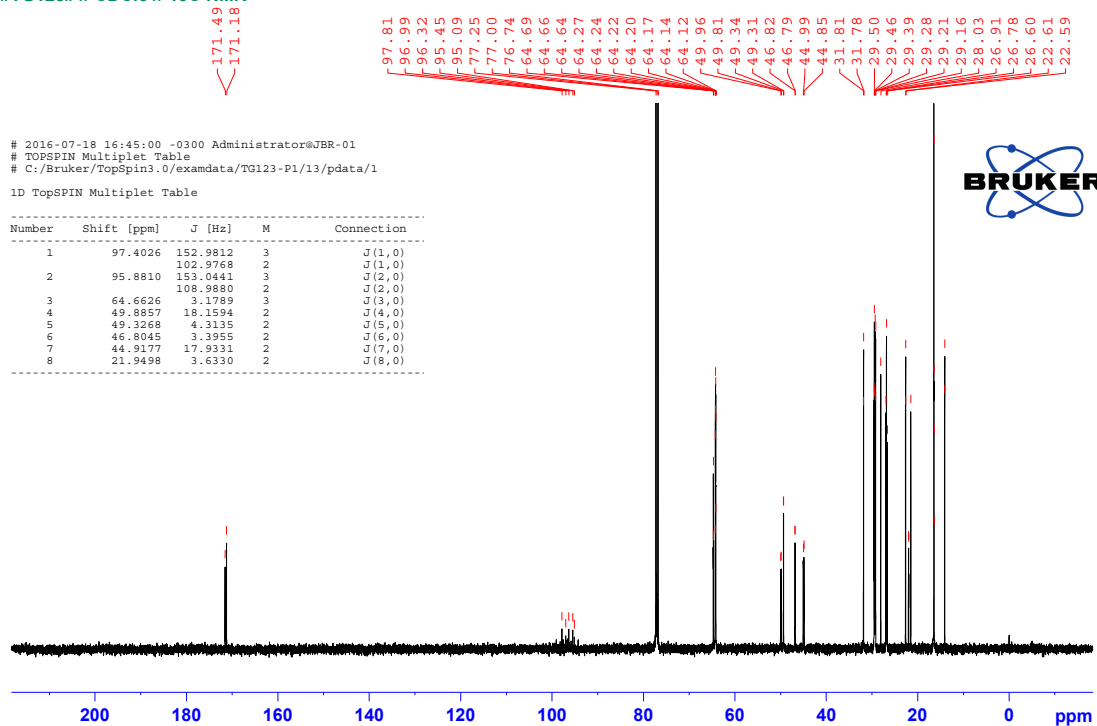


19F NMR spectrum of compound 80.

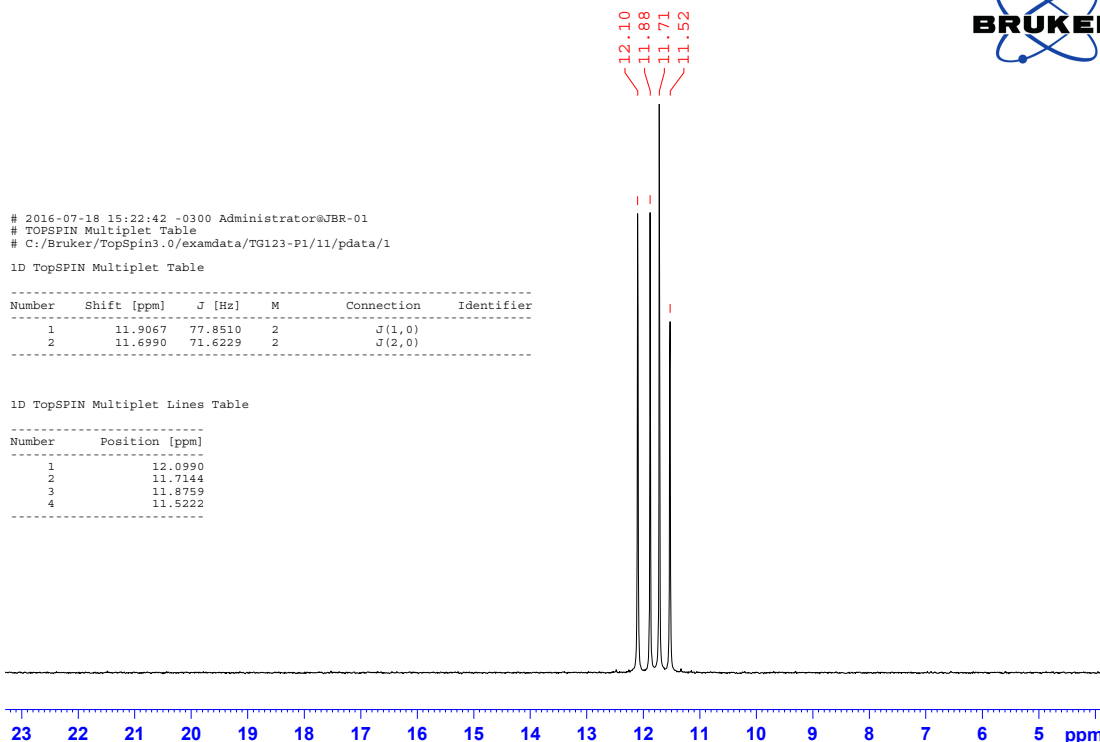
#TG123# // CDCI3 // 1H NMR

¹H NMR spectrum of compound 81.

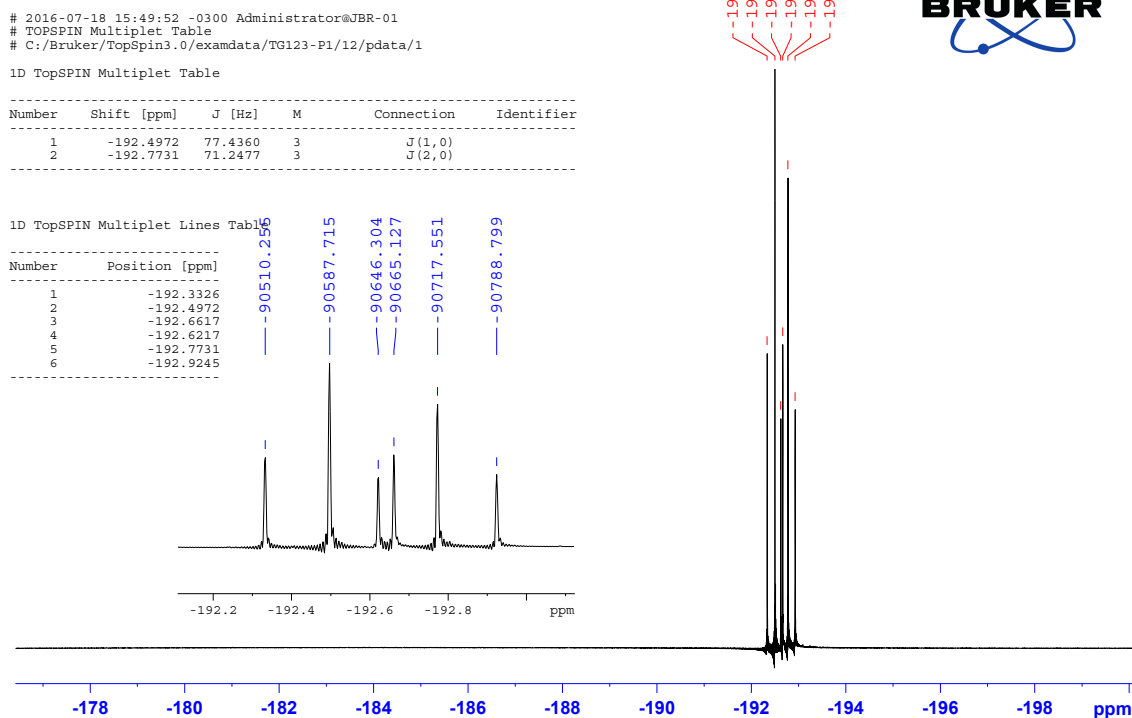
#TG123# // CDCI3 // 13C NMR

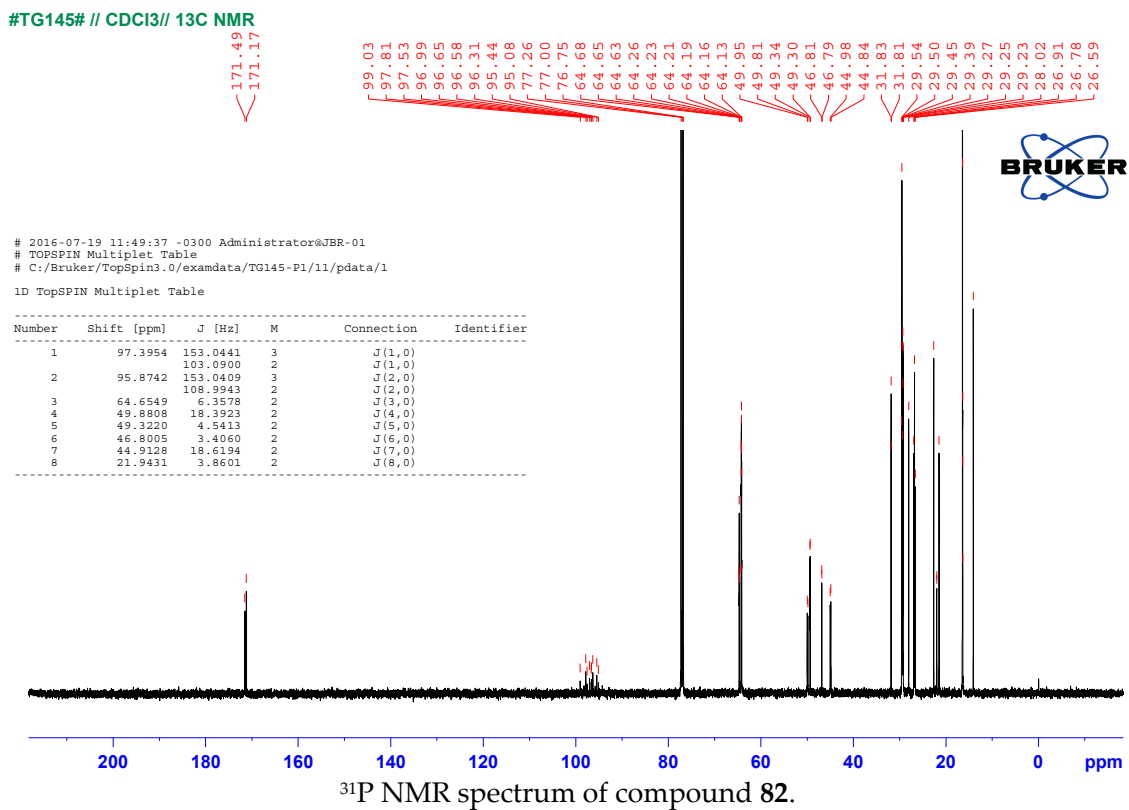
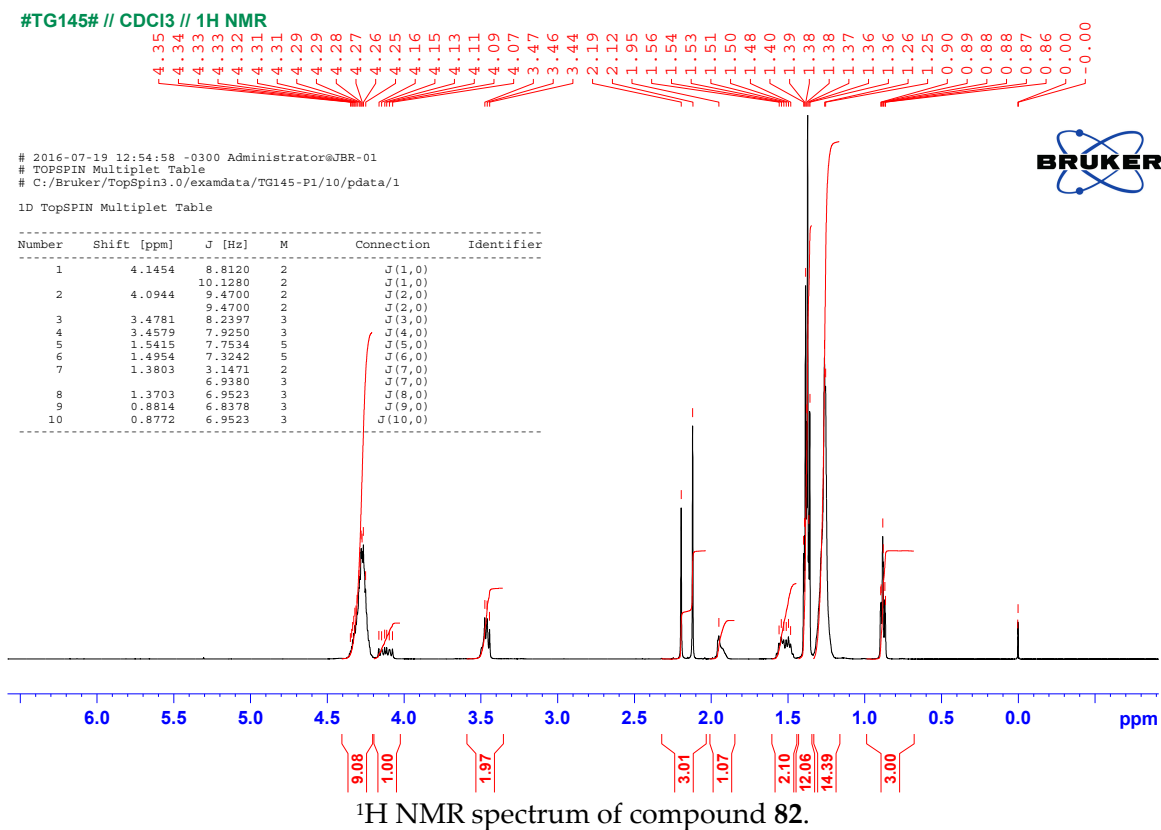
¹³C NMR spectrum of compound 81.

