Electronic Supplementary Information

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

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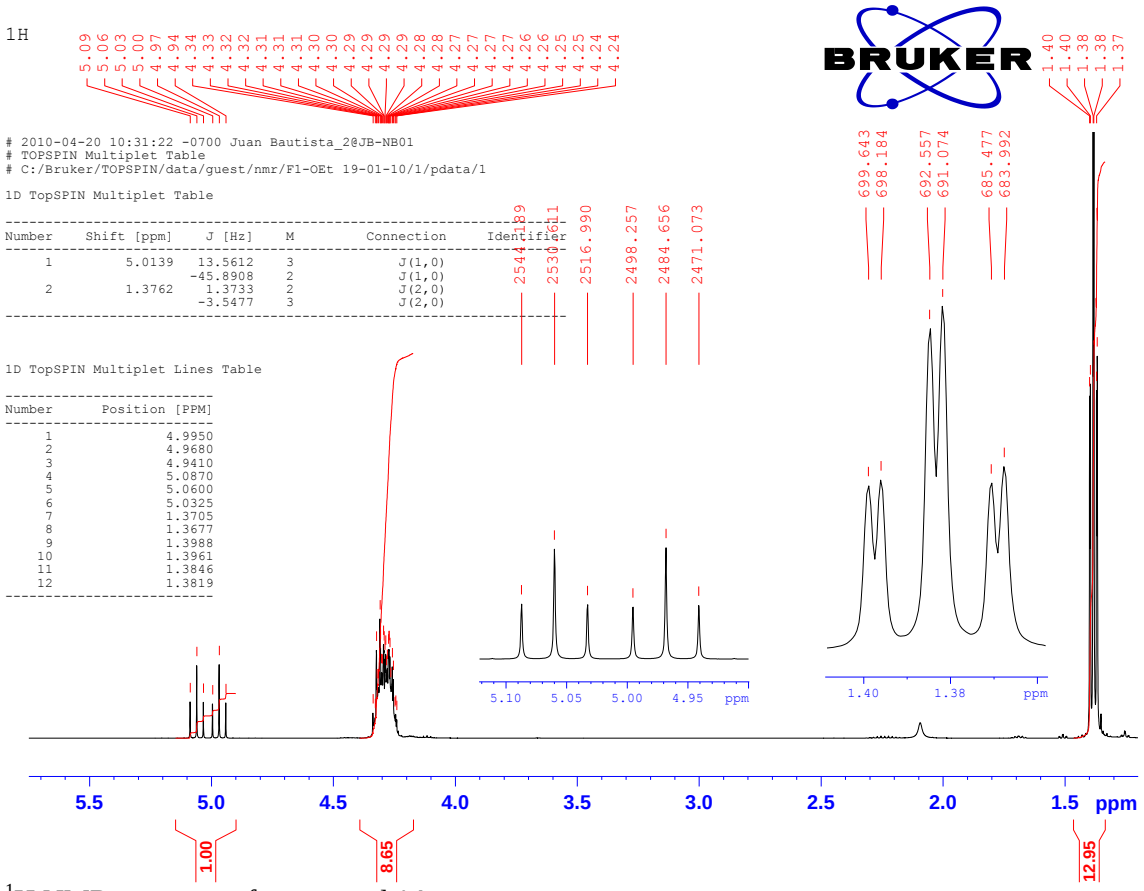

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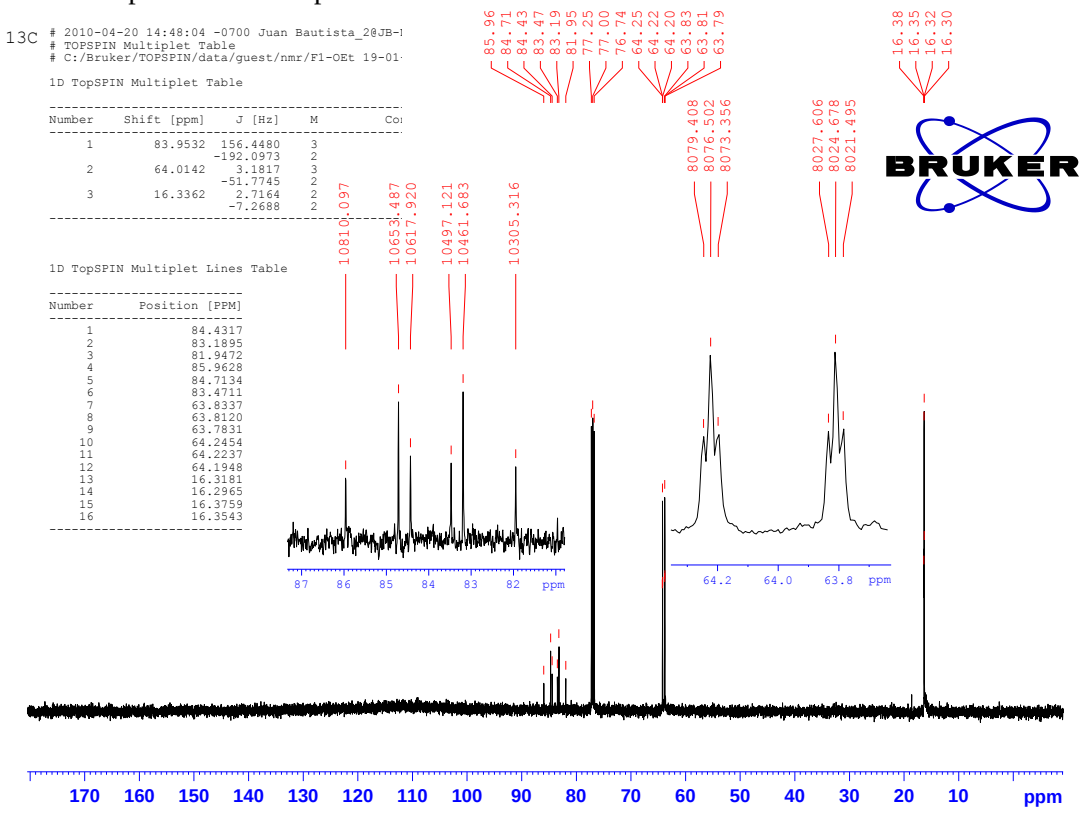

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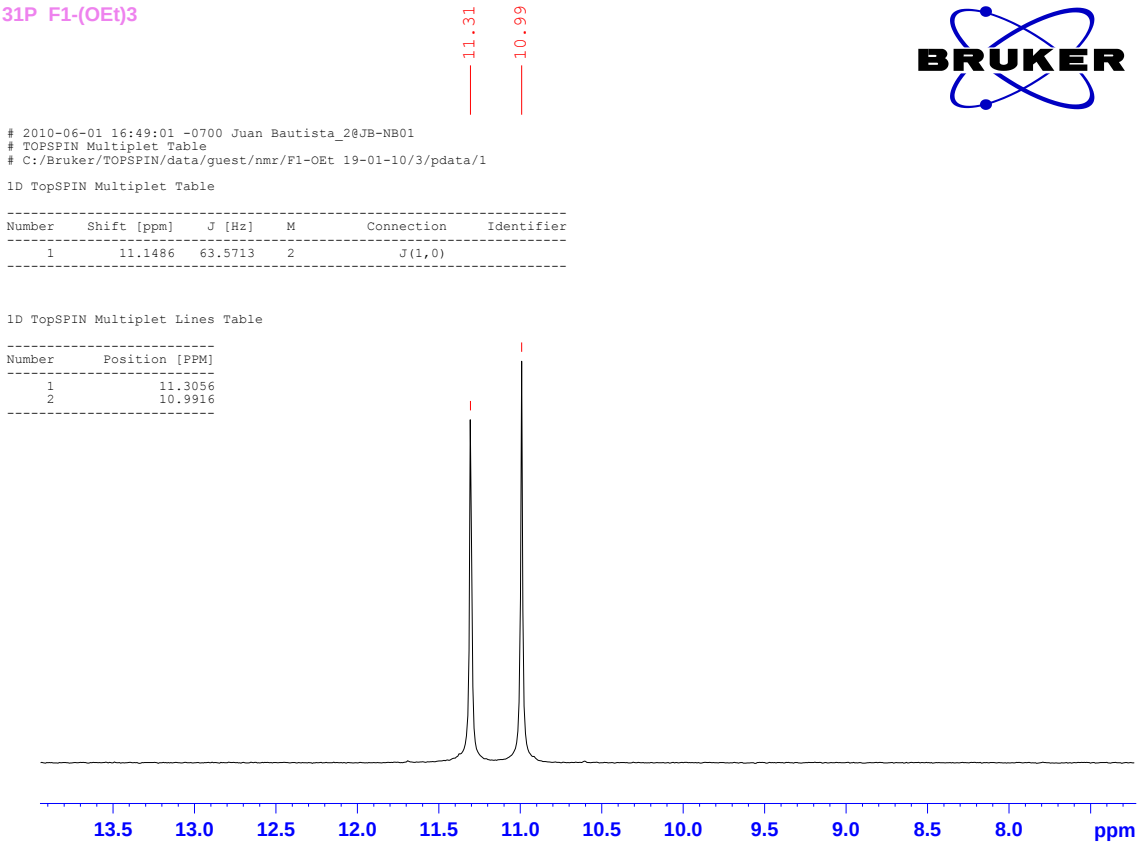

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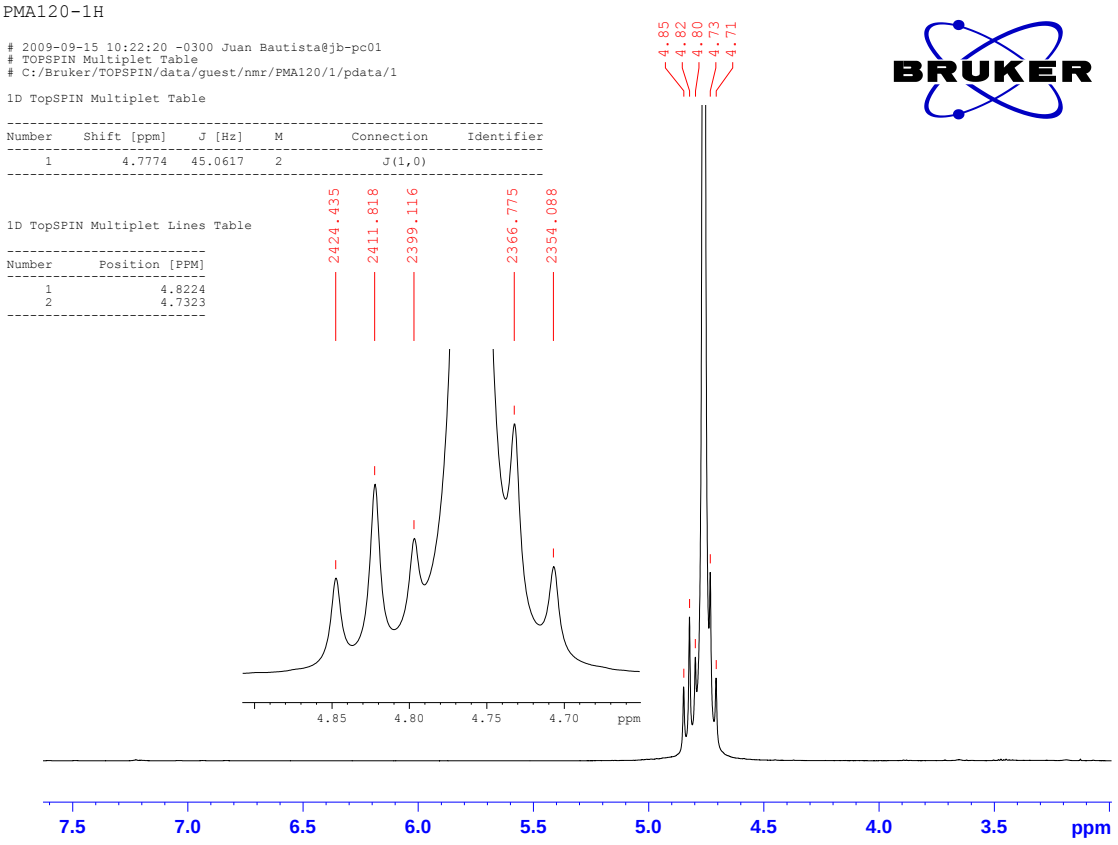

^{1}H NMR spectrum of compound **35**

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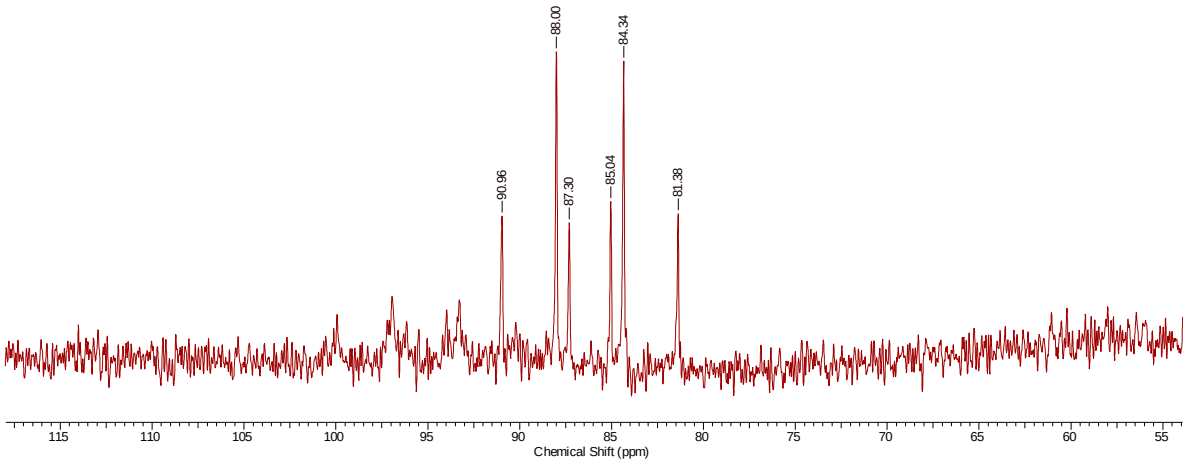