TG123 # //CDCl3 // 31P NMR

³¹P NMR spectrum of compound 81.

#TG123# // CDCI3 // 19F NMR

¹⁹F NMR spectrum of compound 81.



#TG145# // CDCl3 // 31P NMR

2016-07-19 11:35:23 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
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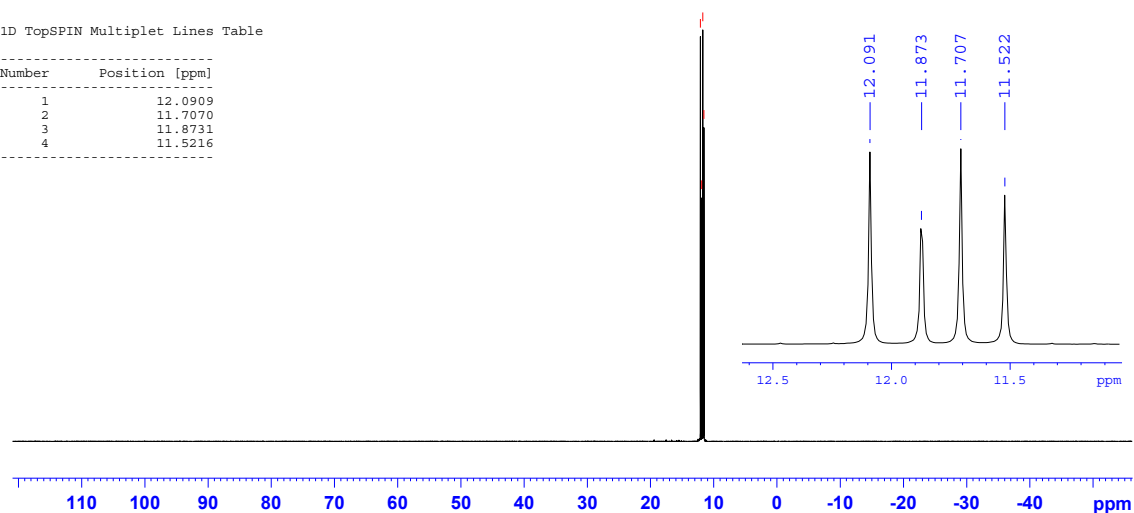
1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Ident
1	11.8990	77.7230	2	J(1,0)	
2	11.6974	71.1634	2	J(2,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	12.0909
2	11.7070
3	11.8731
4	11.5216

12.09
11.87
11.71
11.52

³¹P NMR spectrum of compound 82.

#TG145# // CDCl3 // 19F NMR

2016-07-19 11:02:54 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
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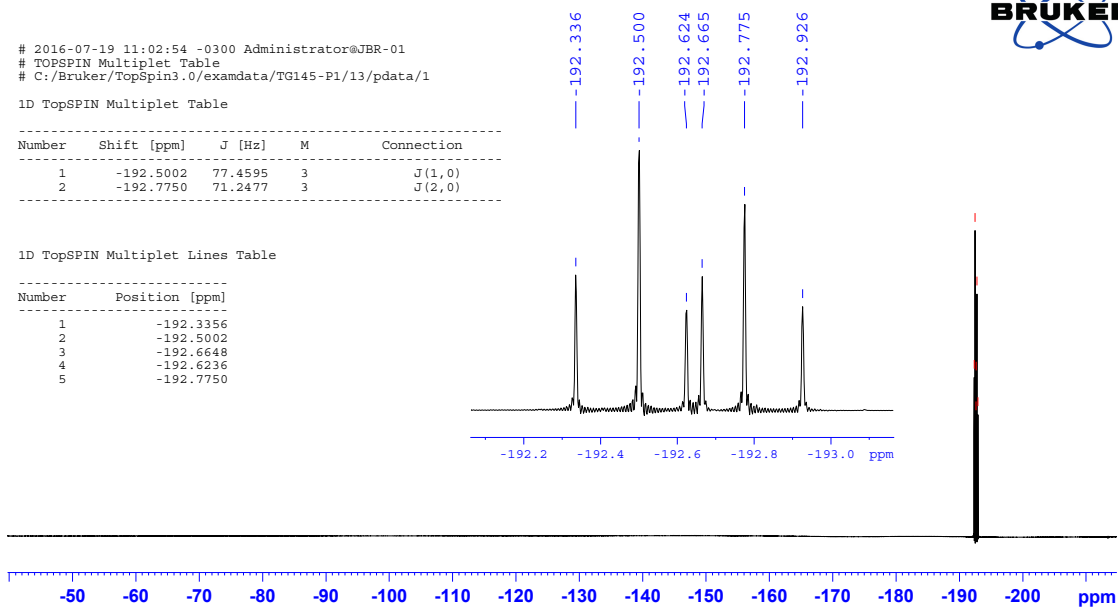
1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection
1	-192.5002	77.4595	3	J(1,0)
2	-192.7750	71.2477	3	J(2,0)

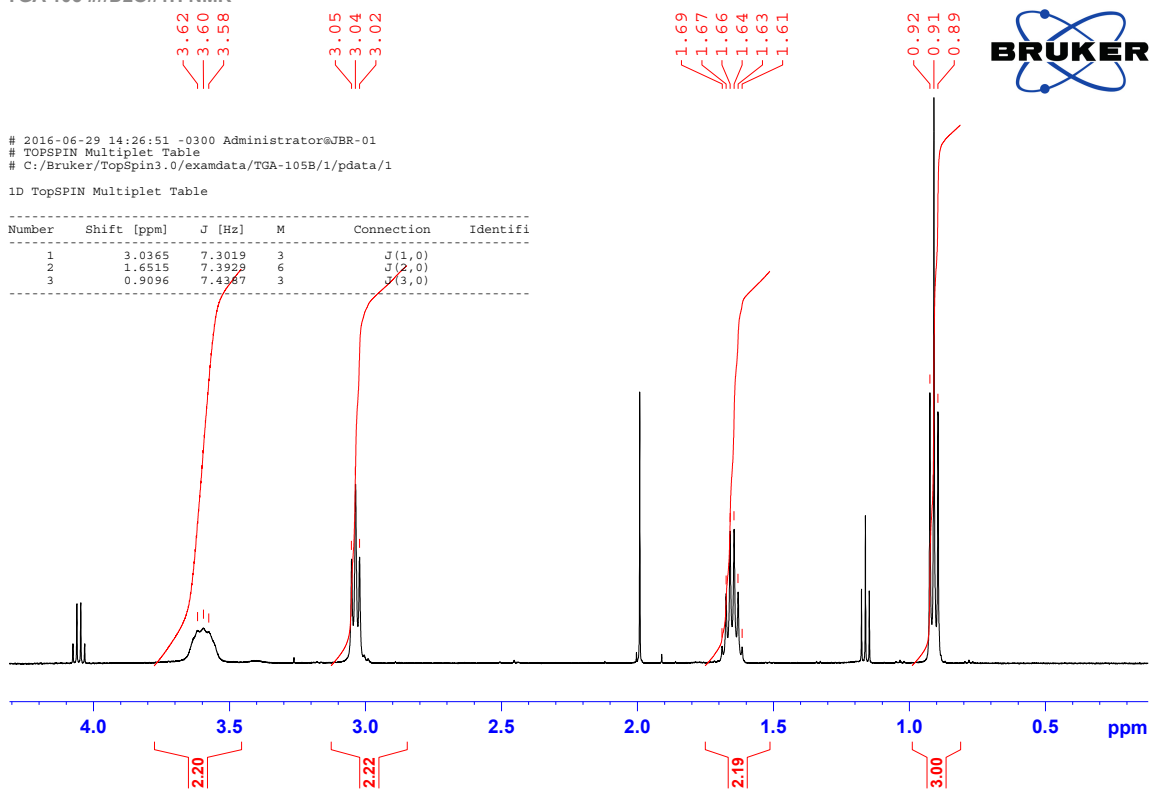
1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	-192.3356
2	-192.5002
3	-192.6648
4	-192.6236
5	-192.7750

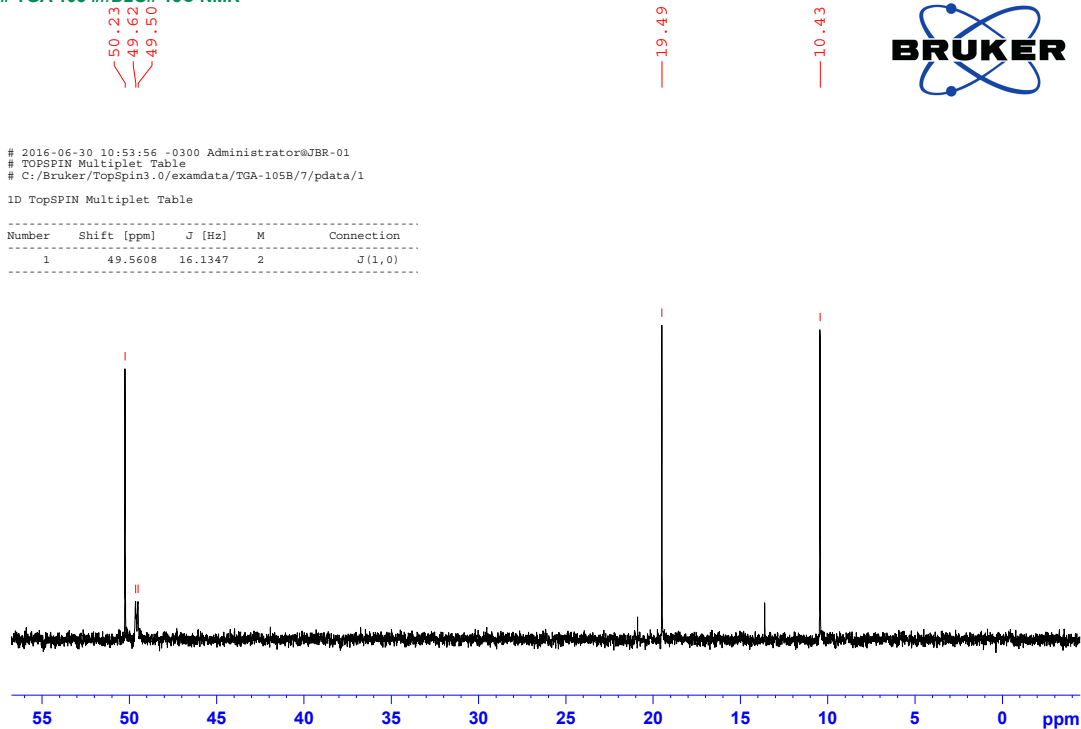
-192.34
-192.50
-192.62
-192.66
-192.78
-192.93

¹⁹F NMR spectrum of compound 82.

TGA 105 #/D2O//1H NMR

¹H NMR spectrum of compound 54.

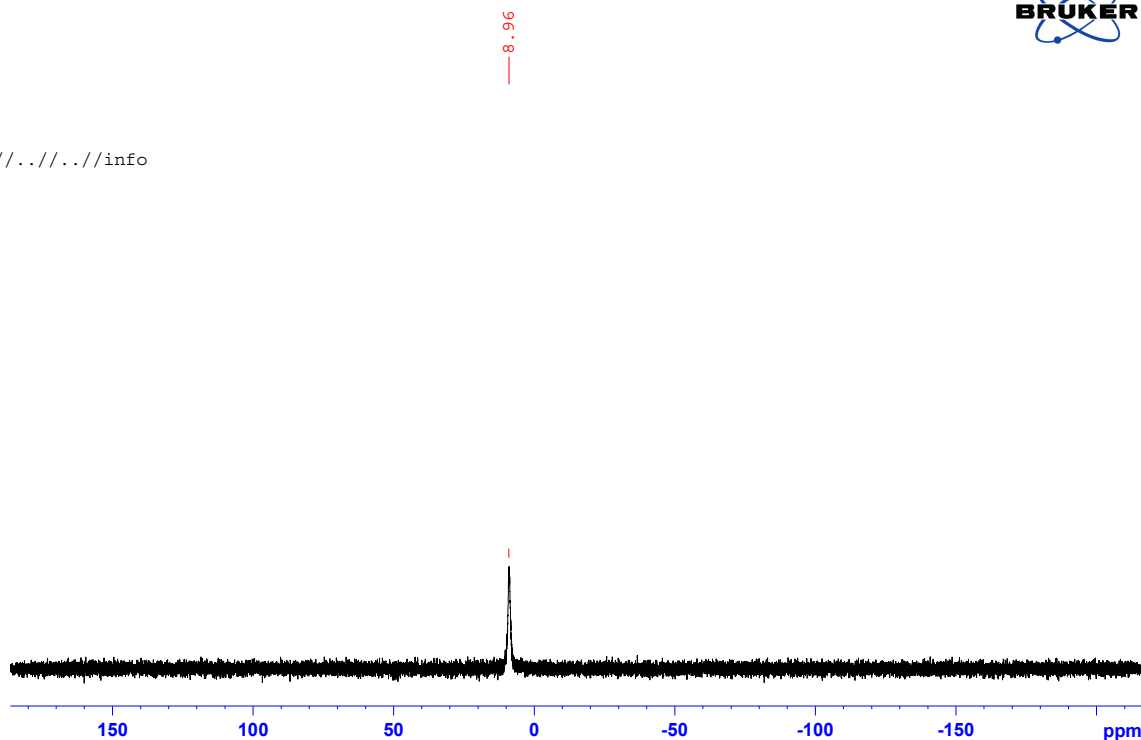
TGA 105 #/D2O// 13C NMR

¹³C NMR spectrum of compound 54.

TGA 105 #/ /D2O// 31P NMR



+//.//.//.//info



³¹P NMR spectrum of compound 54.

#TG105# // CDCI3 // 19F NMR

-193.18
-193.32
-193.46

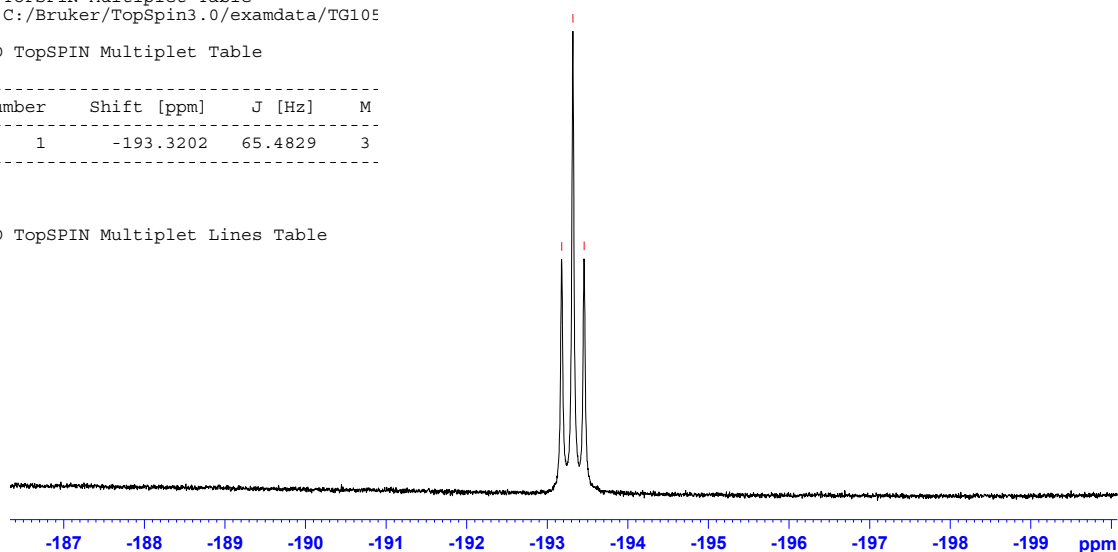


2016-07-19 14:24:23 -0300 Administr
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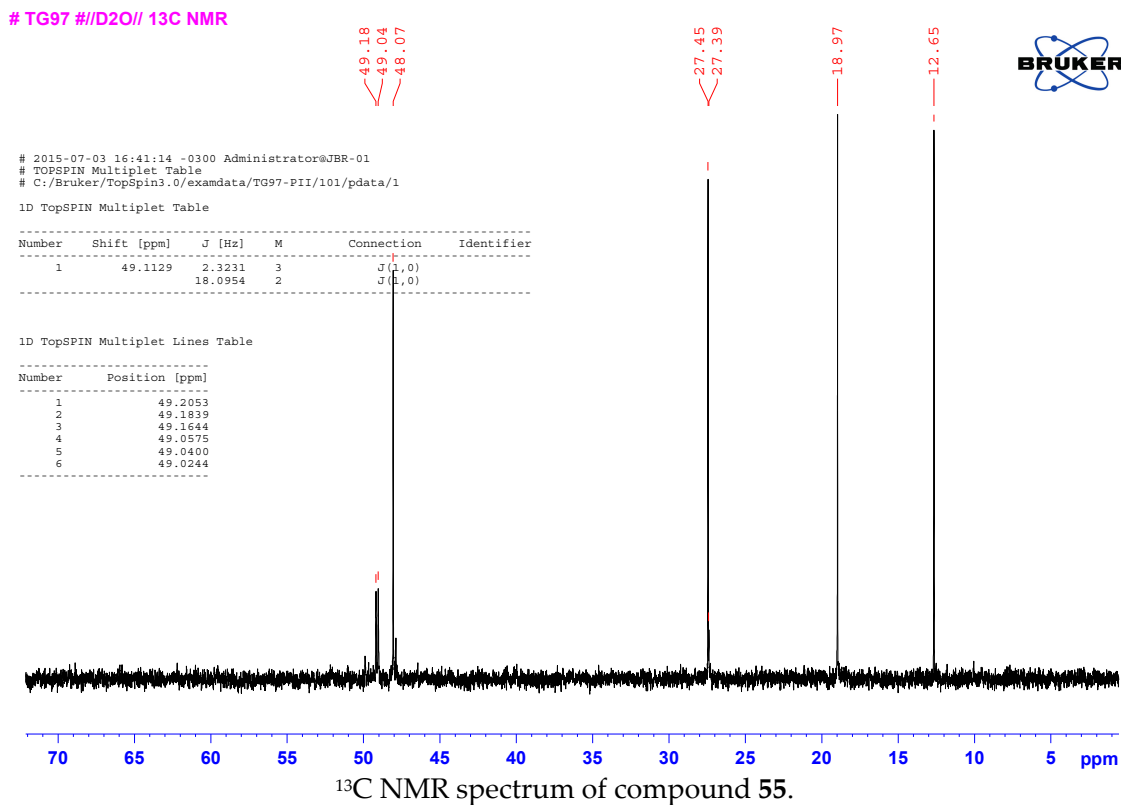
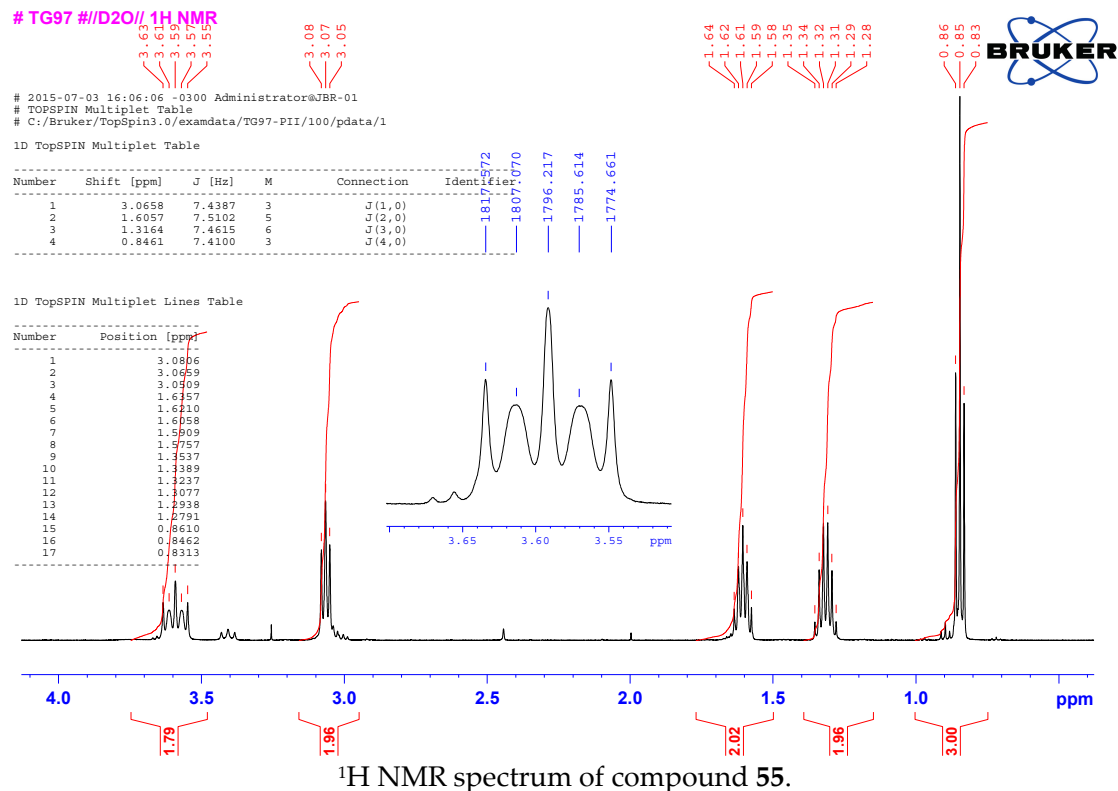
1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M
1	-193.3202	65.4829	3

1D TopSPIN Multiplet Lines Table



¹⁹F NMR spectrum of compound 54.



TG97 #//D2O// 31P NMR

9.01
8.68

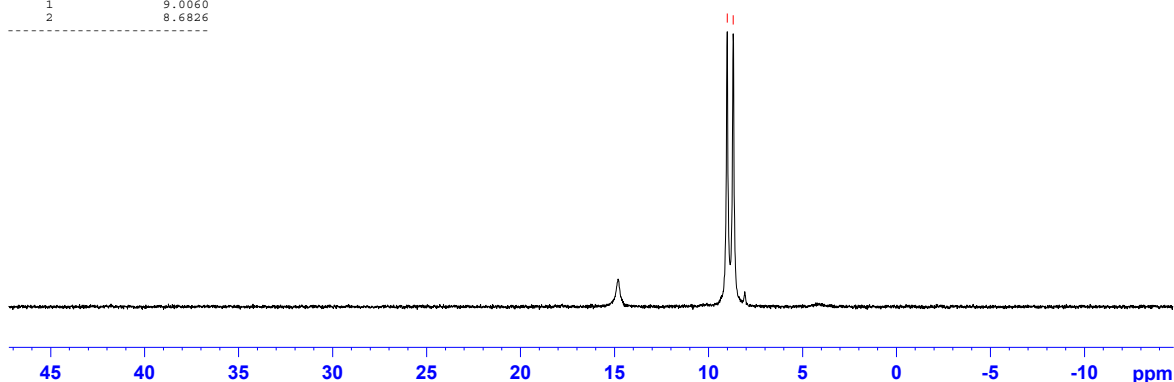
2015-07-03 16:48:52 -0300 Administrator@JBR-01
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1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	8.8443	65.4744	2	J(1,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	9.0060
2	8.6826

³¹P NMR spectrum of compound 55.

TG97 #//D2O// 19F NMR

-193.25
-193.39
-193.53

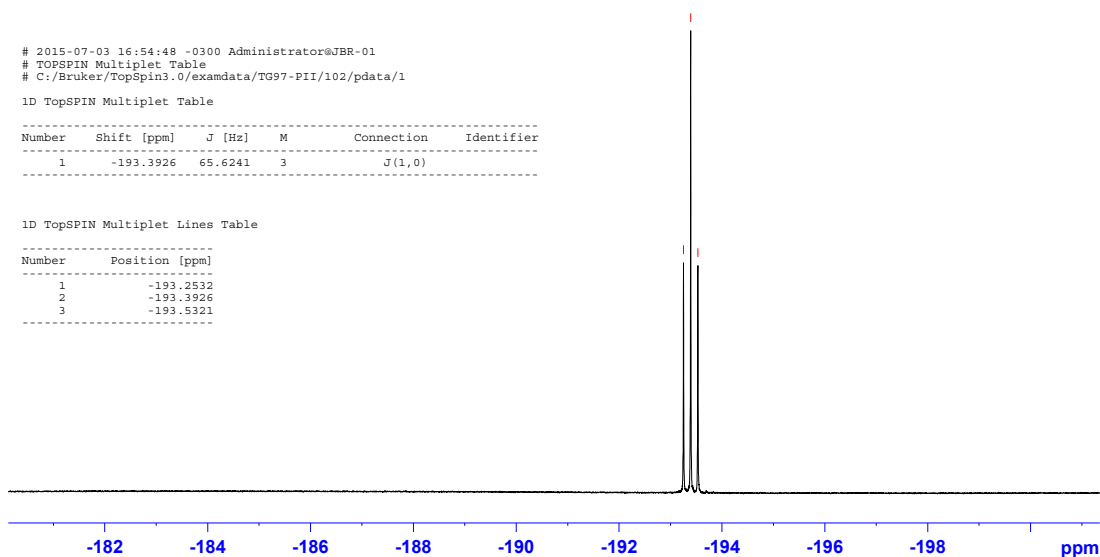
2015-07-03 16:54:48 -0300 Administrator@JBR-01
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1D TopSPIN Multiplet Table