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4	87.30	4393.6	0.0108
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6	90.96	4577.9	0.0114

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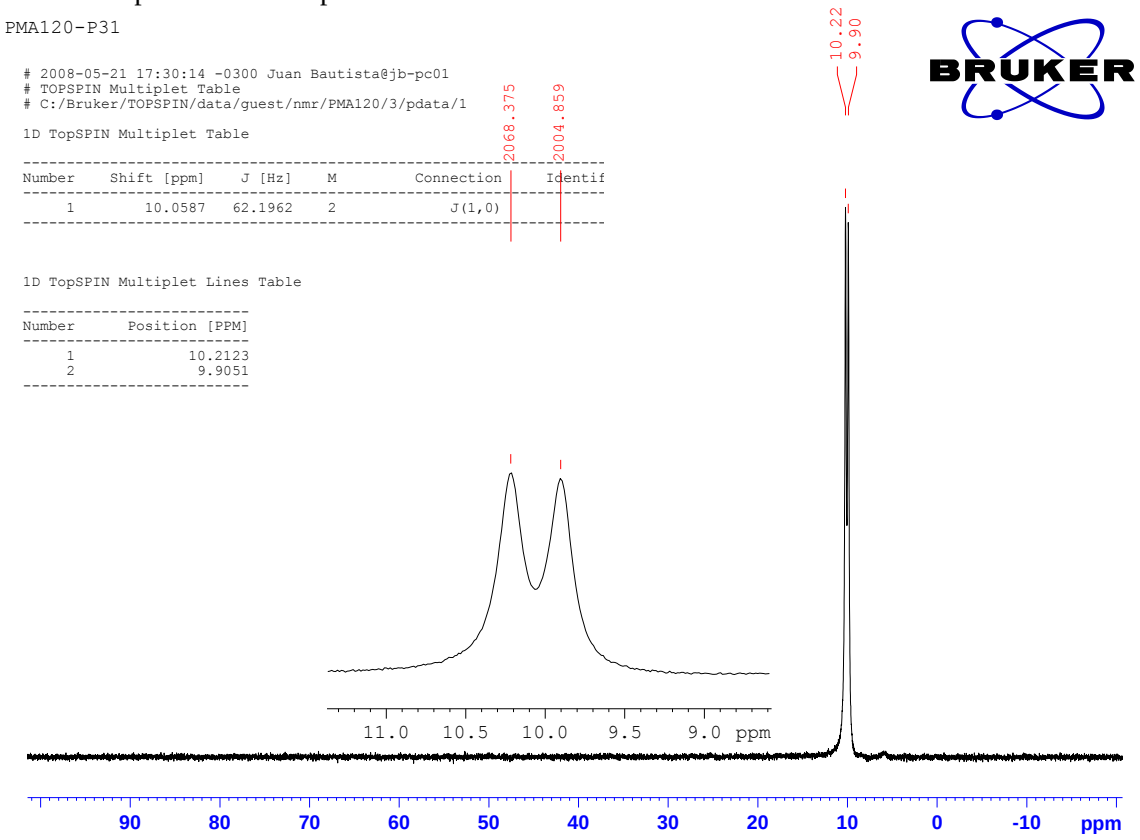

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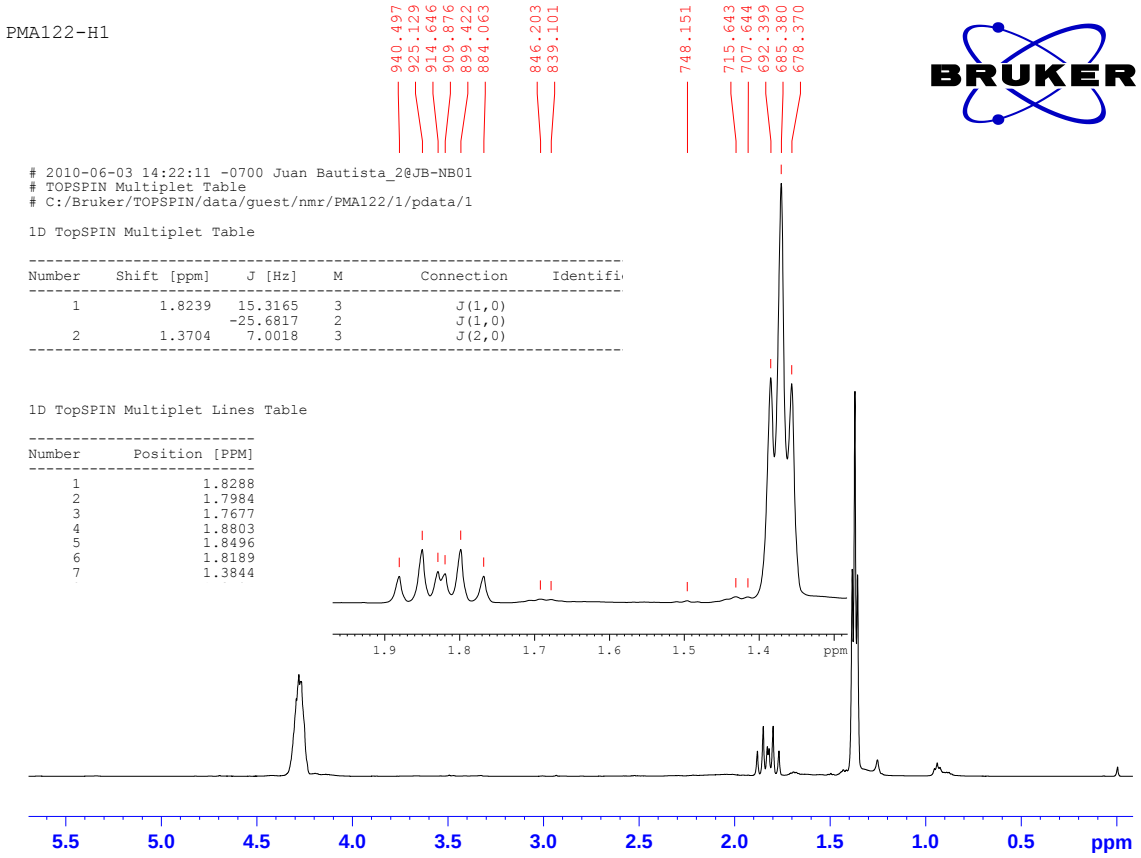

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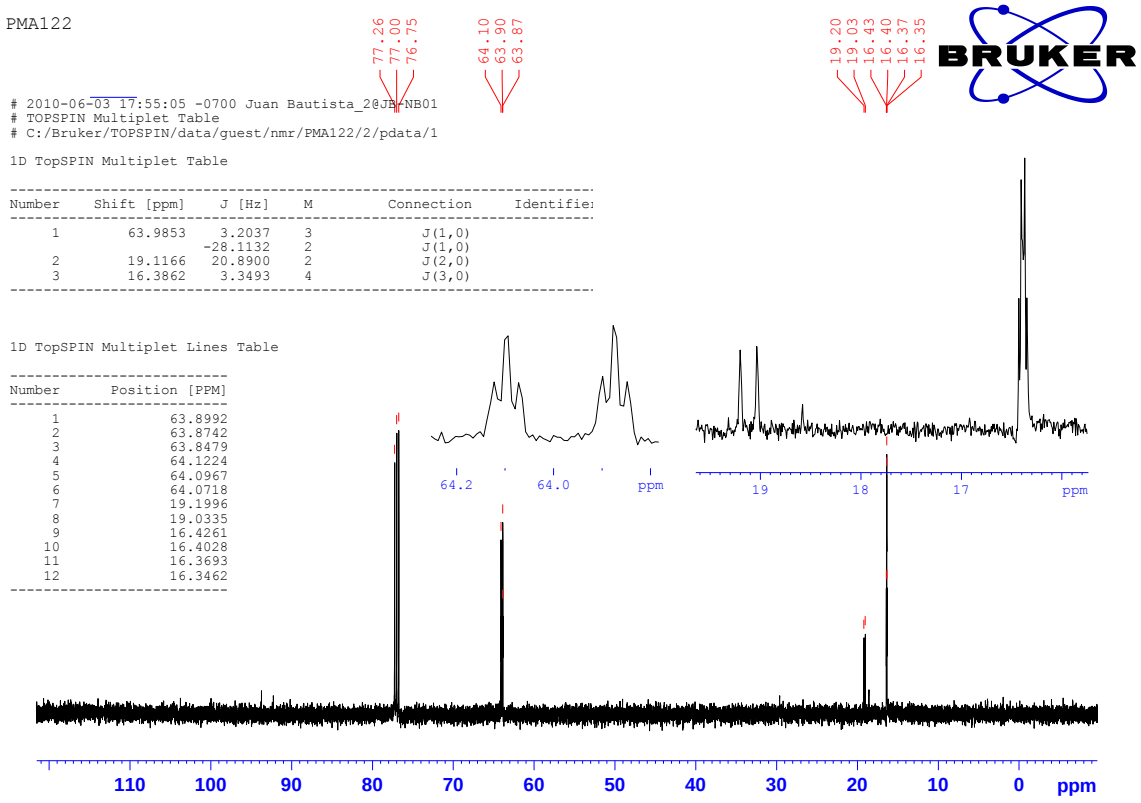

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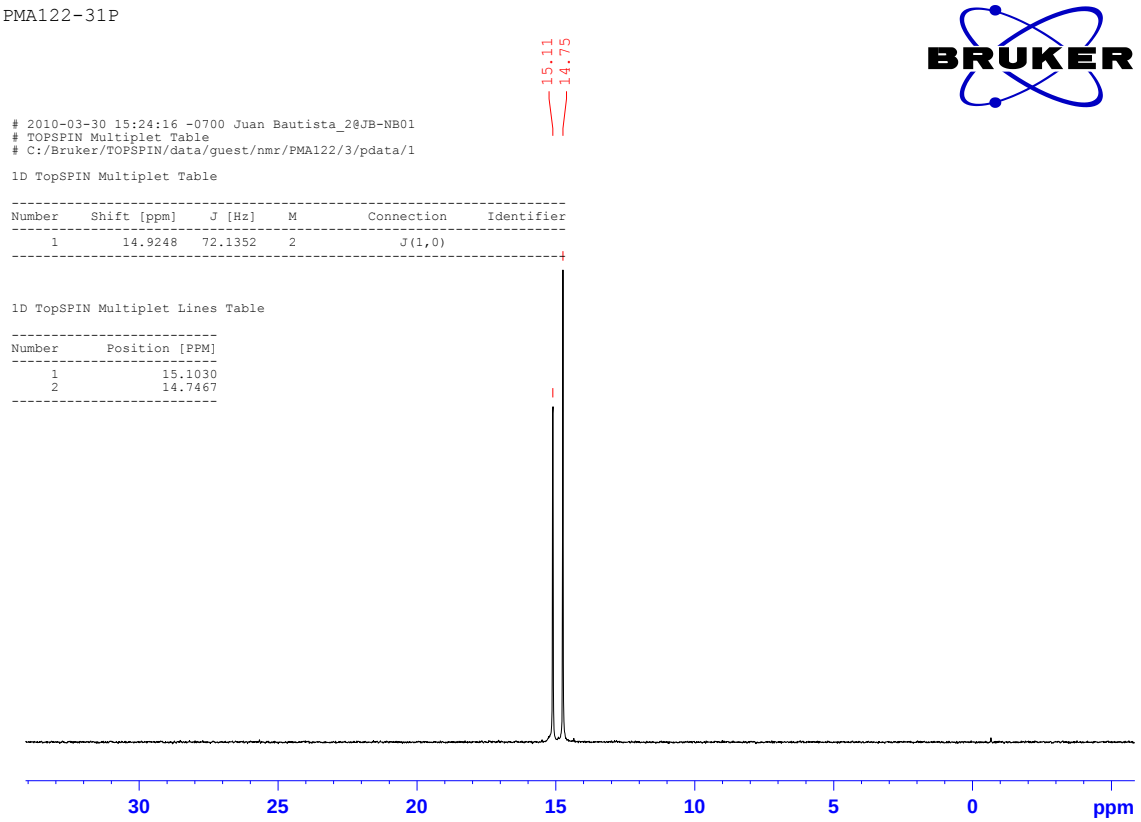

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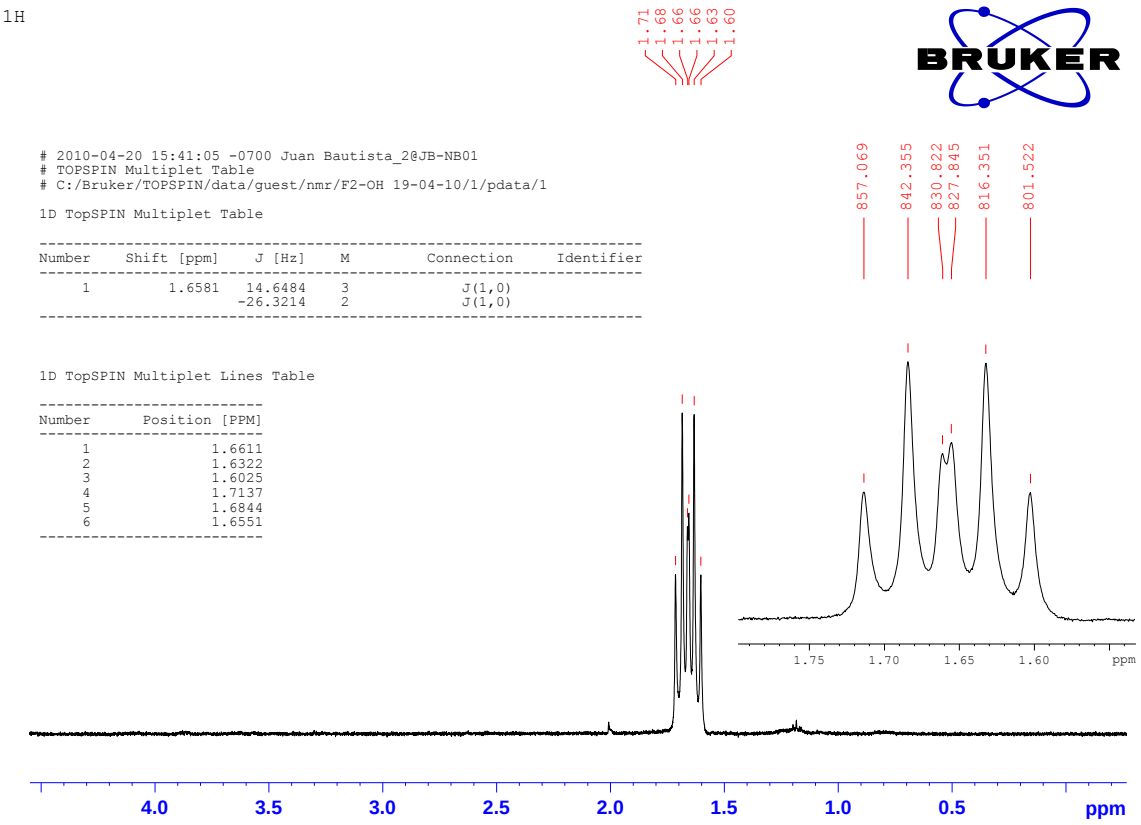

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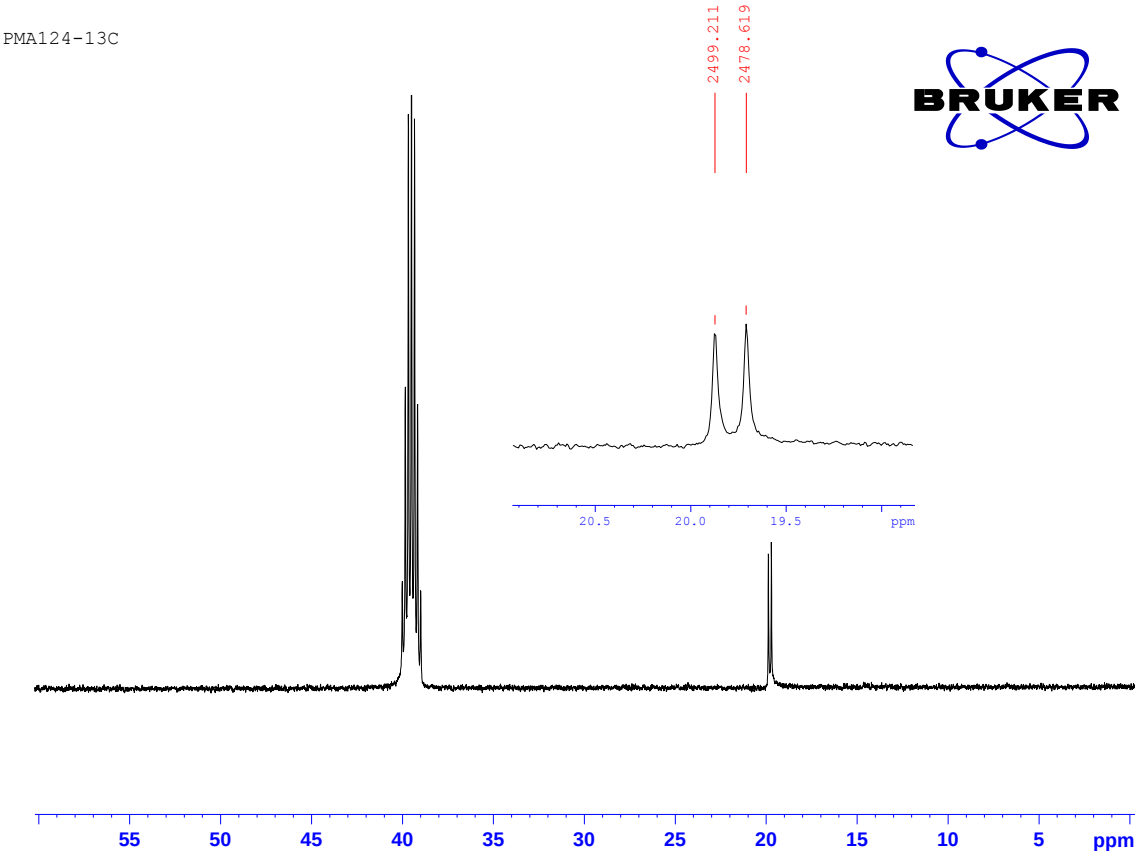

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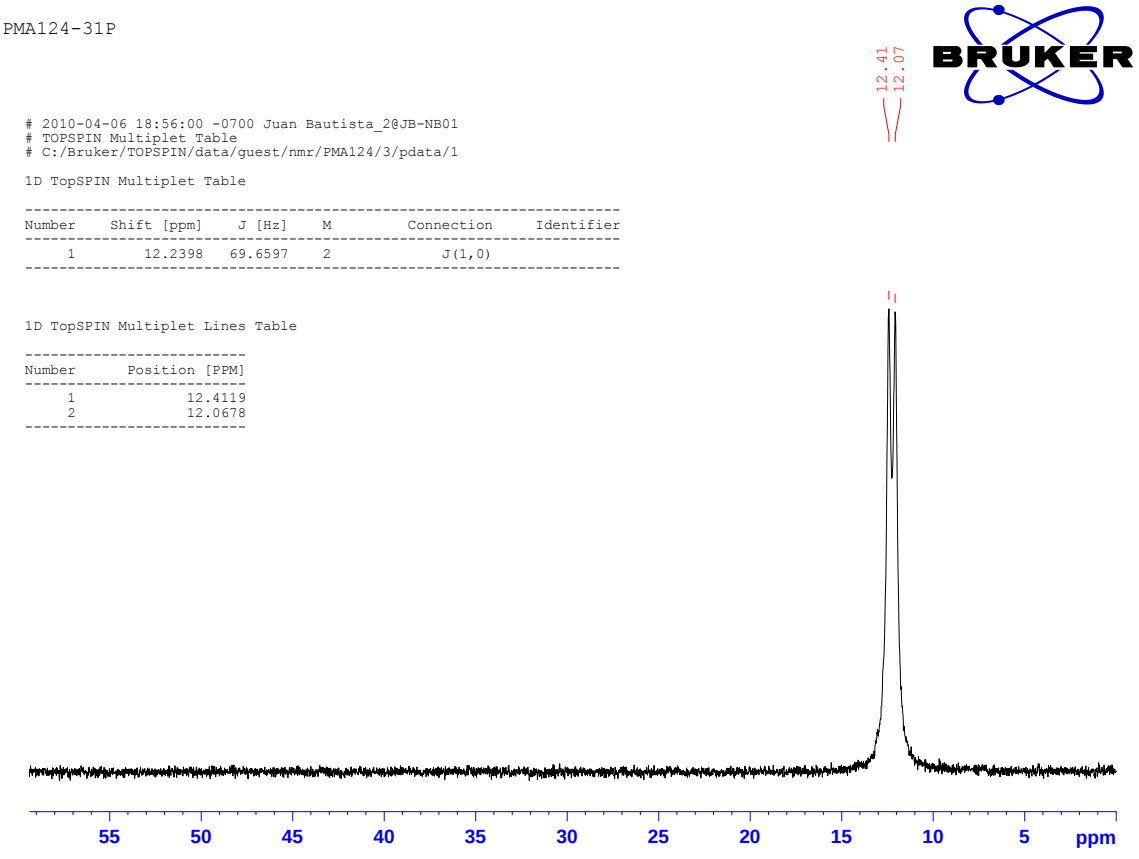

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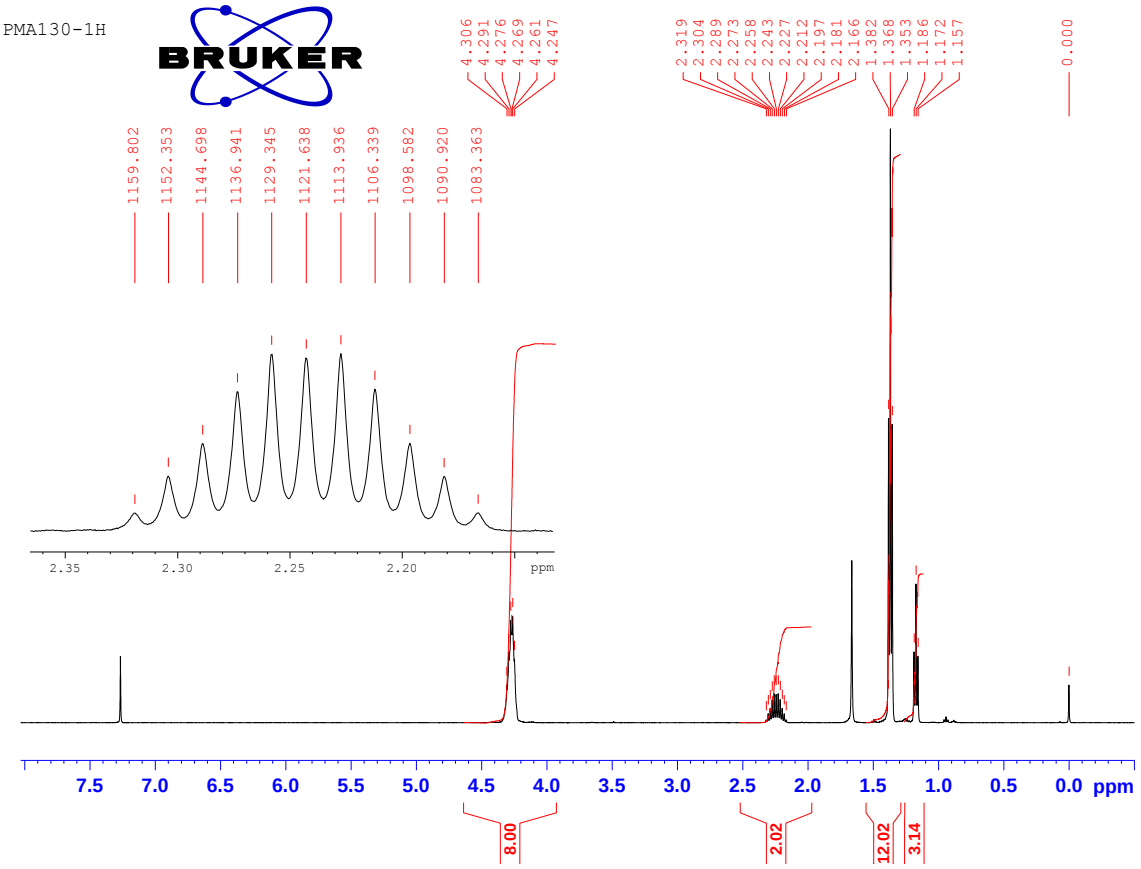

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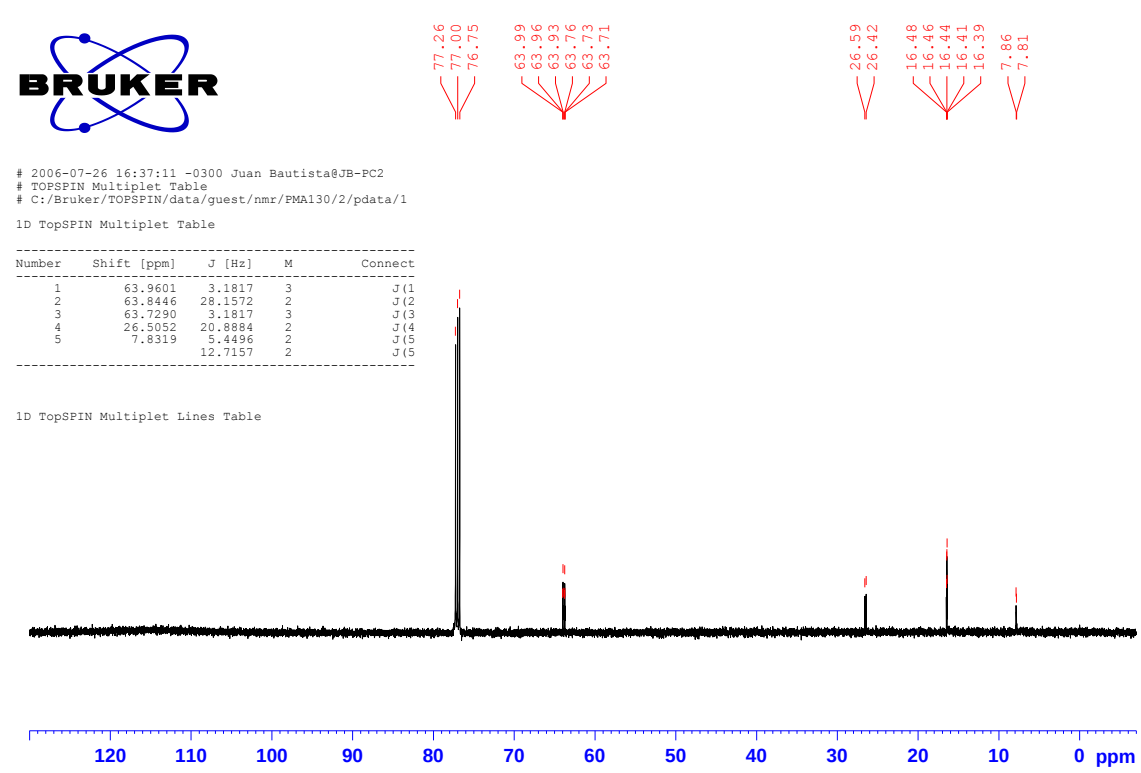