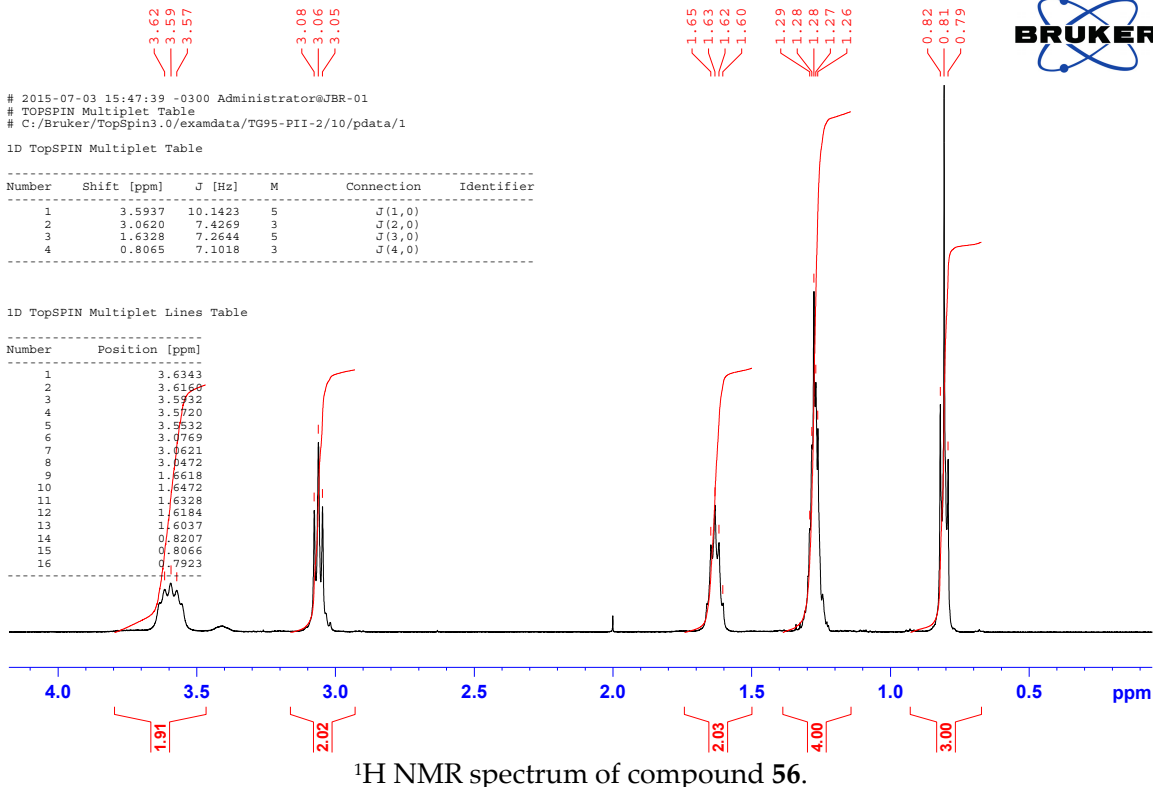
Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	-193.3926	65.6241	3	J(1,0)	

1D TopSPIN Multiplet Lines Table

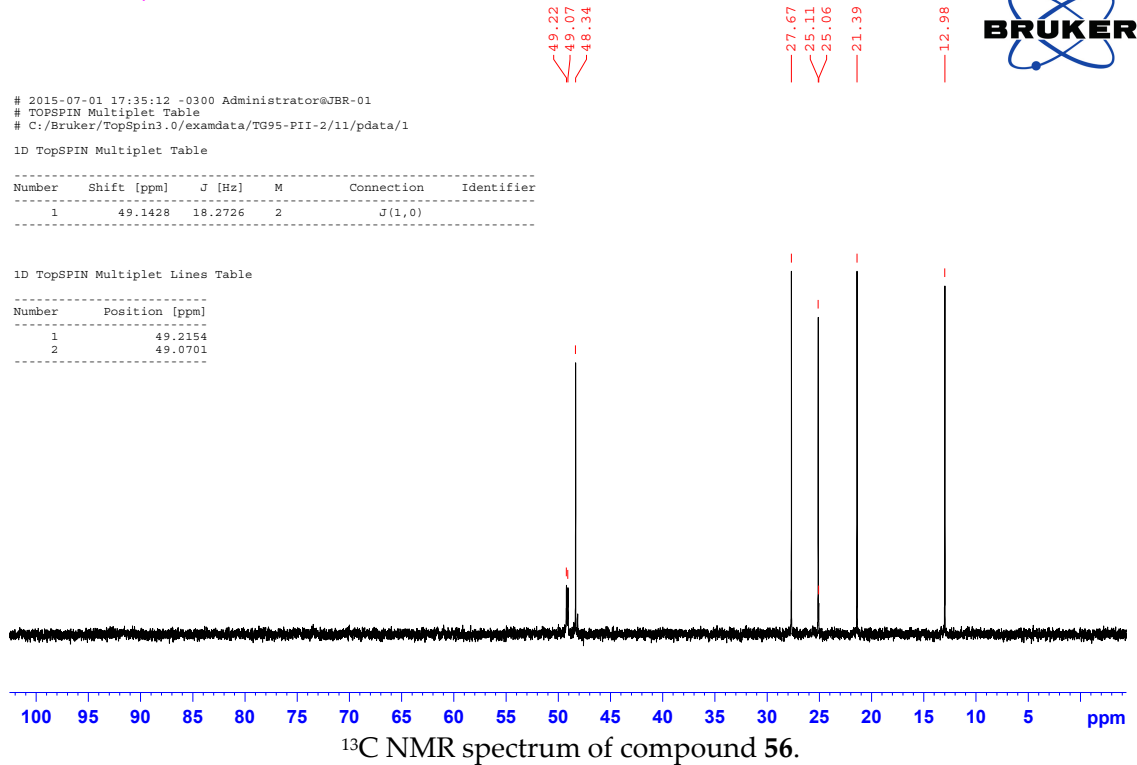
Number	Position [ppm]
1	-193.2532
2	-193.3926
3	-193.5321

¹⁹F NMR spectrum of compound 55.

TG95 #/D2O// 1H NMR



TG95#/D2O//13C NMR



TG95 #//D2O// 31P NMR



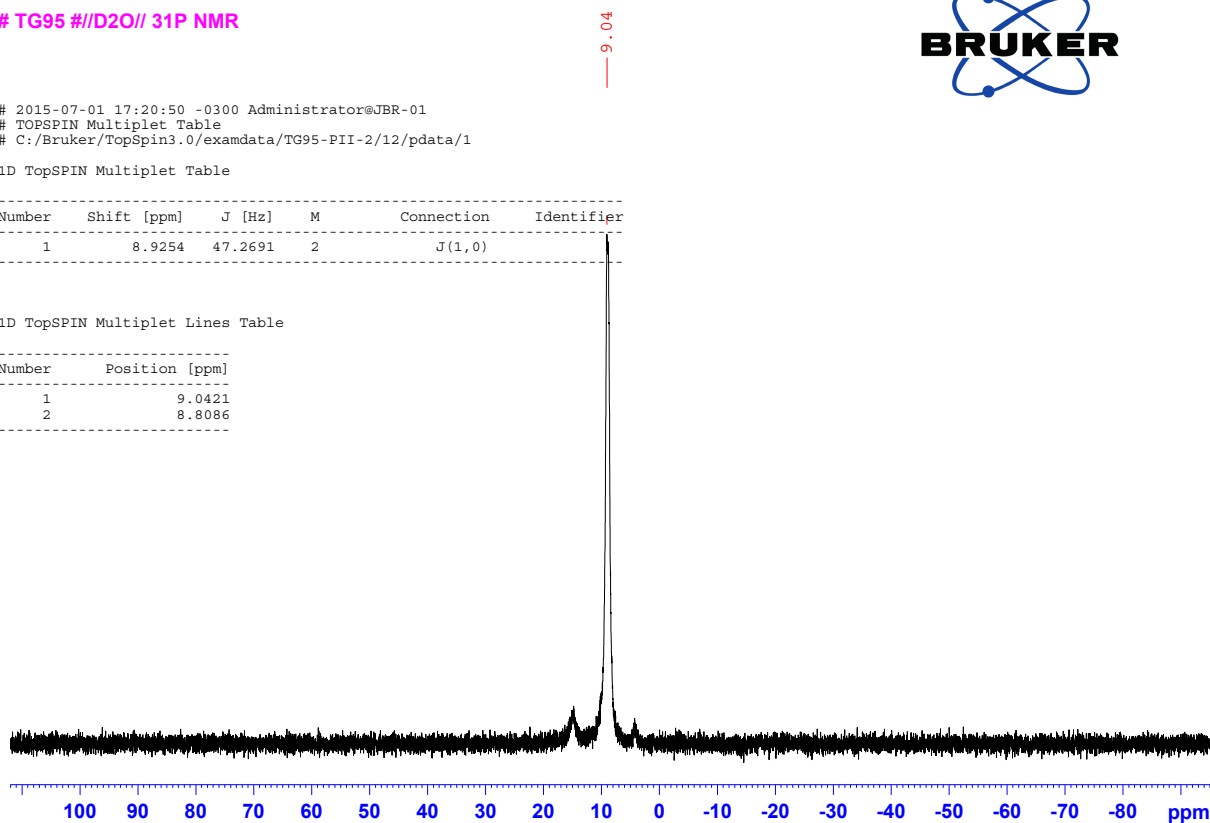
2015-07-01 17:20:50 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG95-PII-2/12/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	8.9254	47.2691	2	J(1,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	9.0421
2	8.8086



^{31}P NMR spectrum of compound 56.

TG95#//D2O// 19F NMR



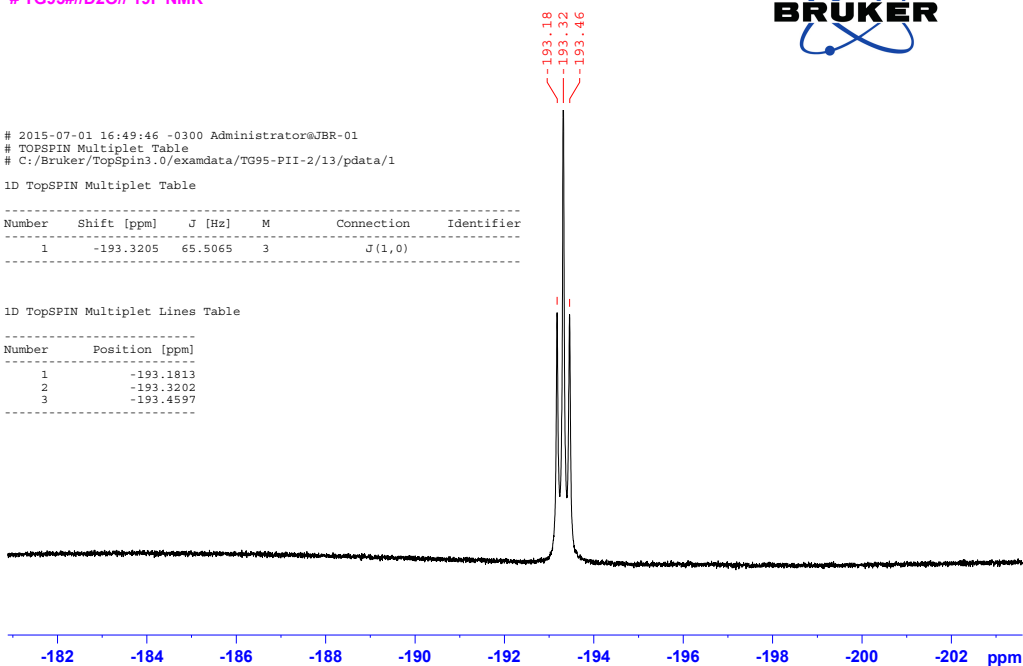
2015-07-01 16:49:46 -0300 Administrator@JBR-01
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C:/Bruker/TopSpin3.0/examdata/TG95-PII-2/13/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	-193.3205	65.5065	3	J(1,0)	

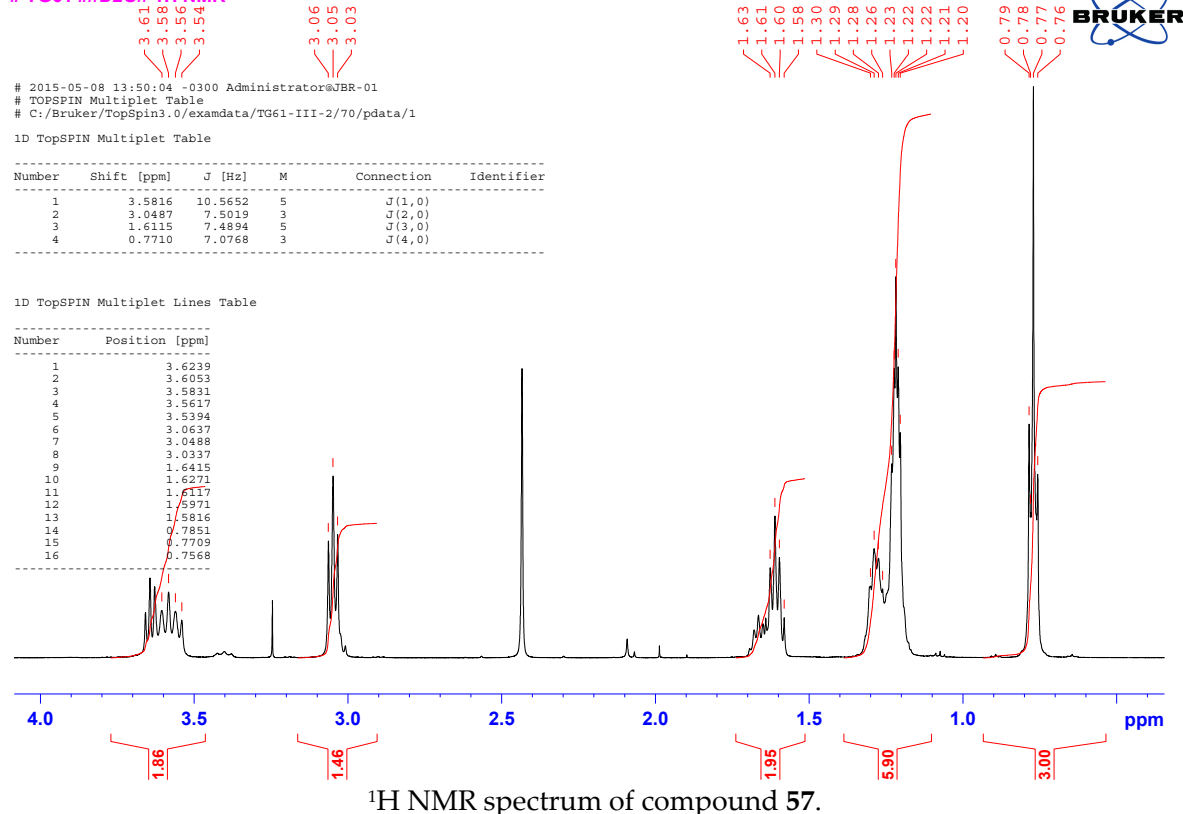
1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	-193.1813
2	-193.3202
3	-193.4597

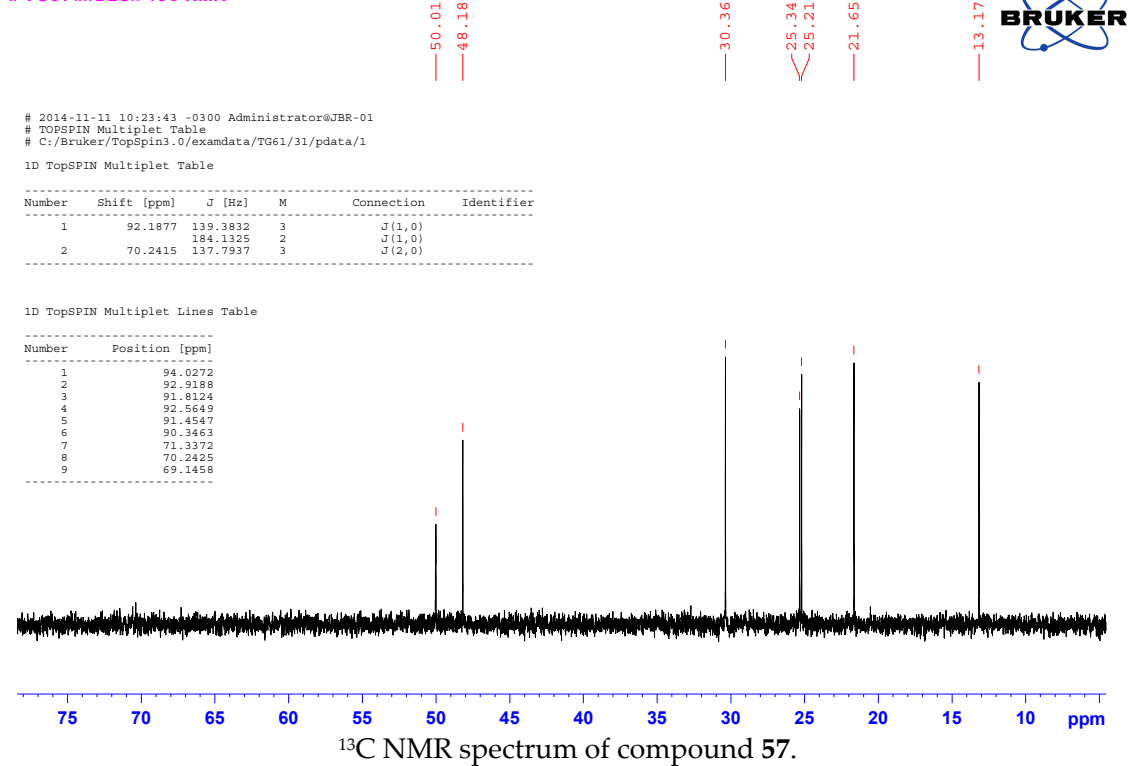


^{19}F NMR spectrum of compound 56.

TG61 #/D2O// 1H NMR



TG61 #/D2O// 13C NMR



TG61 #/D2O// 31P NMR



9.06
8.76

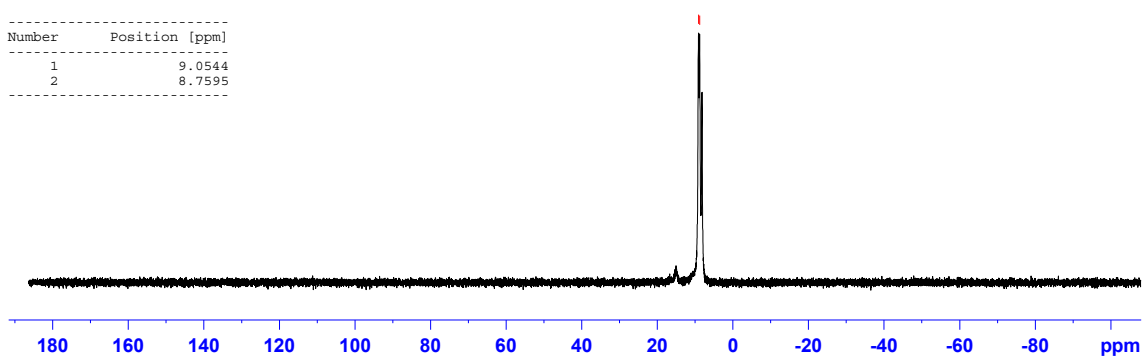
2015-05-08 12:08:48 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
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1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	8.9069	59.7083	2	J(1,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	9.0544
2	8.7595



³¹P NMR spectrum of compound 57.

TG-61 #/D2O// 19F NMR



-193.54

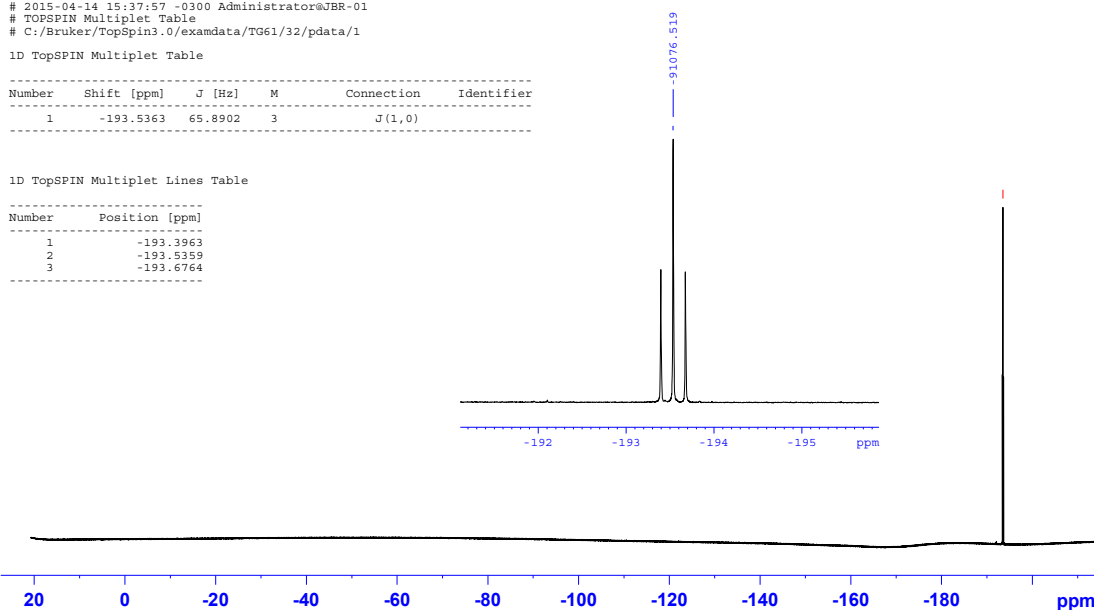
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1D TopSPIN Multiplet Table

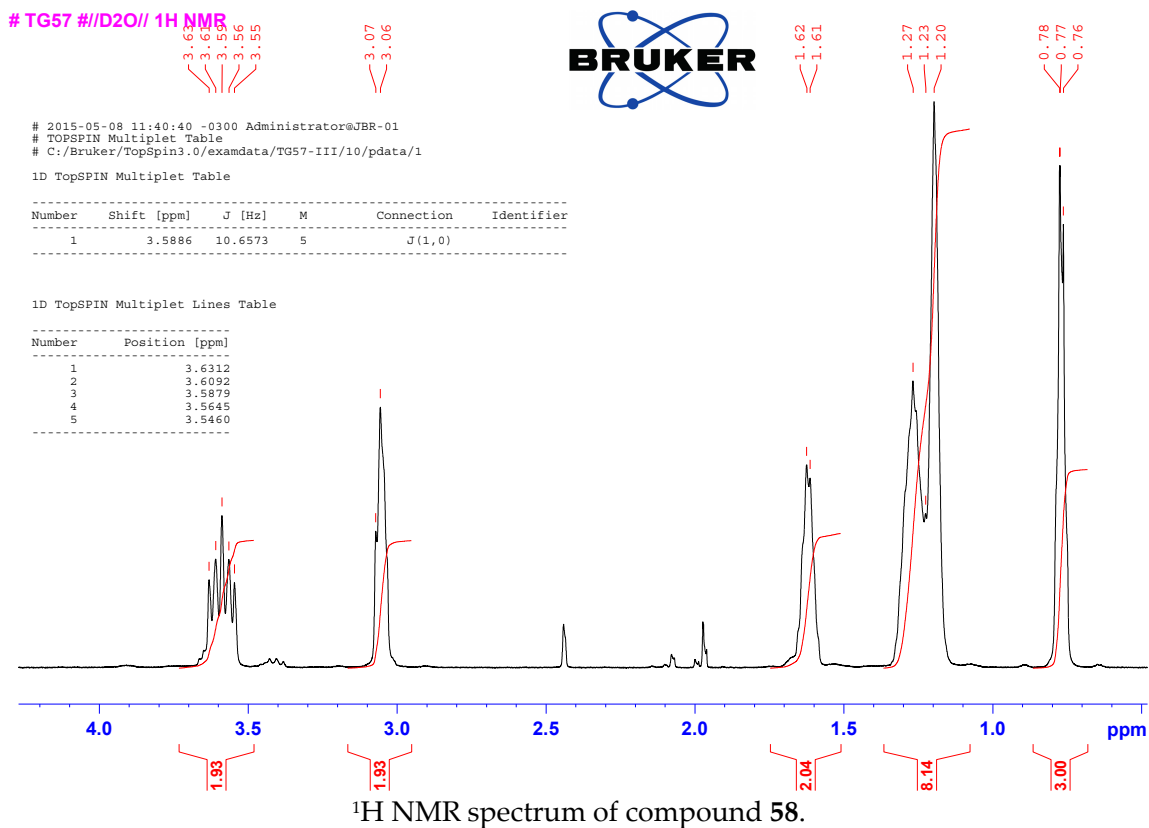
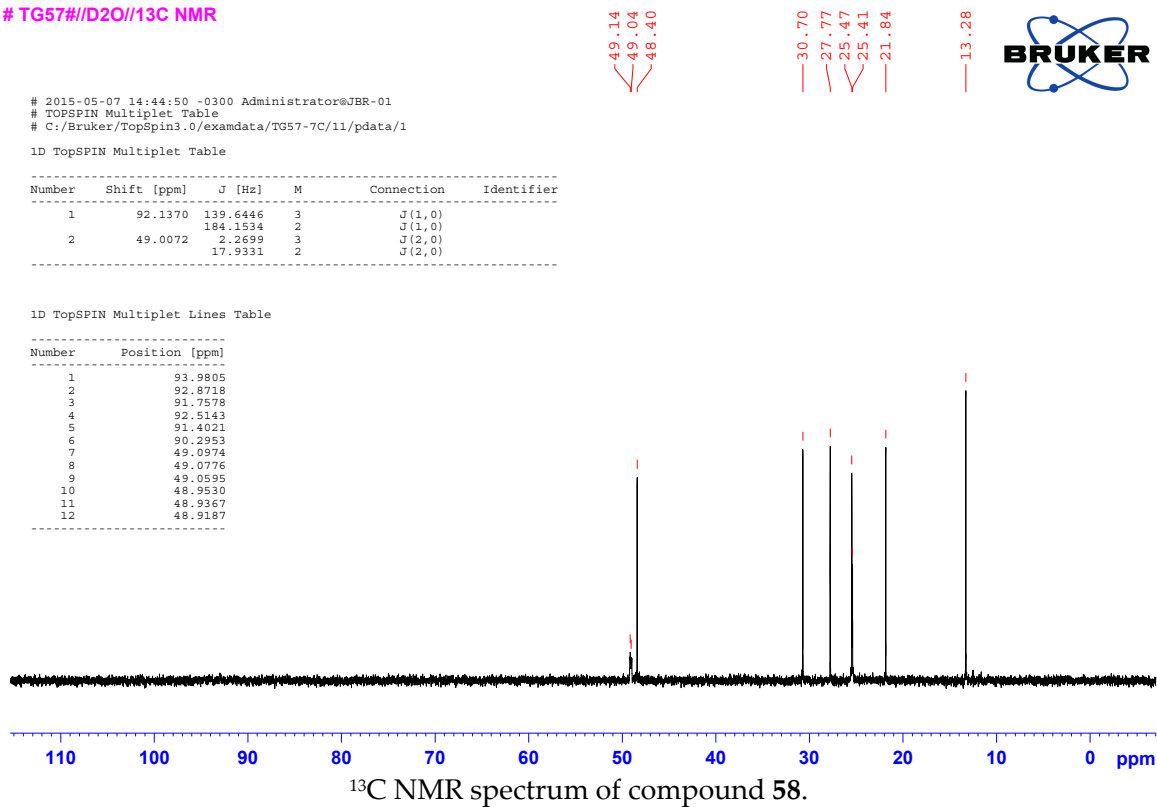
Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	-193.5363	65.8902	3	J(1,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	-193.3963
2	-193.5359
3	-193.6764



¹⁹F NMR spectrum of compound 57.