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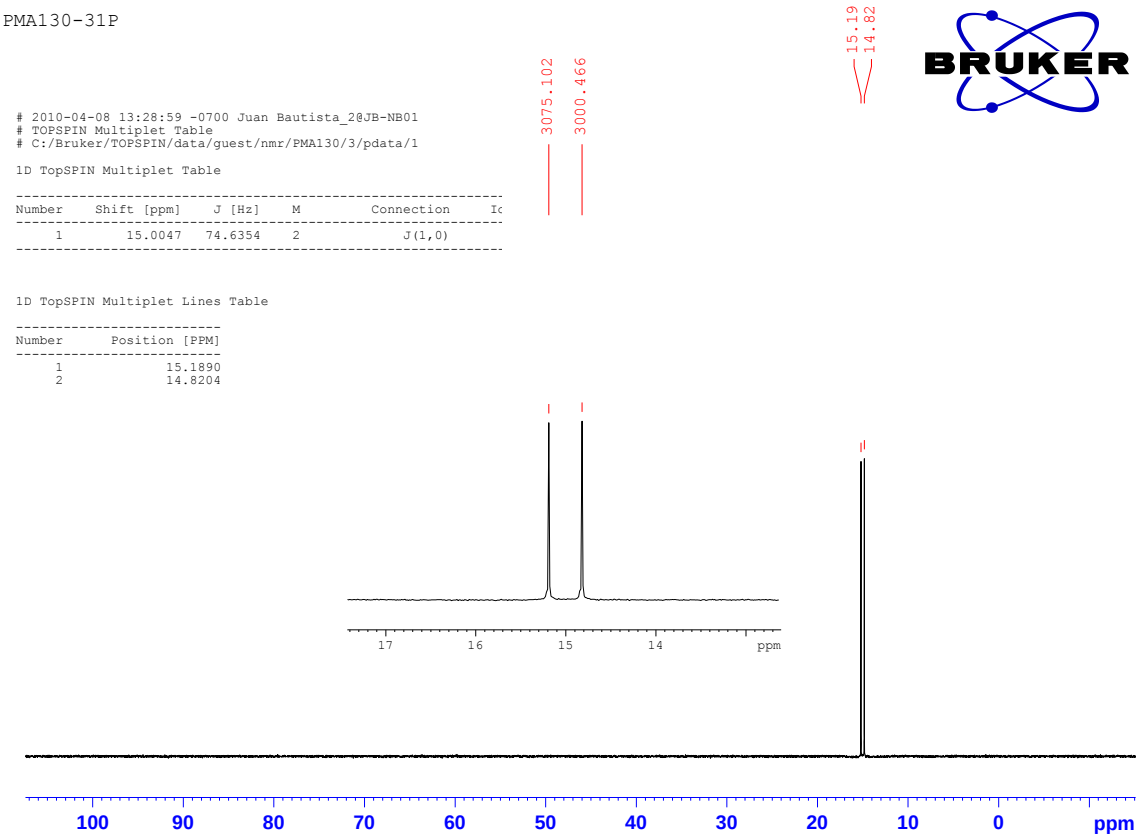

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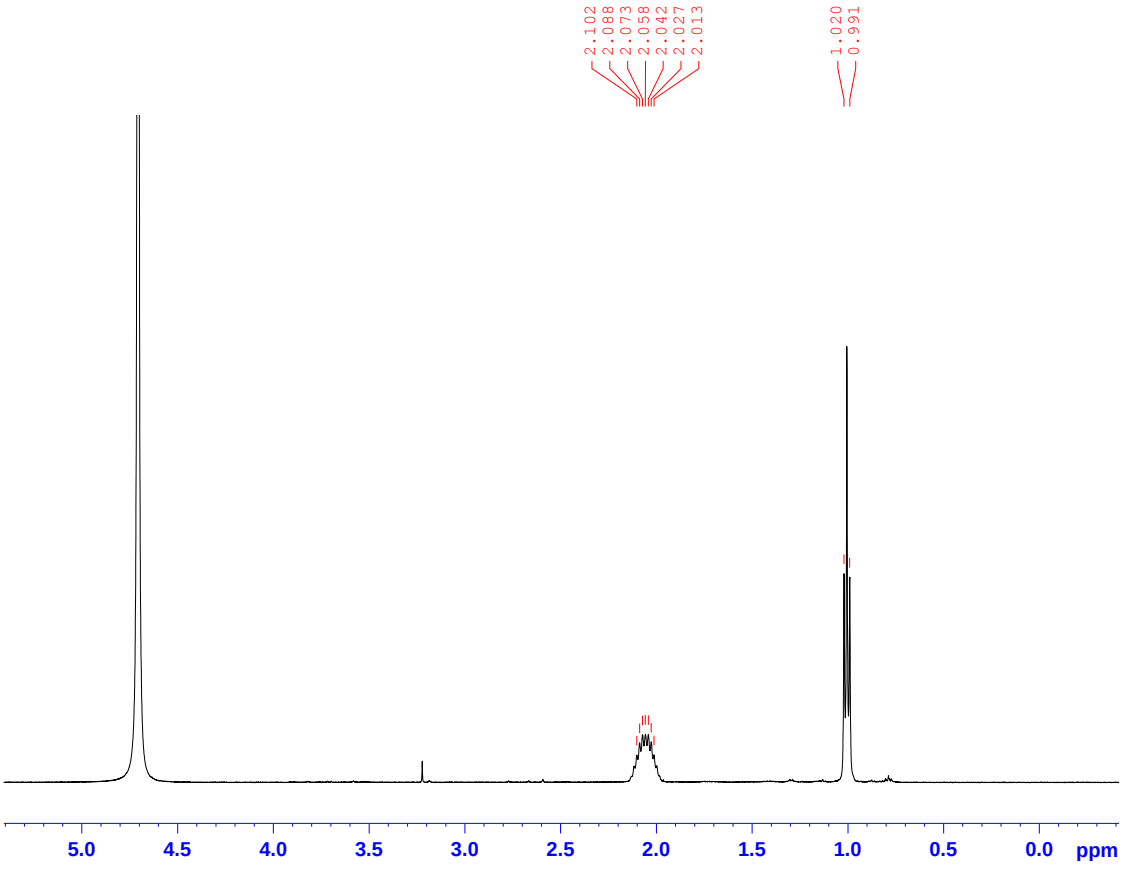

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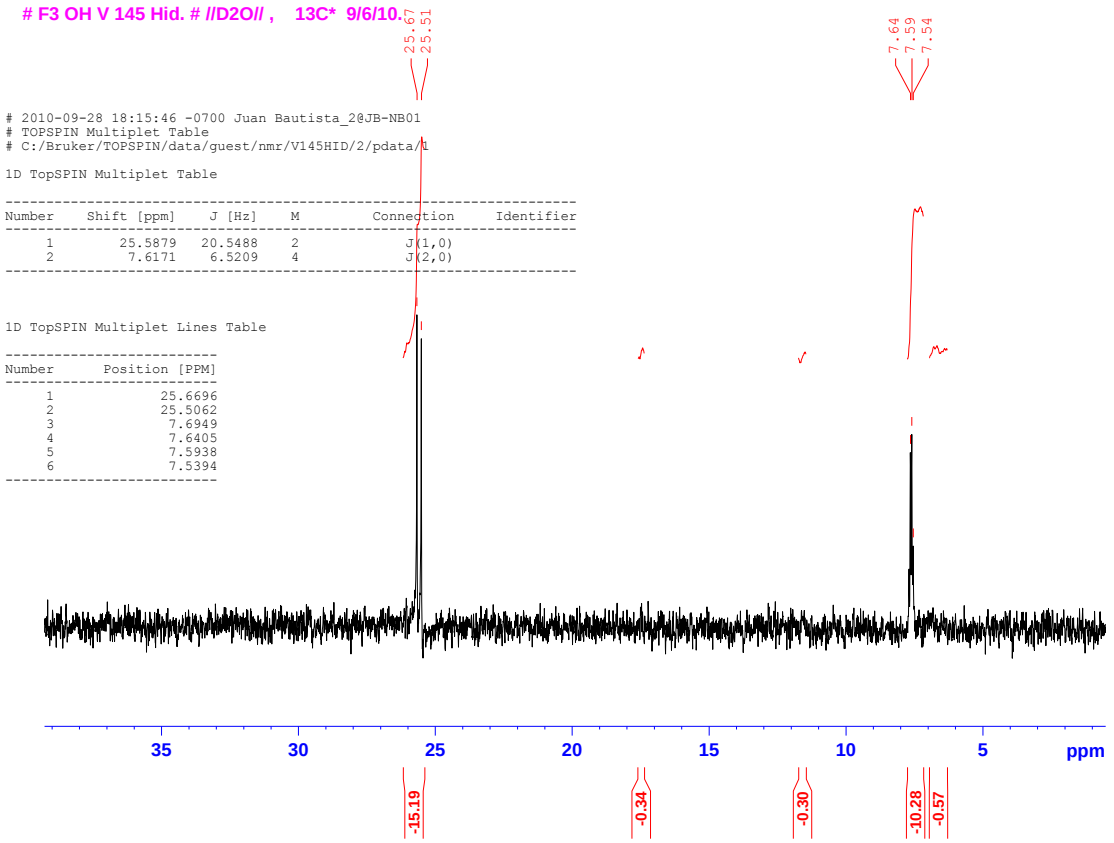

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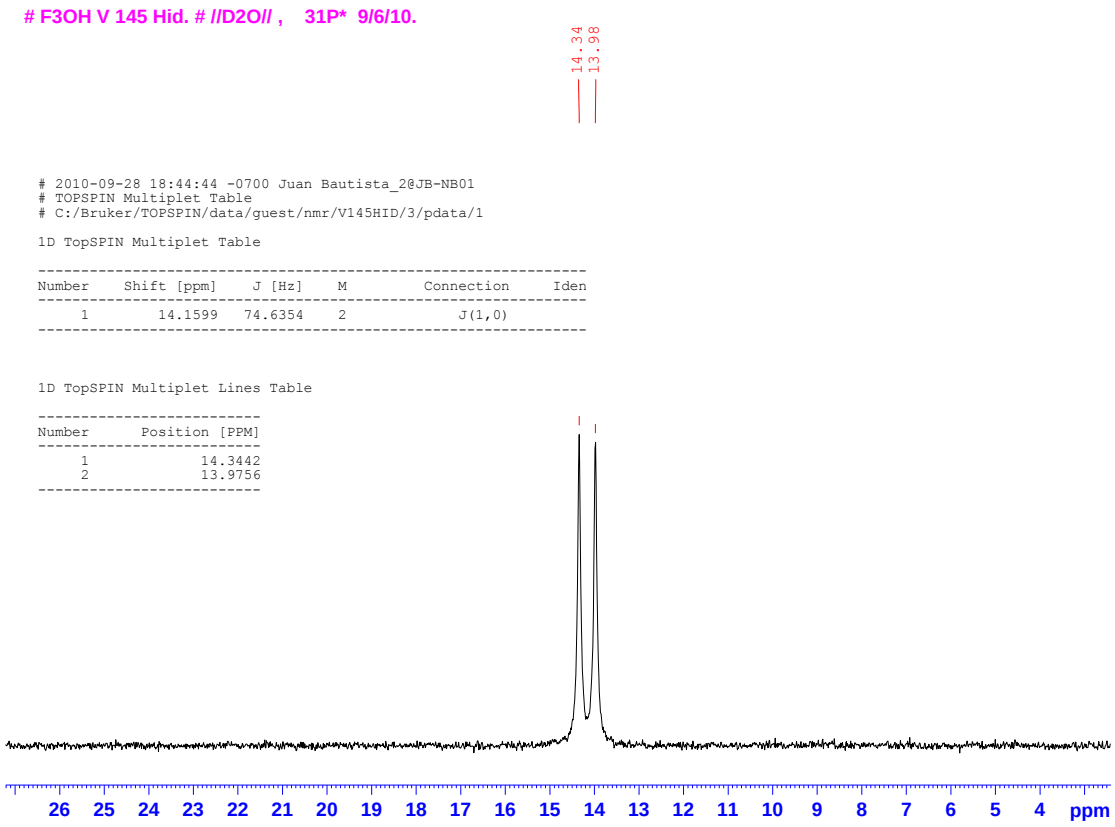

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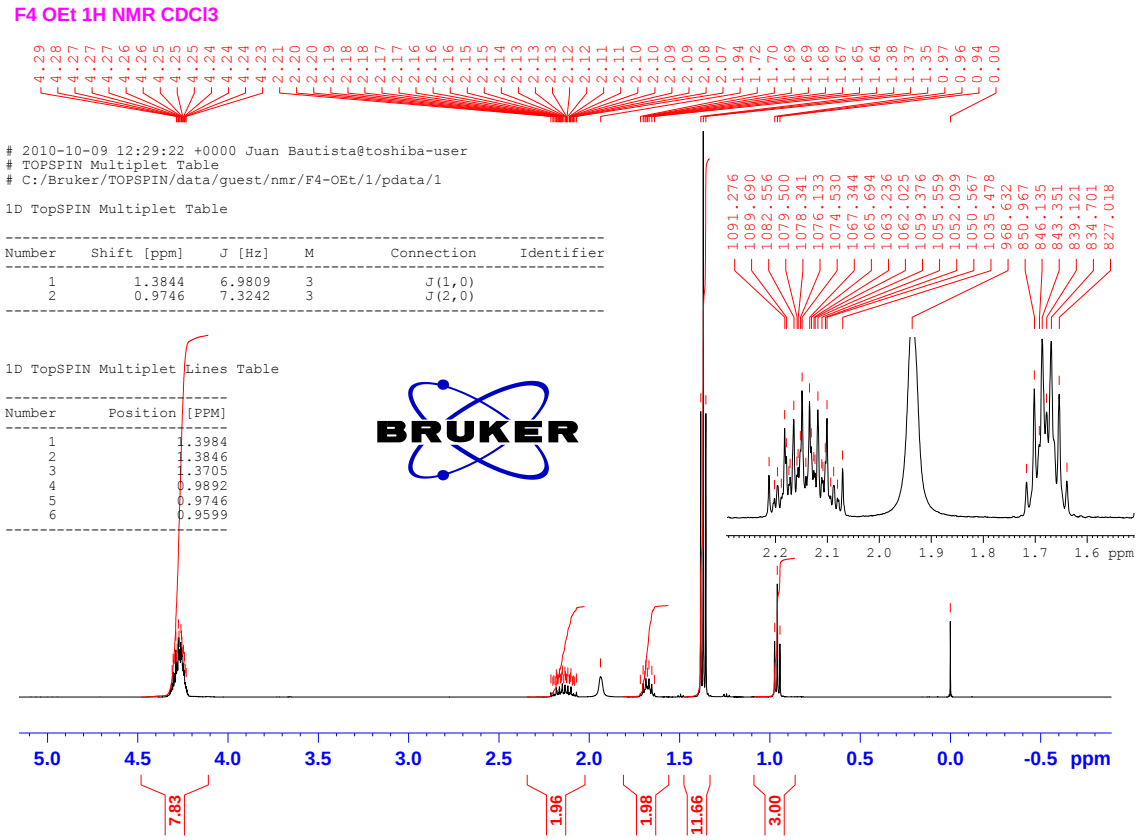

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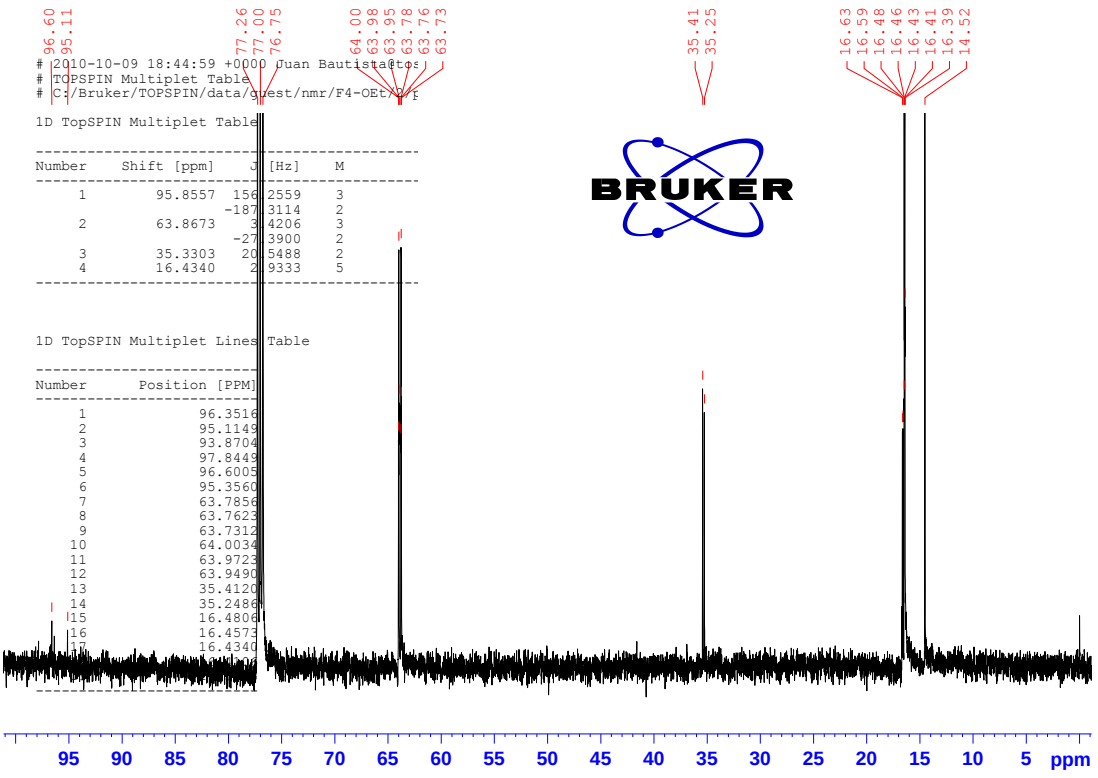

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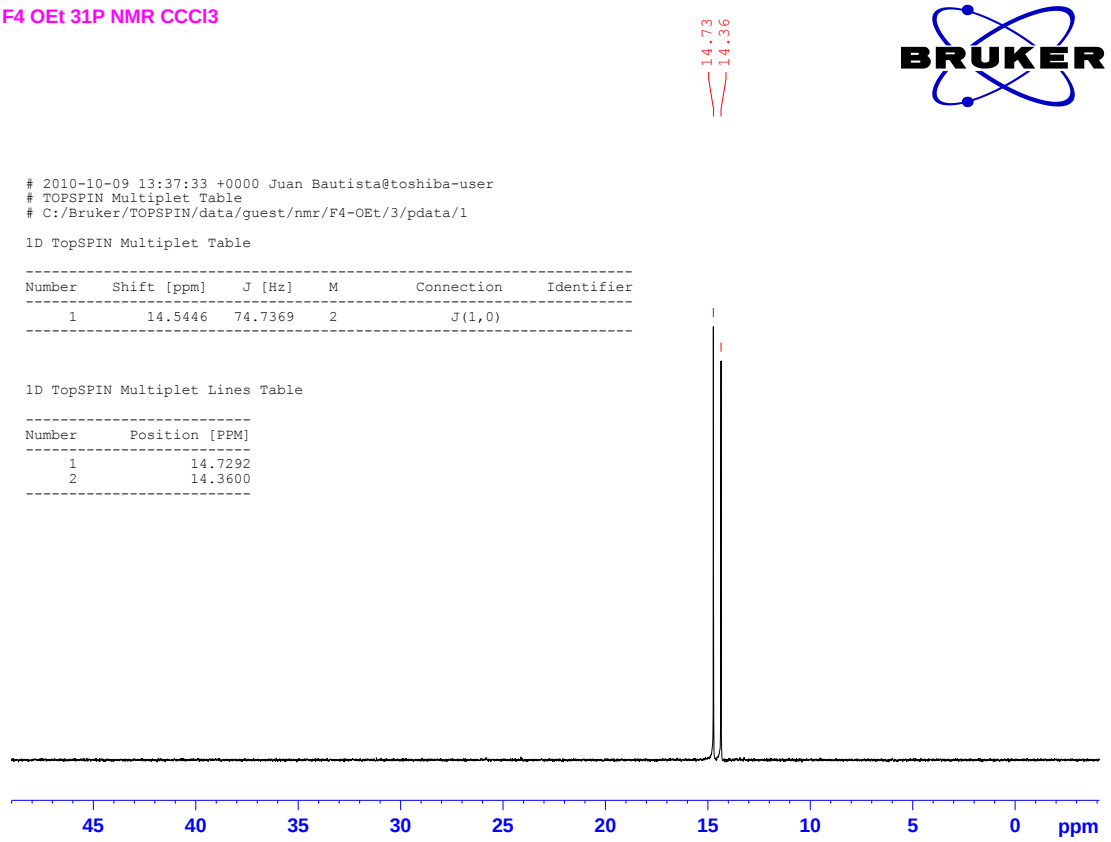

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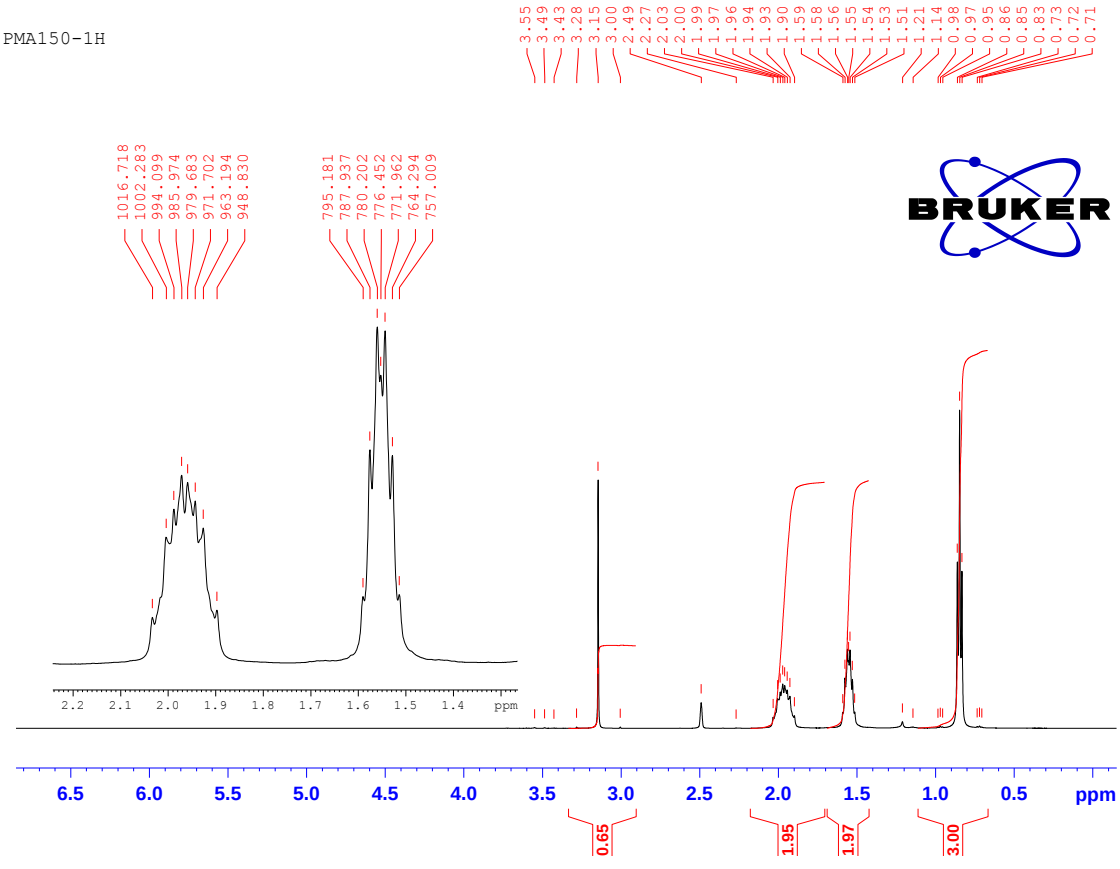

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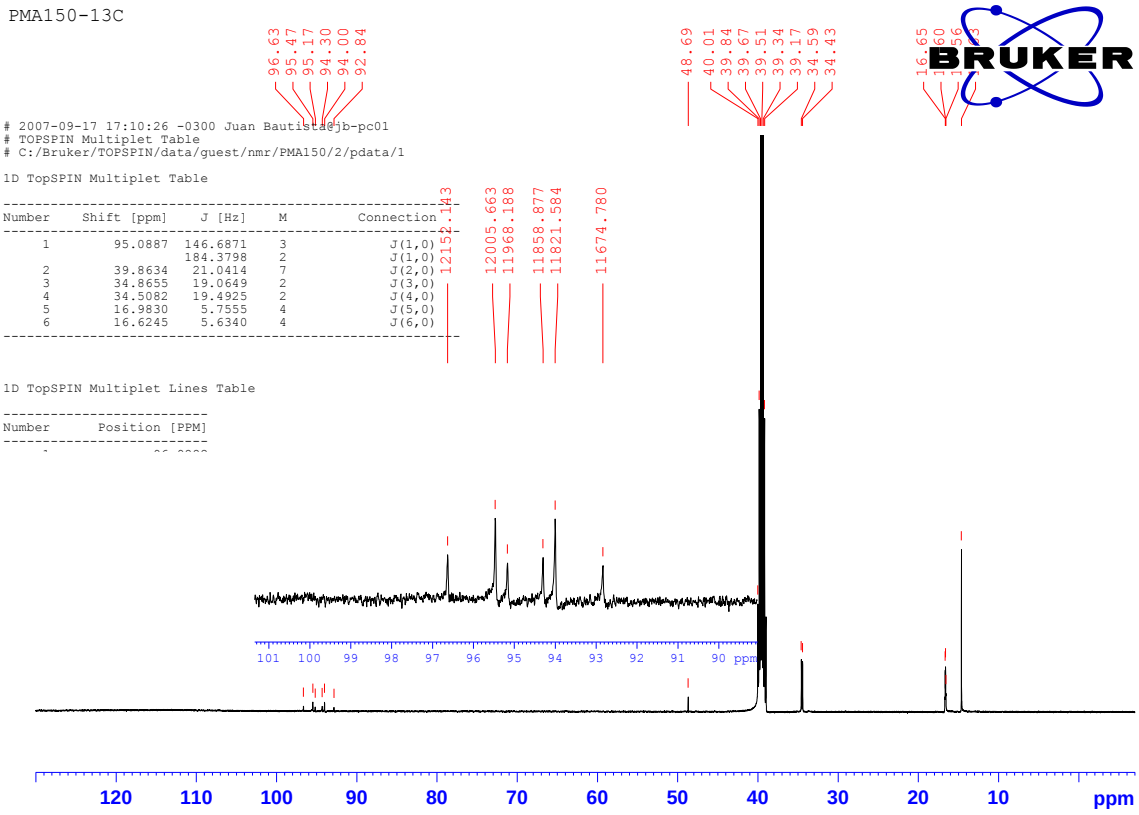