# TG57#/ID20//¹³C NMR

TG57-#//D2O// 31P NMR



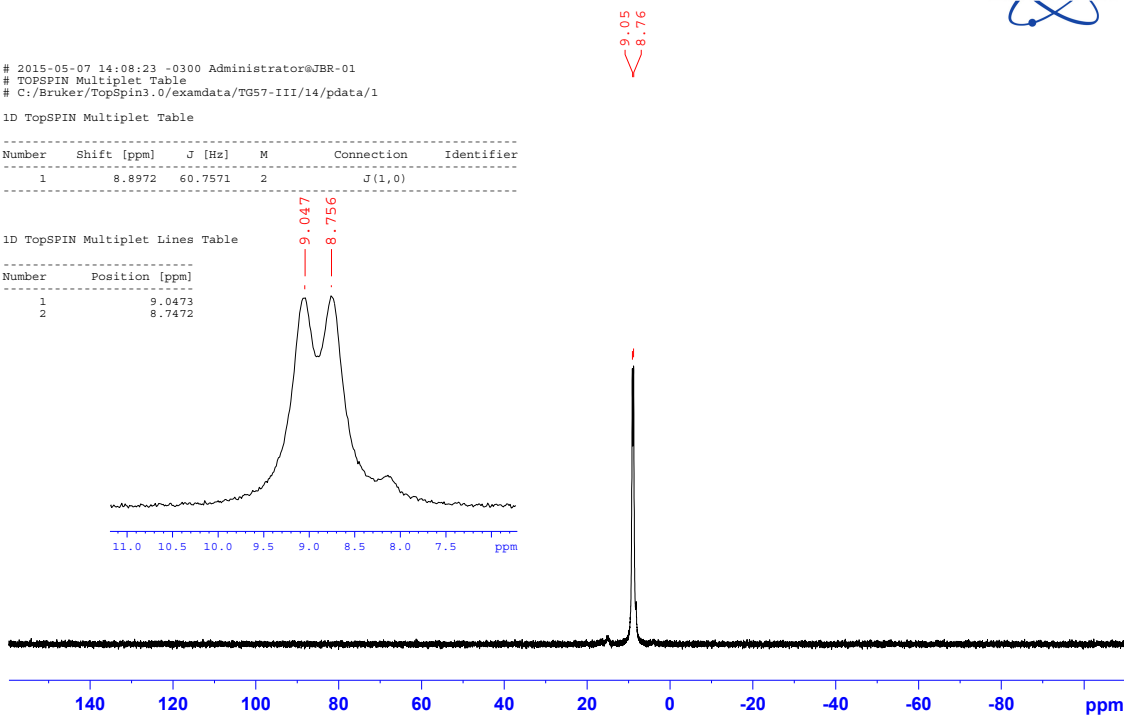
2015-05-07 14:08:23 -0300 Administrator@JBR-01
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1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	8.8972	60.7571	2	J(1,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	9.0473
2	8.7472



³¹P NMR spectrum of compound 58.

TG57-7C // D2O // 19F NMR



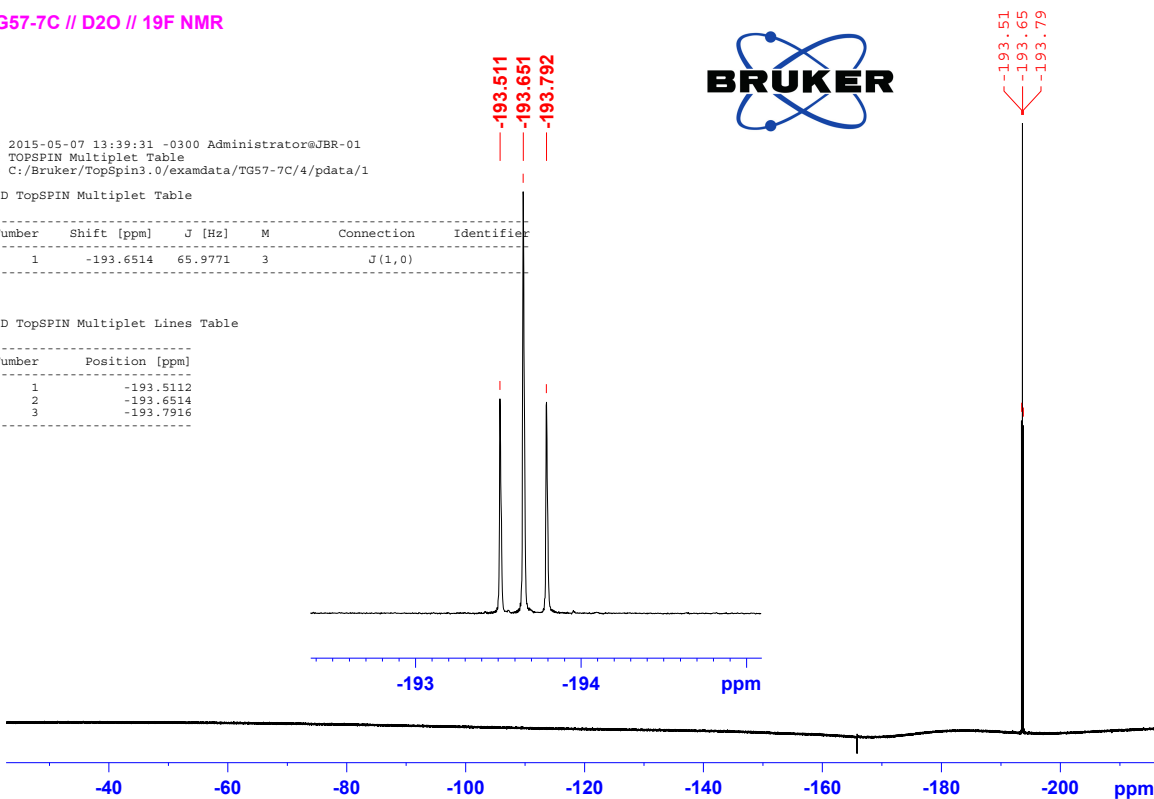
2015-05-07 13:39:31 -0300 Administrator@JBR-01
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 # C:/Bruker/TopSpin3.0/examdata/TG57-7C/4/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	-193.6514	65.9771	3	J(1,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	-193.5112
2	-193.6514
3	-193.7916



¹⁹F NMR spectrum of compound 58.

#TG73 #I/D2O// 1H NMR



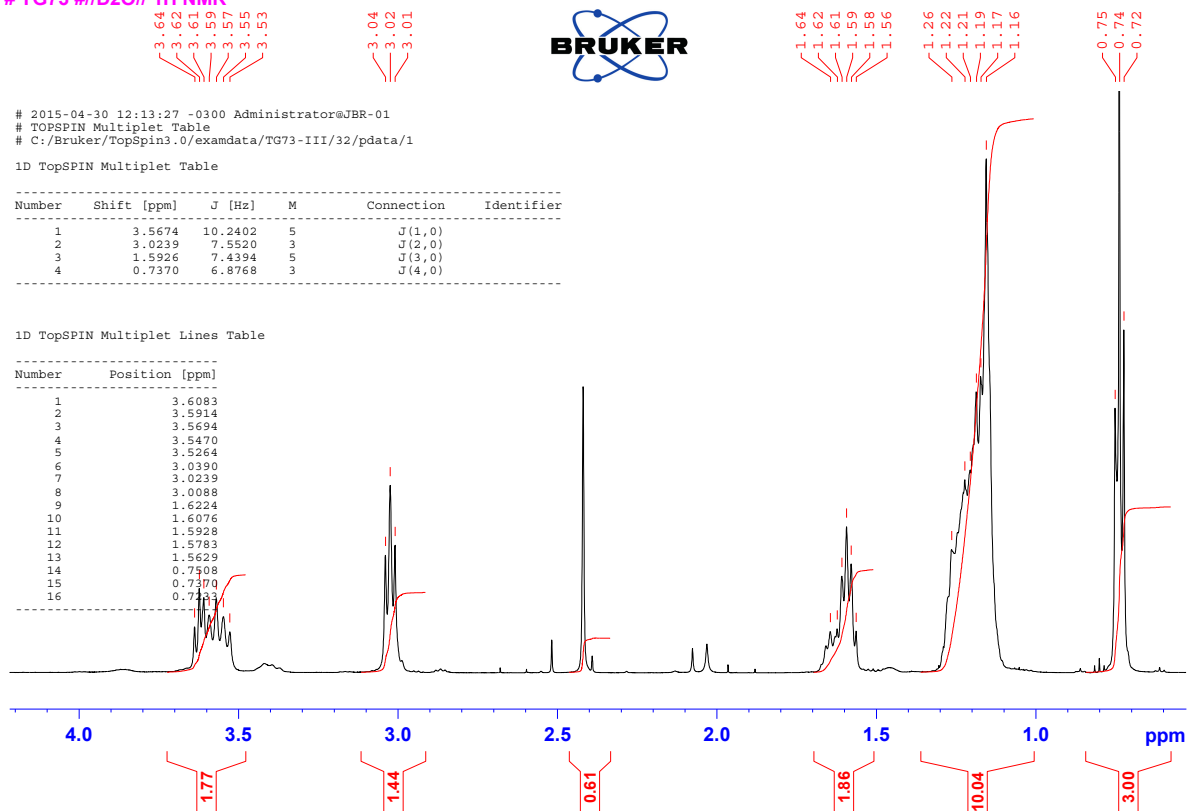
2015-04-30 12:13:27 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG73-III/32/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	3.5674	10.2402	5	J(1,0)	
2	3.0239	7.5520	3	J(2,0)	
3	1.5926	7.4394	5	J(3,0)	
4	0.7370	6.8768	3	J(4,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	3.6083
2	3.5914
3	3.5694
4	3.5470
5	3.5264
6	3.0390
7	3.0239
8	3.0088
9	1.6224
10	1.6076
11	1.5928
12	1.5783
13	1.5629
14	0.7508
15	0.7370
16	0.7232

¹H NMR spectrum of compound 59.

#TG73 #I/D2O// 13C NMR



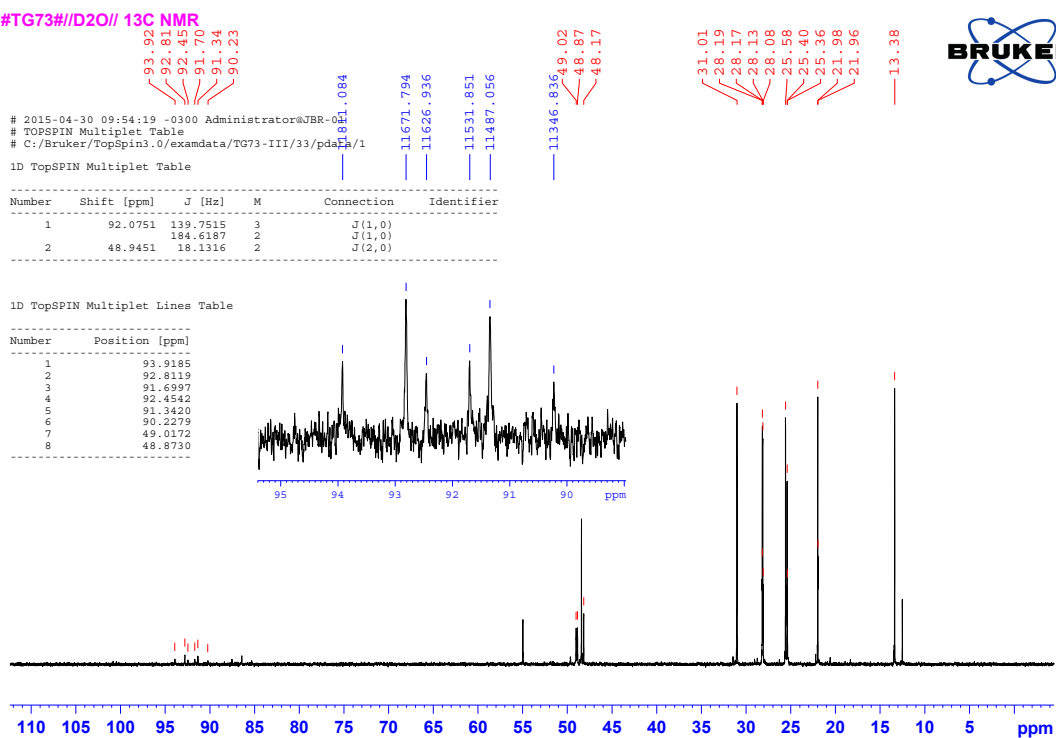
2015-04-30 09:54:19 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG73-III/33/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	92.0751	139.7515	3	J(1,0)	
2	48.9451	18.1316	2	J(2,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	93.9185
2	92.8119
3	91.6997
4	92.4542
5	91.3420
6	90.2279
7	49.0172
8	48.8730

¹³C NMR spectrum of compound 59.

TG73 #//D2O// 13C NMR



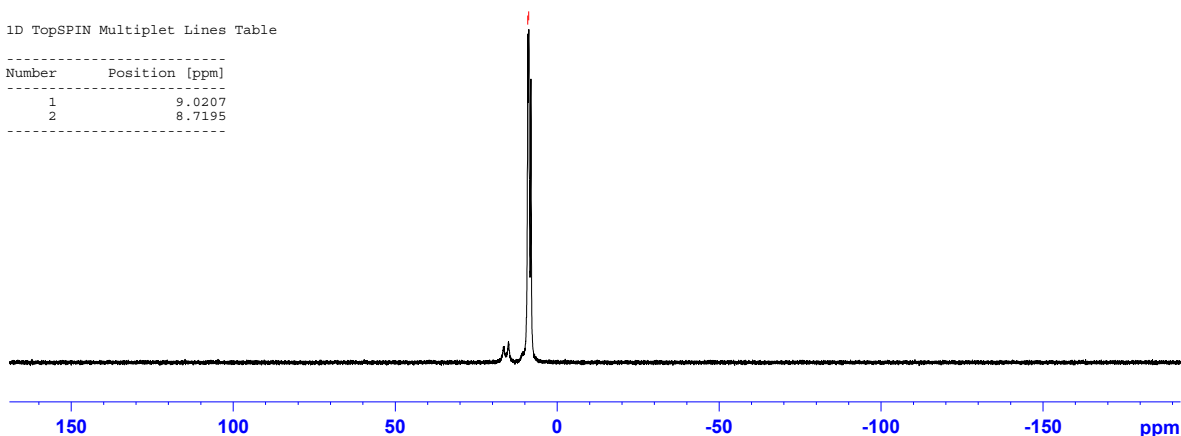
2015-04-30 09:42:34 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG73-III/34/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	8.8701	60.9798	2	J(1,0)	

1D TopSPIN Multiplet Lines Table

Number	Position [ppm]
1	9.0207
2	8.7195



³¹P NMR spectrum of compound 59.

#TG73#// D2O // 19F NMR



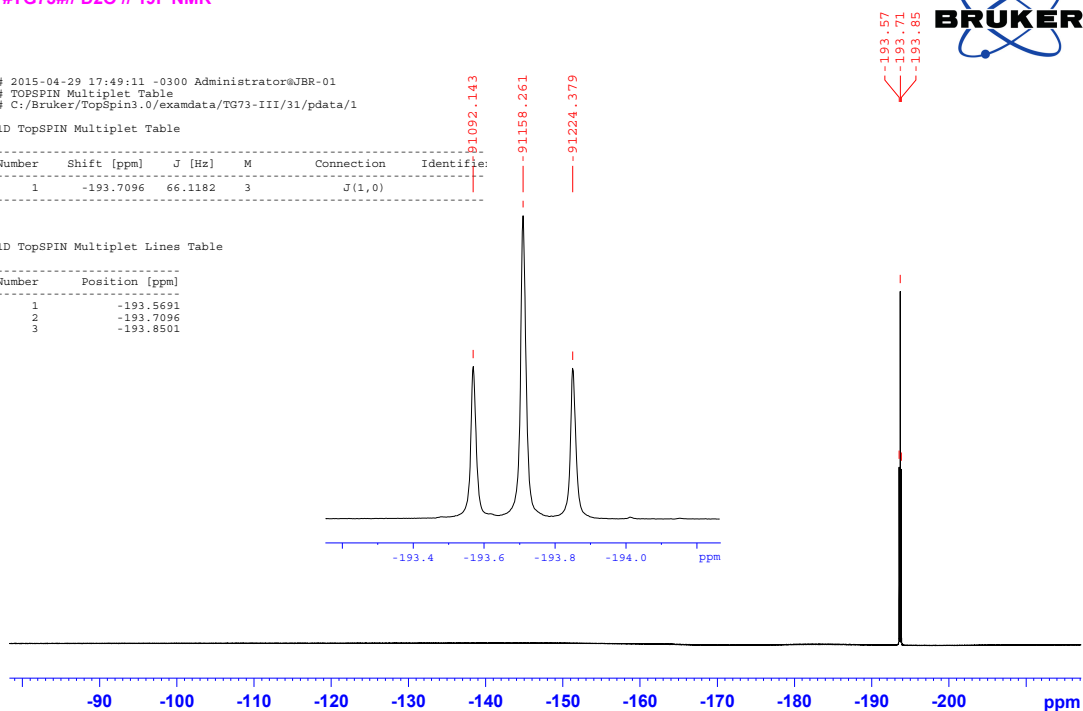
2015-04-29 17:49:11 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
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1D TopSPIN Multiplet Table

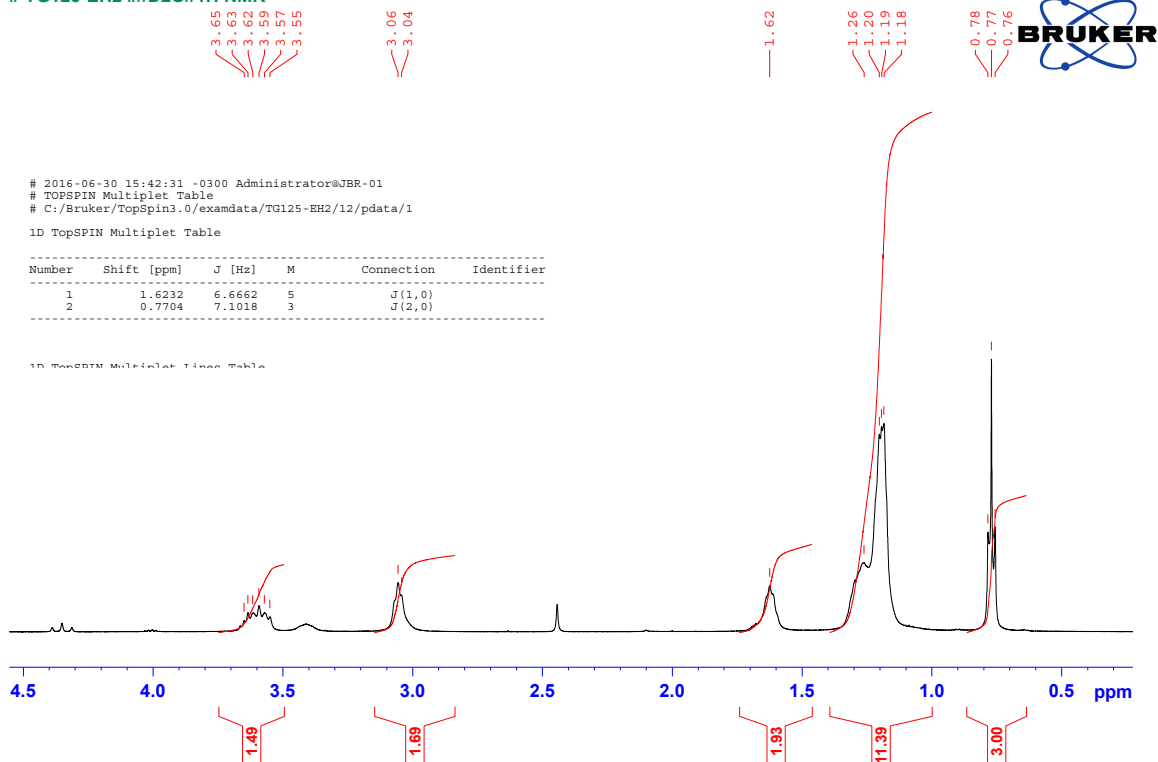
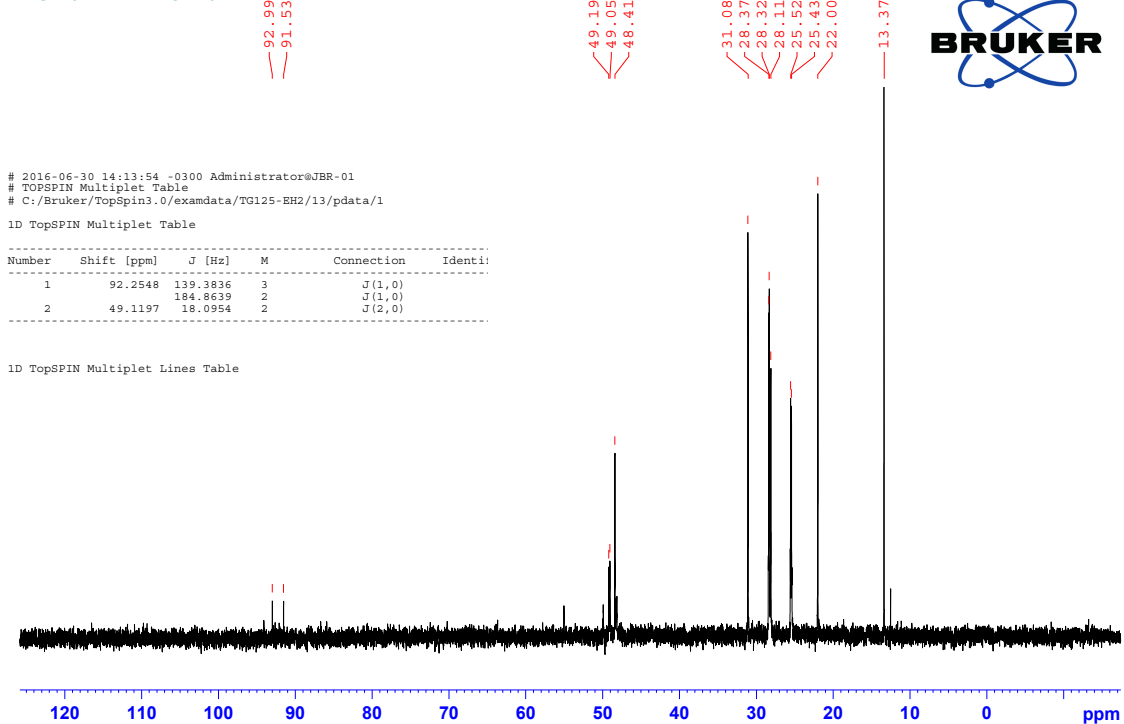
Number	Shift [ppm]	J [Hz]	M	Connection	Identifie:
1	-193.7096	66.1182	3	J(1,0)	

1D TopSPIN Multiplet Lines Table

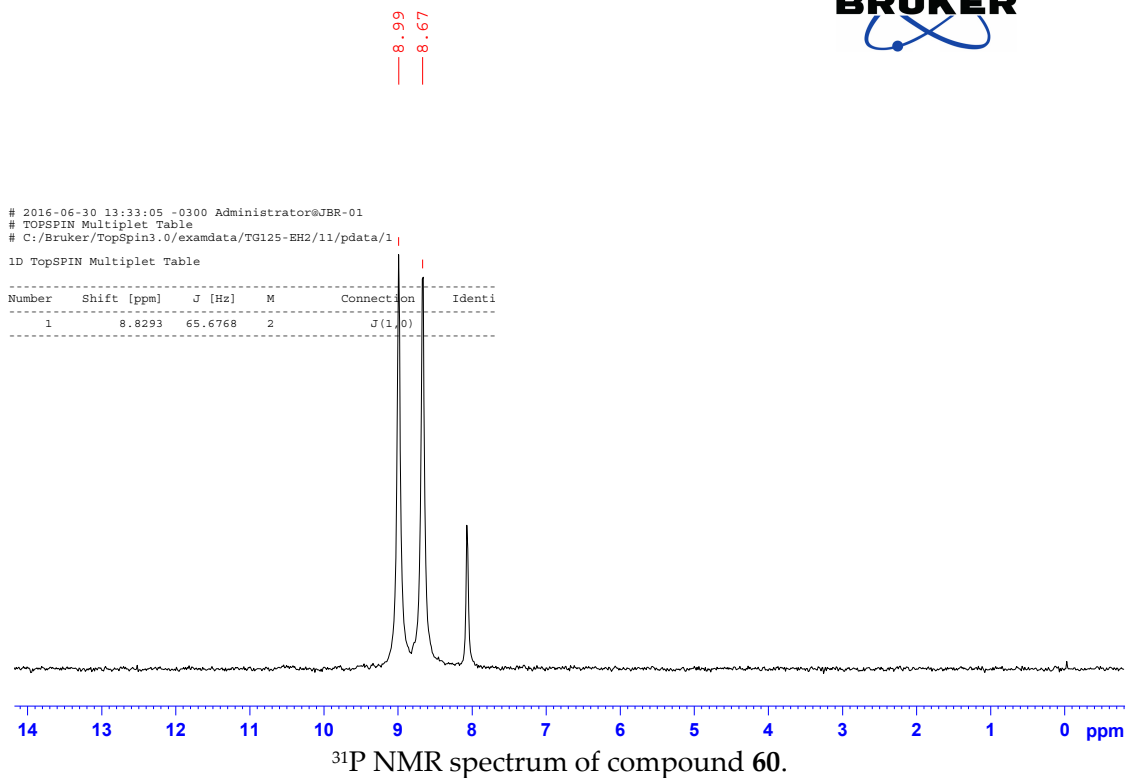
Number	Position [ppm]
1	-193.5691
2	-193.7096
3	-193.8501