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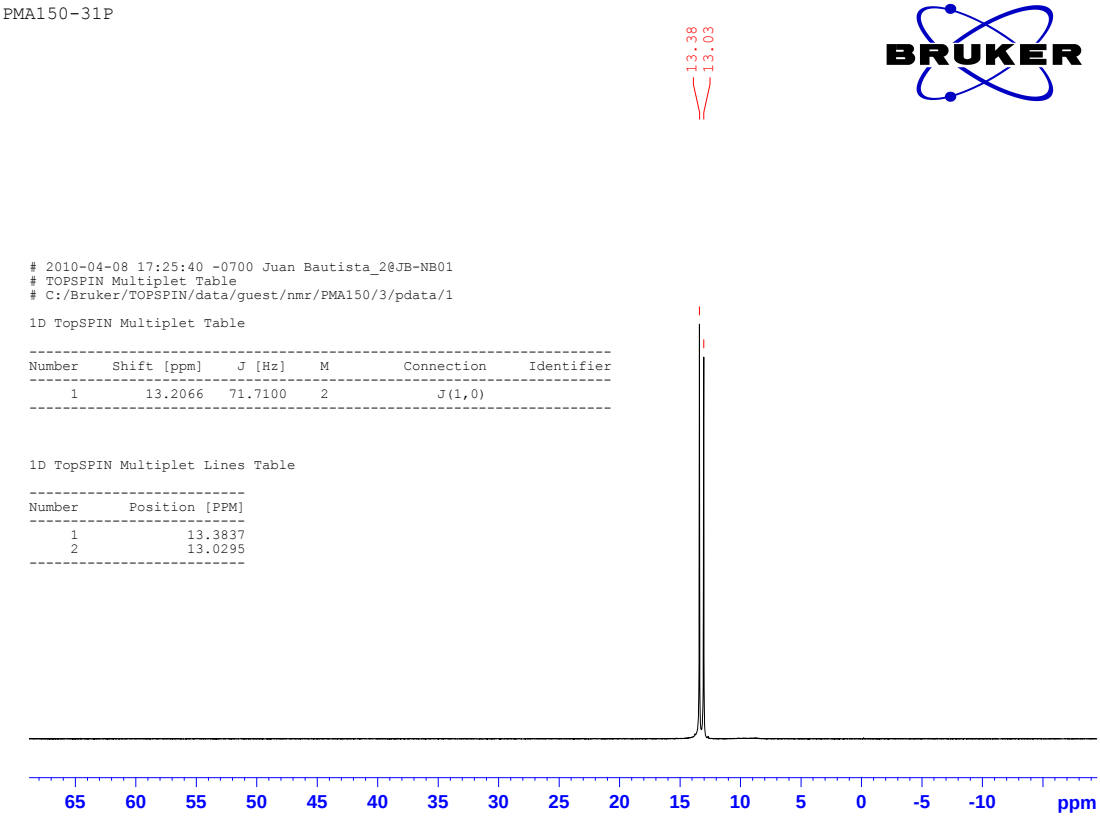

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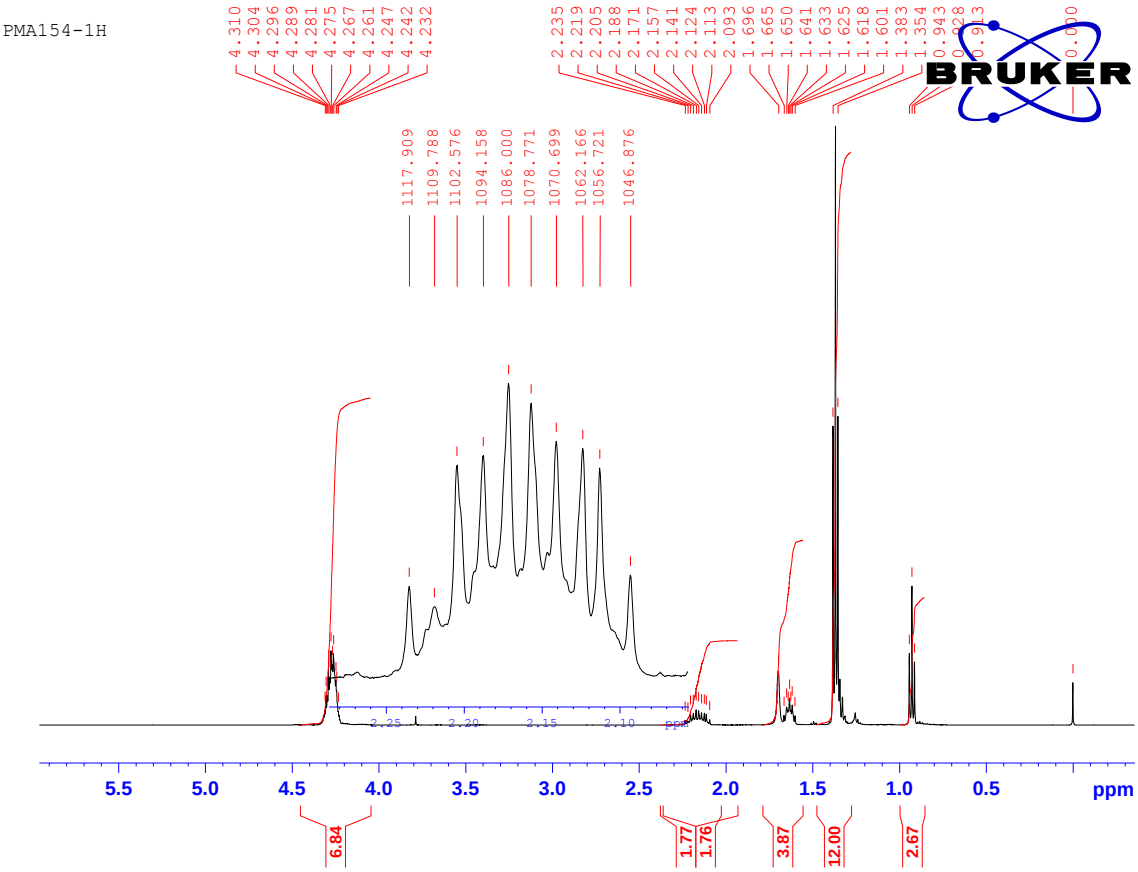

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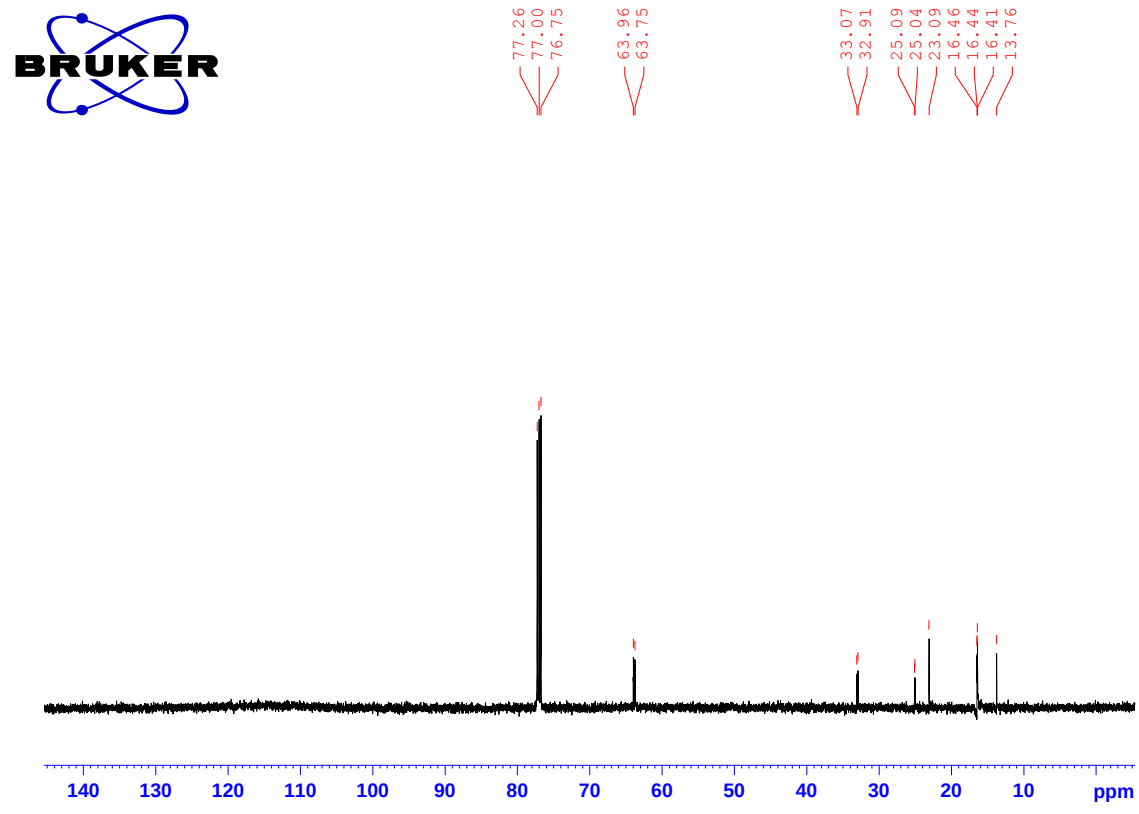

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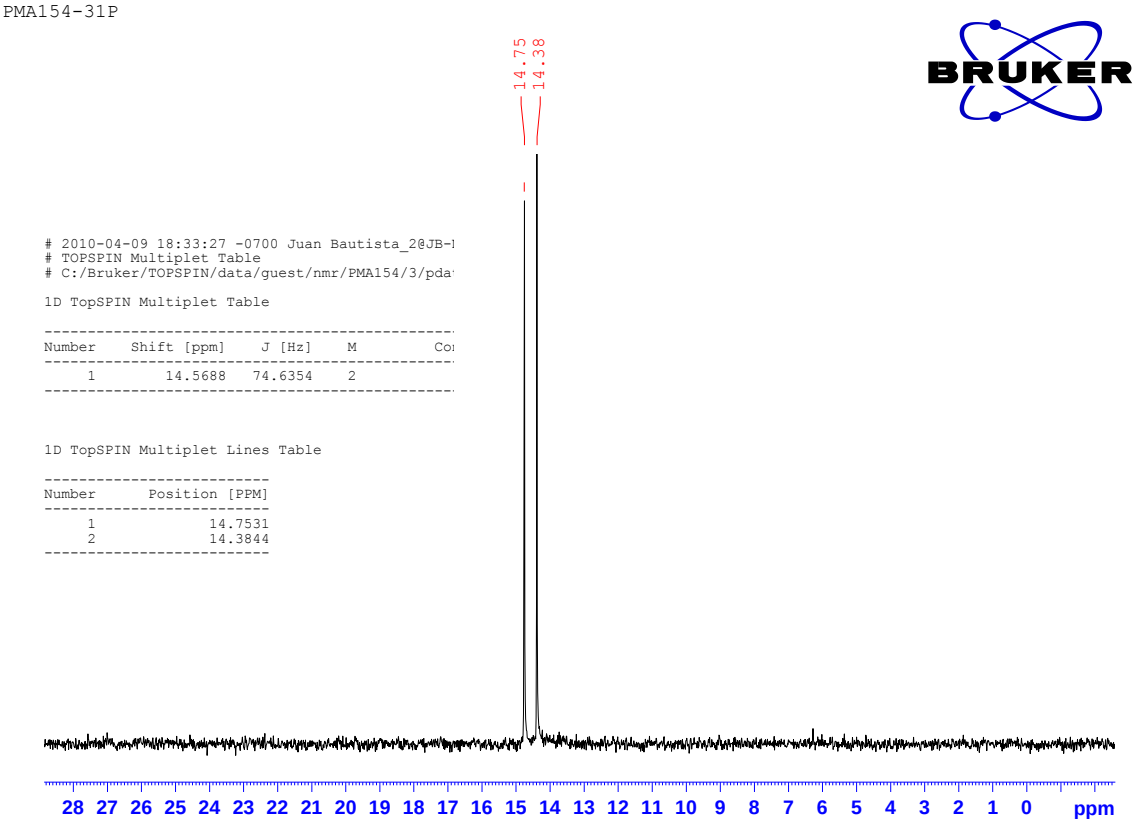