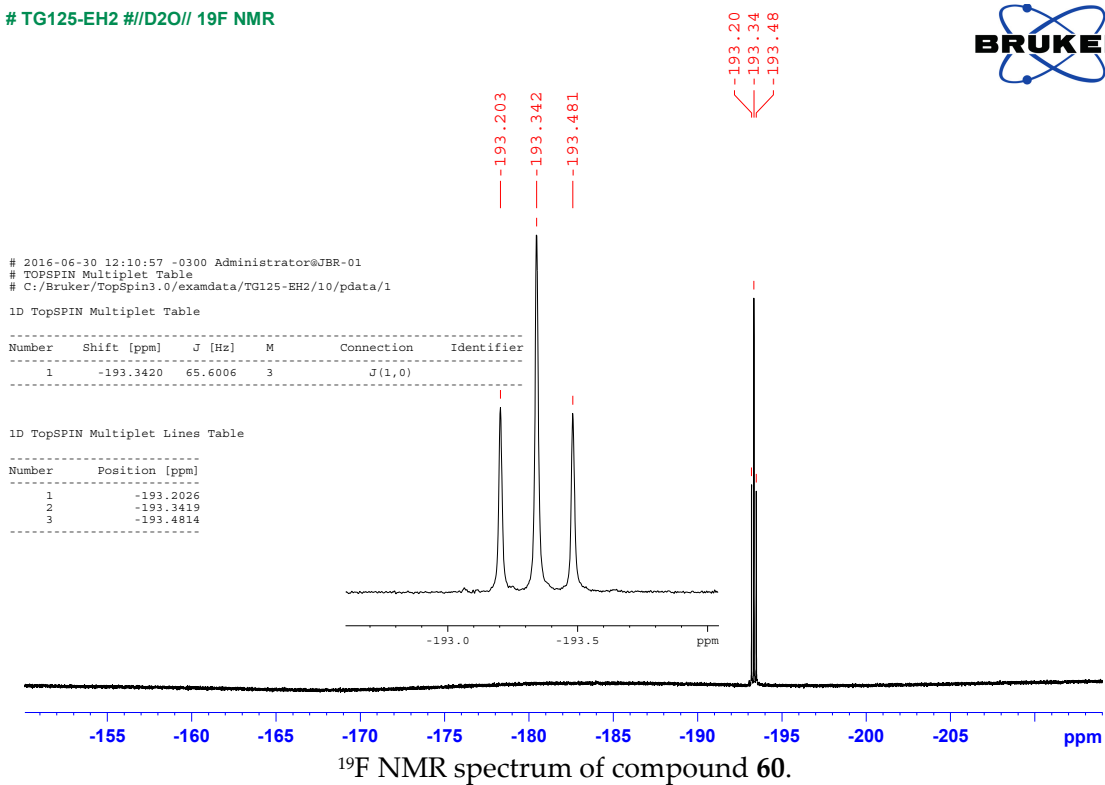
¹⁹F NMR spectrum of compound 59.

TG125-EH2 #/D2O//¹H NMR¹H NMR spectrum of compound 60.# TG125-EH2 #/D2O// ¹³C NMR¹³C NMR spectrum of compound 60.

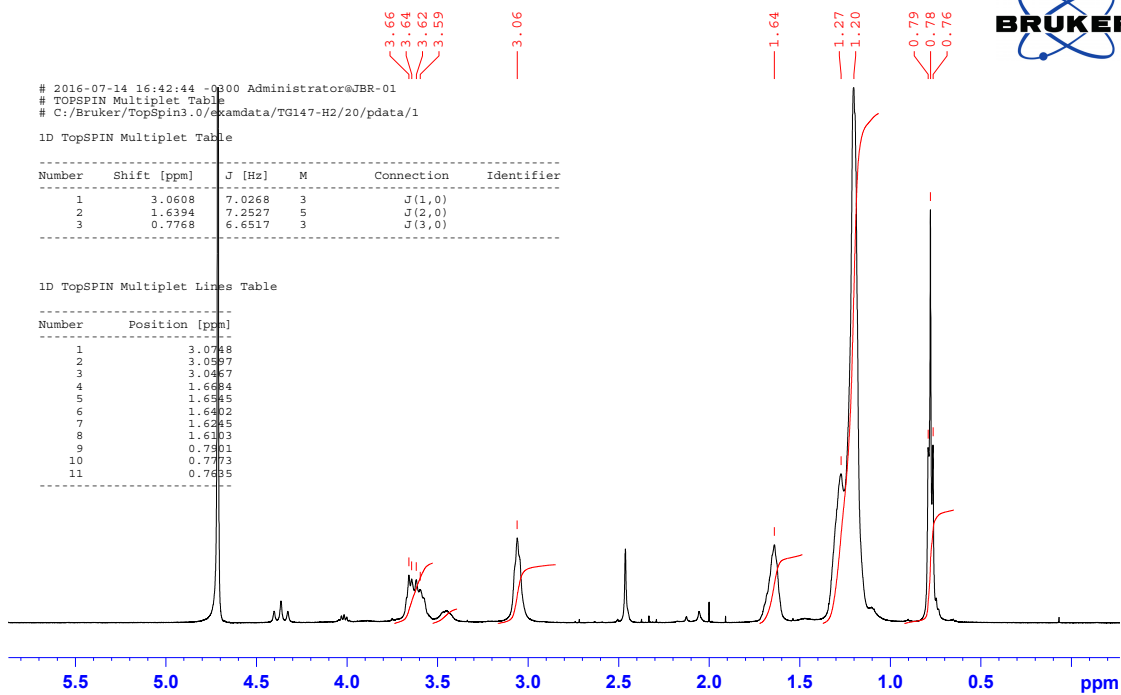
TG125-EH2 #//D2O// 31P NMR



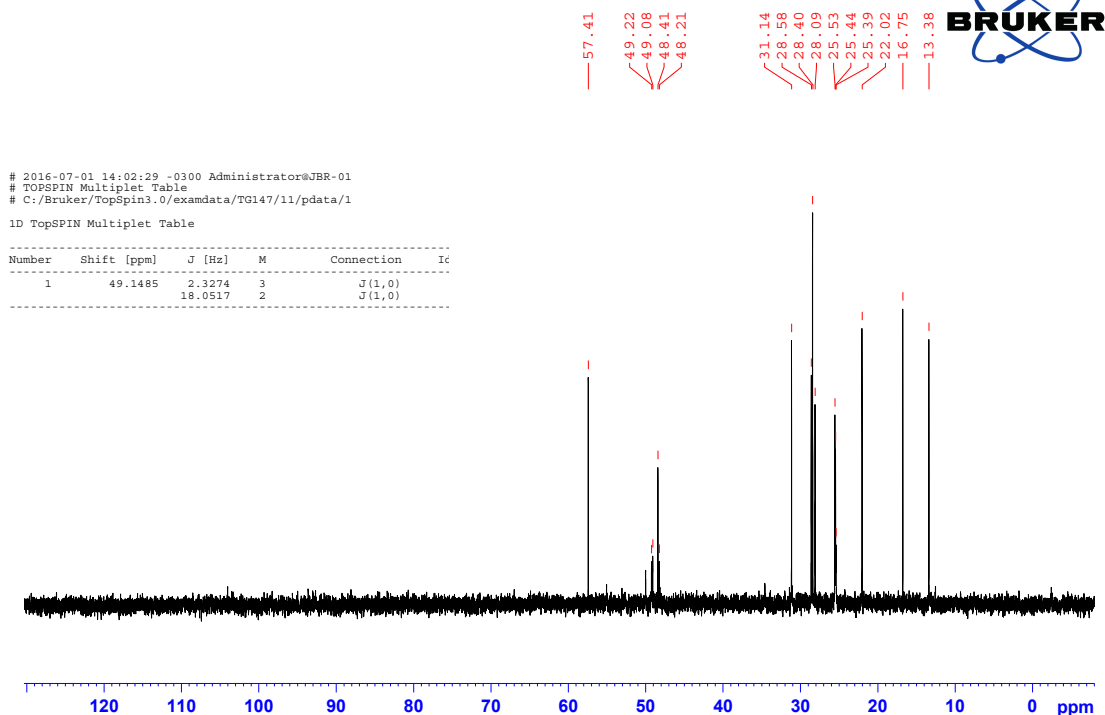
TG125-EH2 #//D2O// 19F NMR



TG147-H2 #//D2O// 1H NMR

¹H NMR spectrum of compound 61.

#TG147# //D2O// 13C NMR

¹³C NMR spectrum of compound 61.

#TG147# D2O // 31P NMR

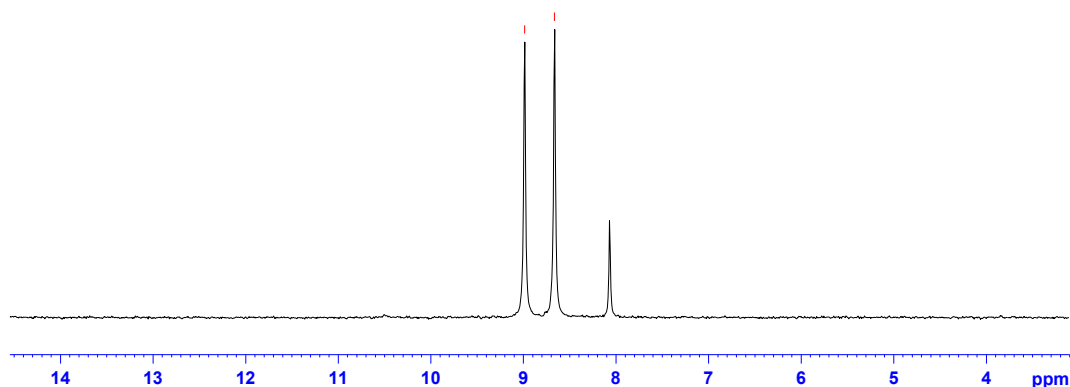


8.99
8.66

2016-07-01 10:43:22 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG147/14/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection	Identifier
1	8.8244	65.4946	2	J(1,0)	



³¹P NMR spectrum of compound 61.

TG147-H2 #/D2O// 19F NMR

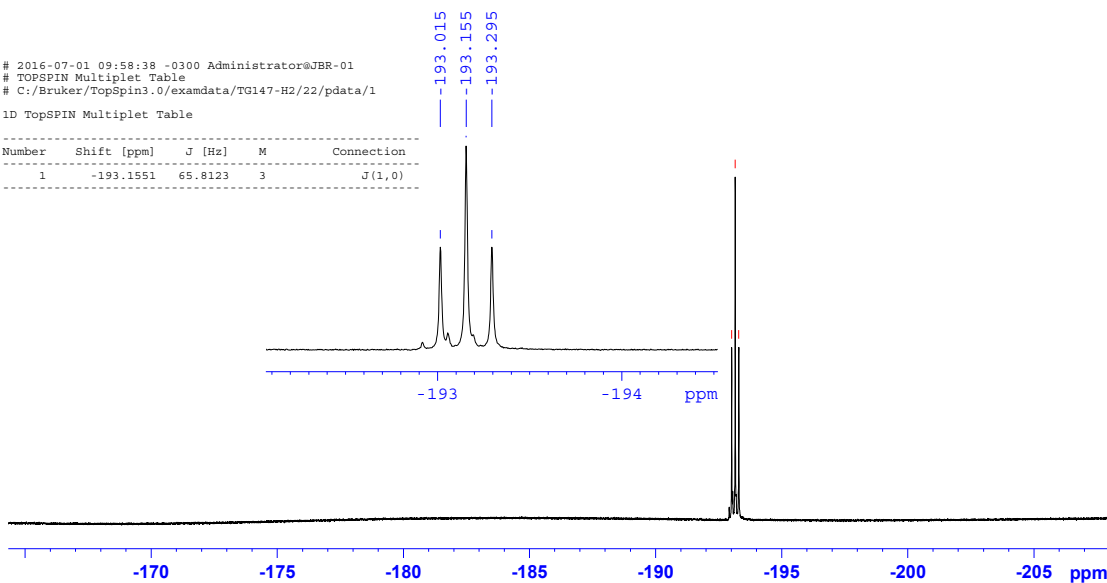


-193.02
-193.16
-193.29

2016-07-01 09:58:38 -0300 Administrator@JBR-01
TOPSPIN Multiplet Table
C:/Bruker/TopSpin3.0/examdata/TG147-H2/22/pdata/1

1D TopSPIN Multiplet Table

Number	Shift [ppm]	J [Hz]	M	Connection
1	-193.1551	65.8123	3	J(1,0)



¹⁹F NMR spectrum of compound 61.