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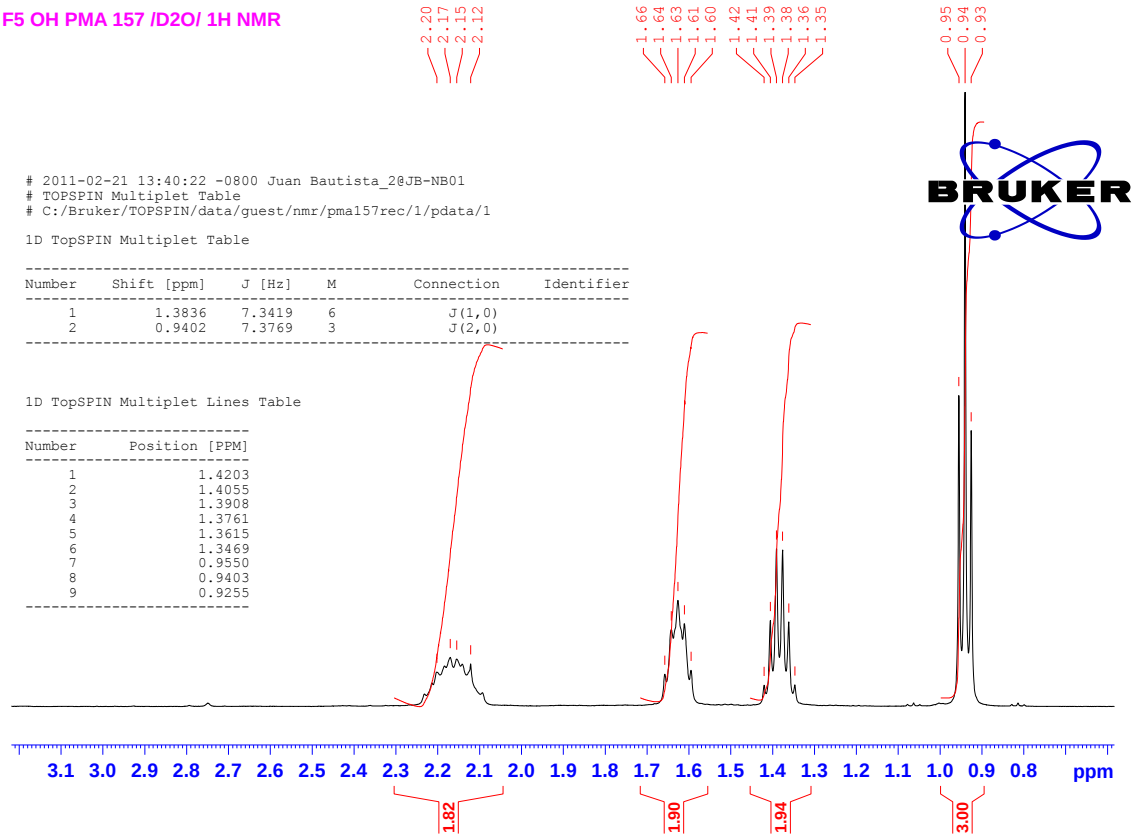

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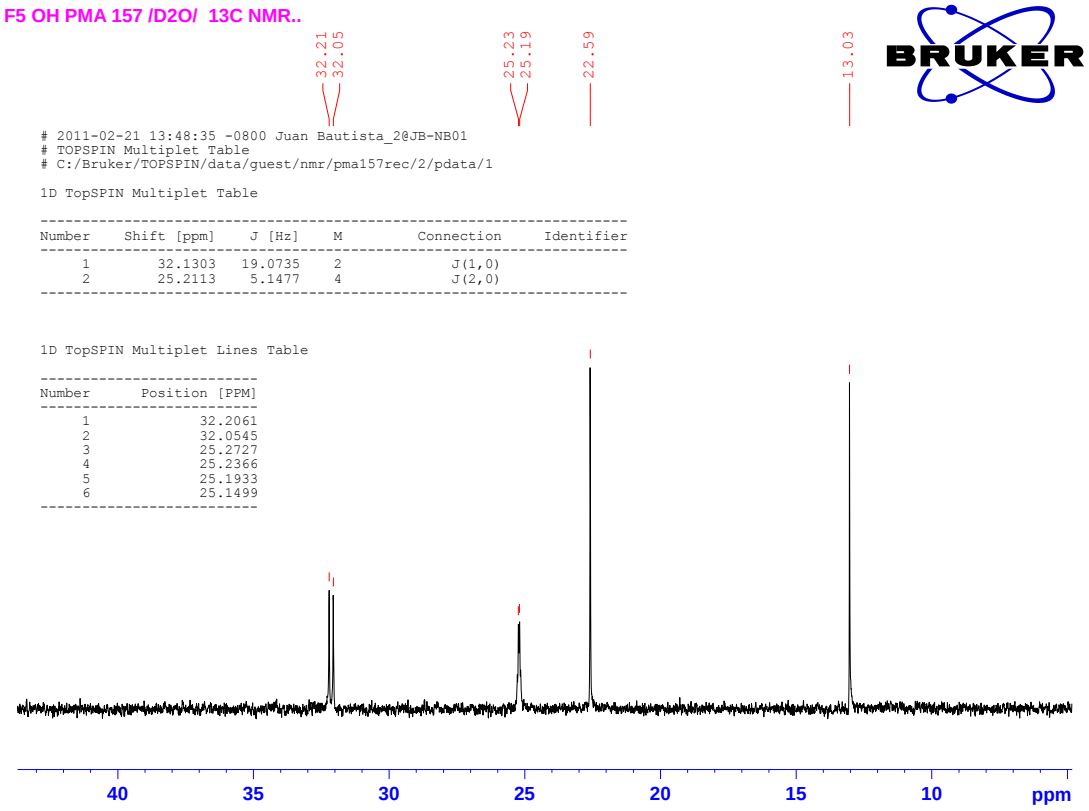

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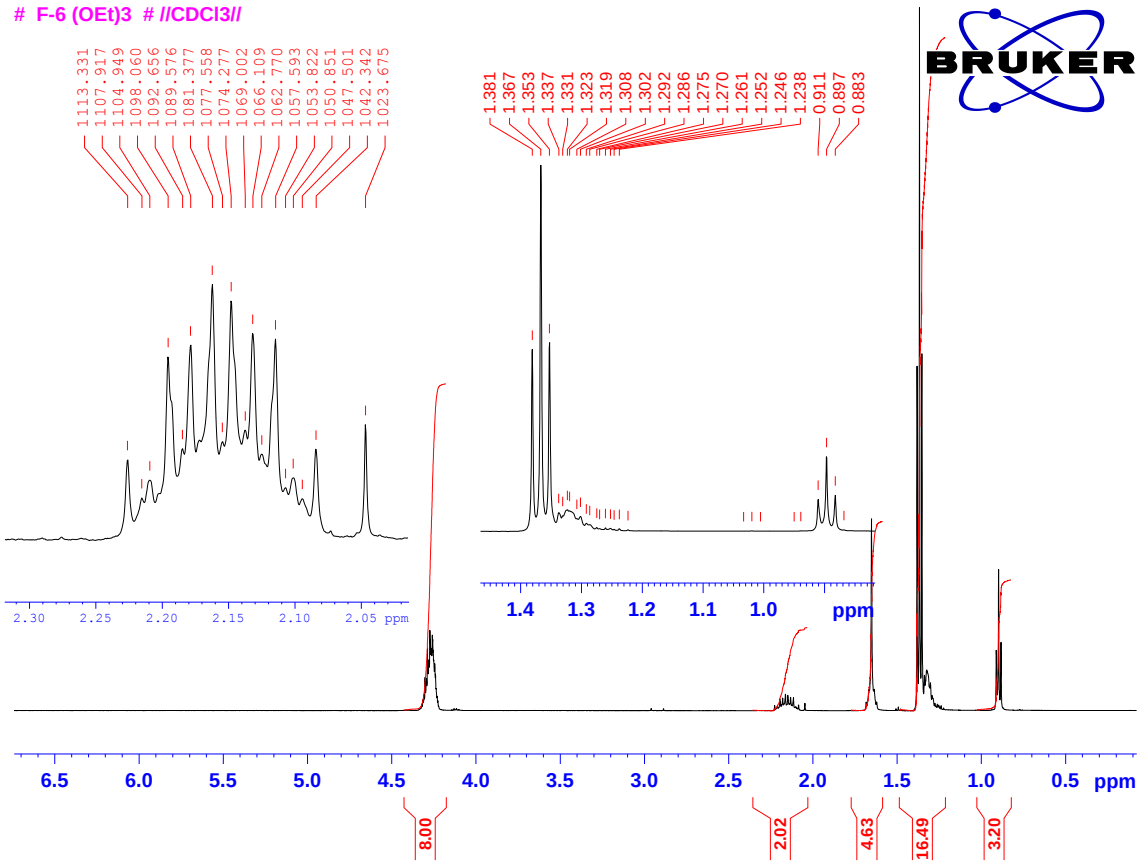

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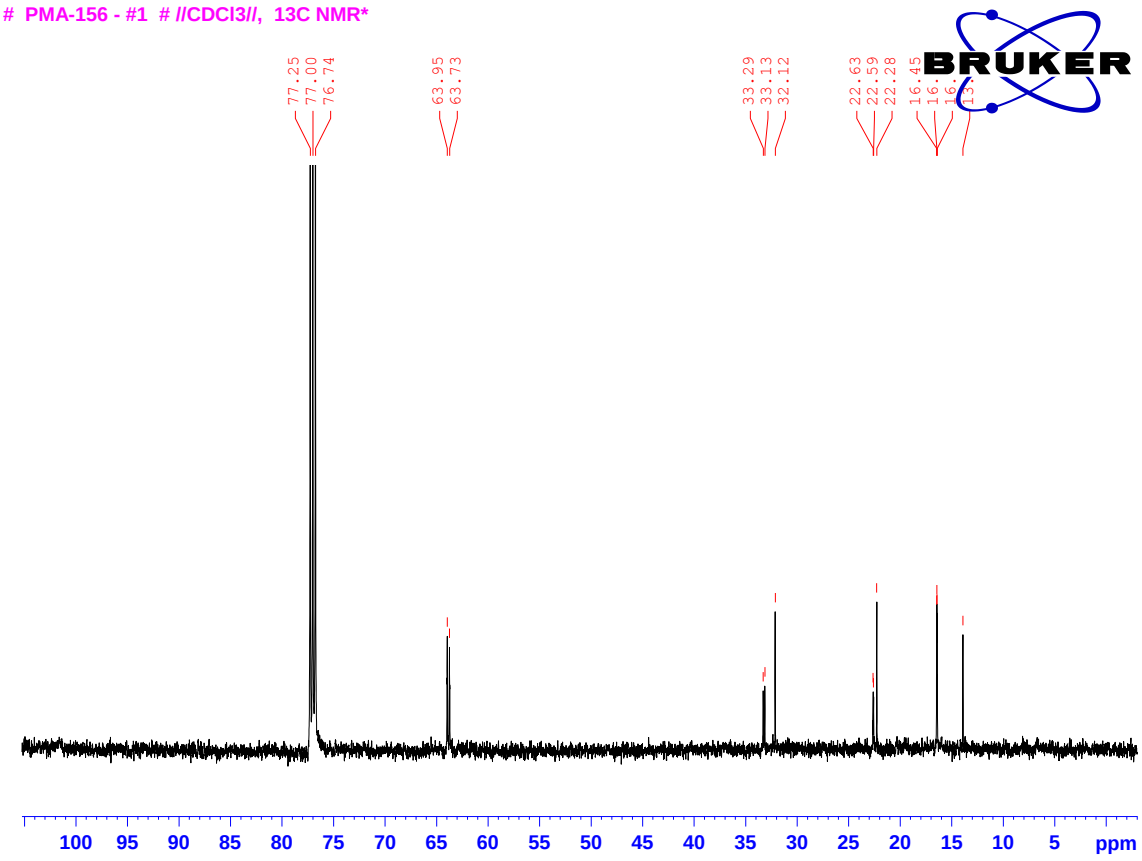

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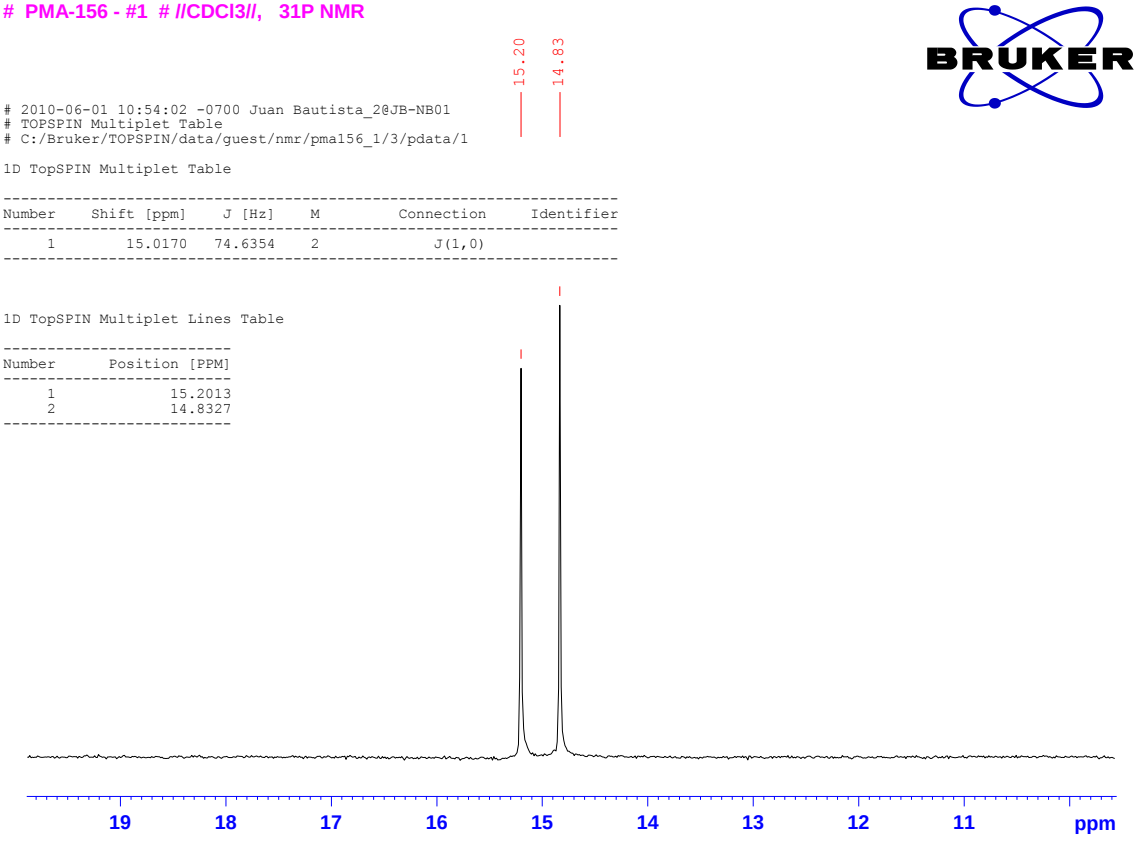

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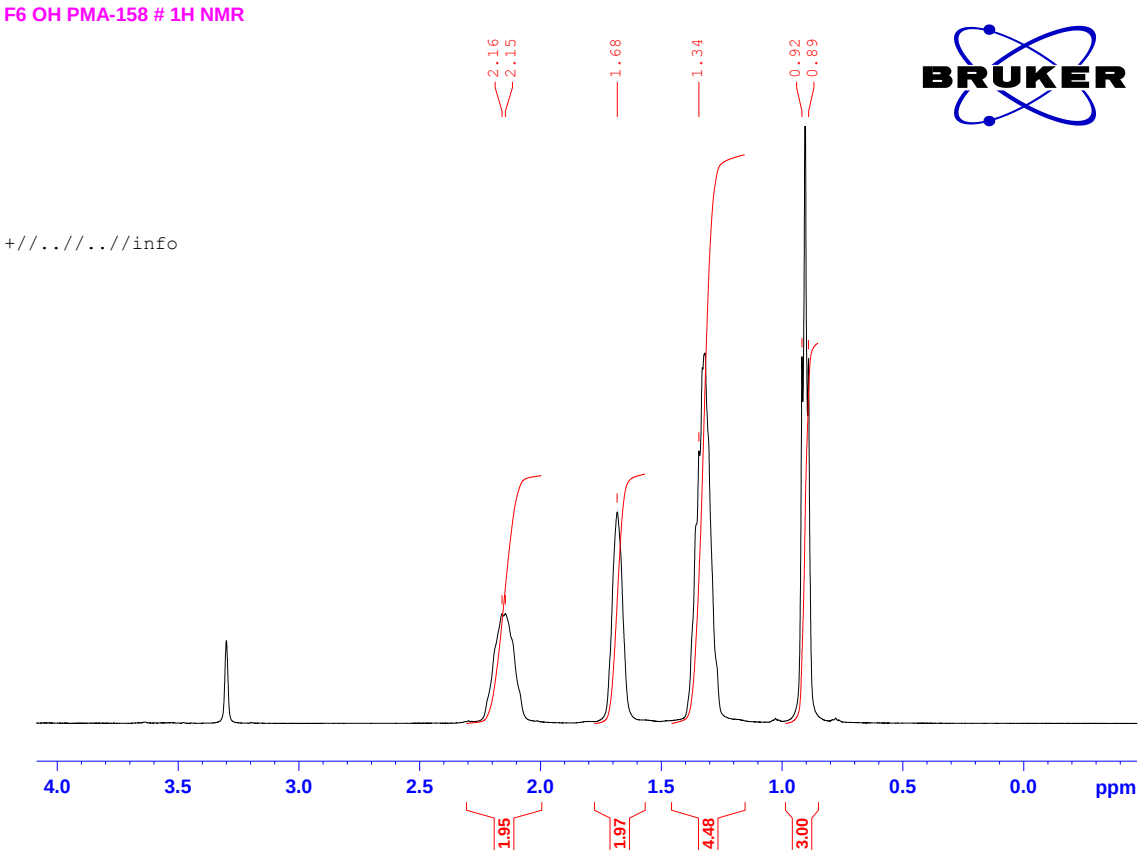

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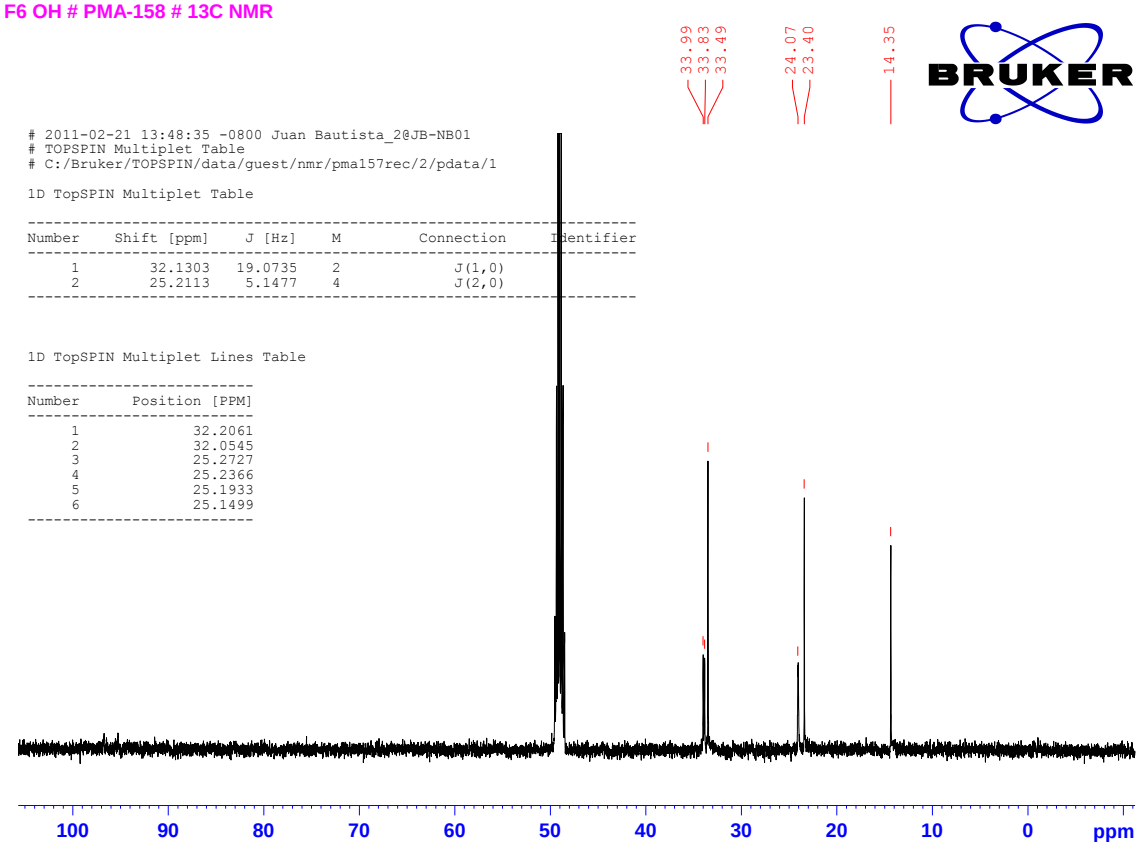

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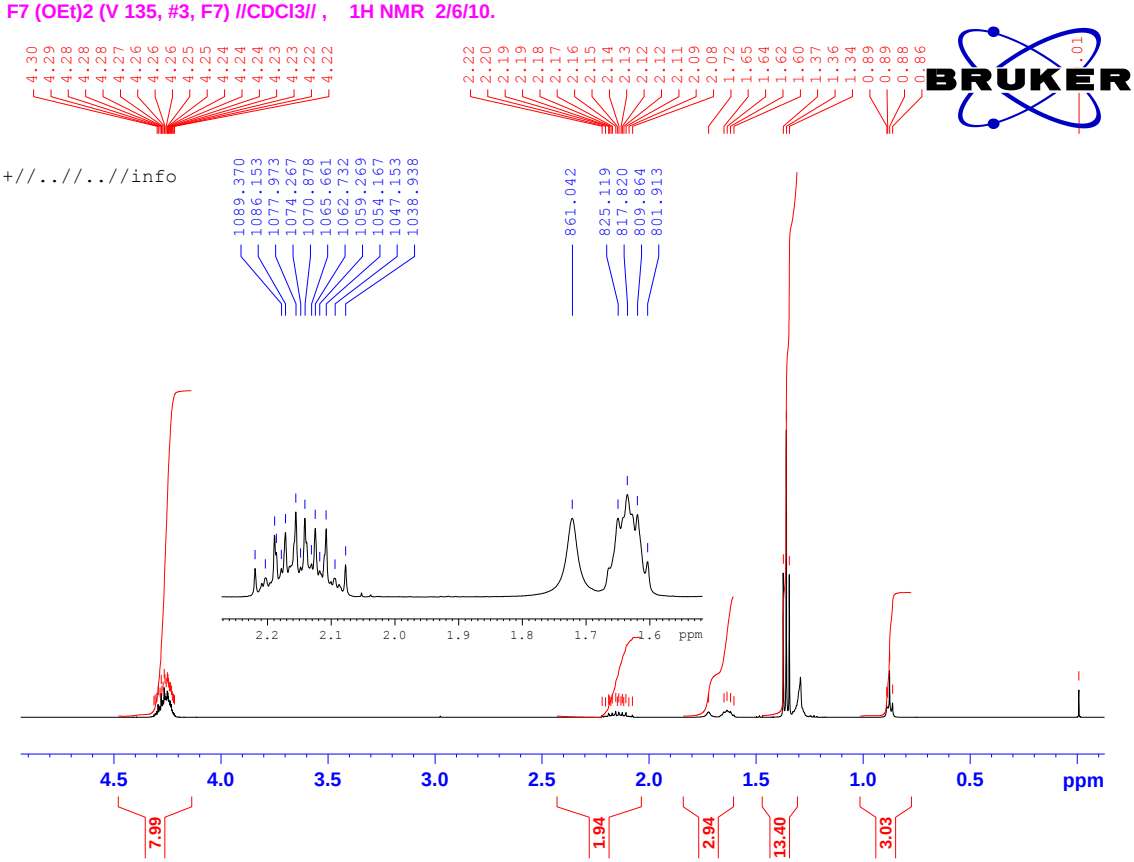

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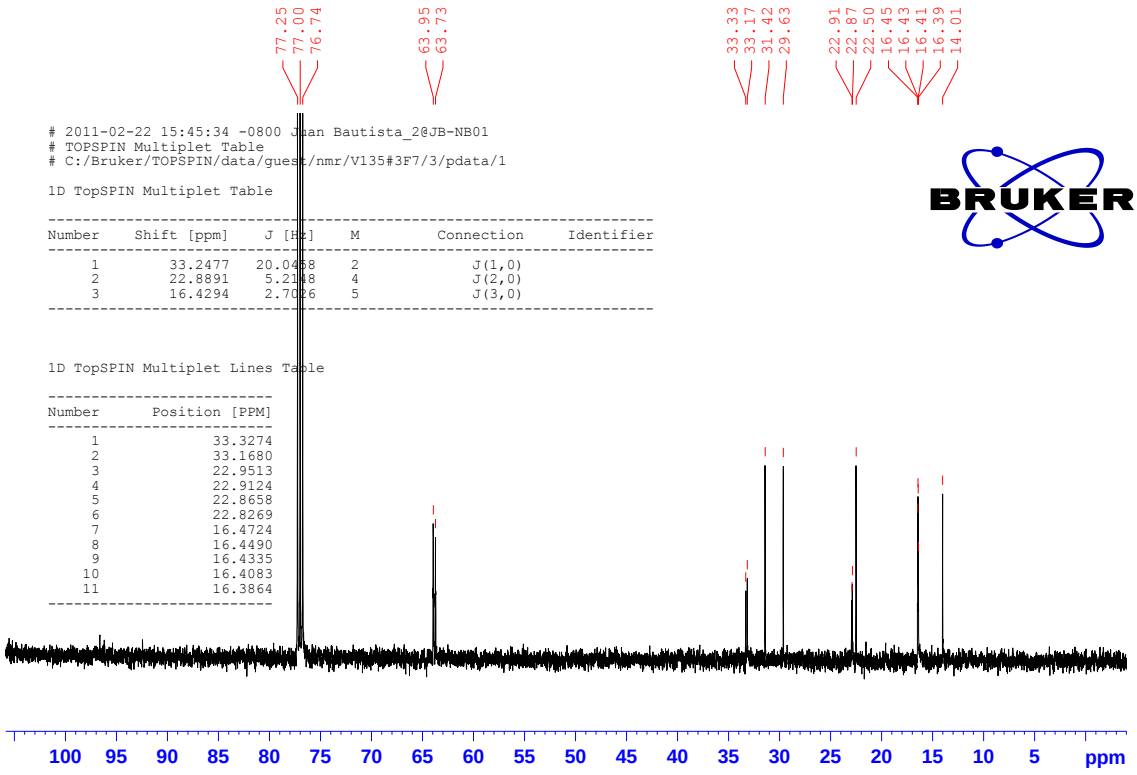

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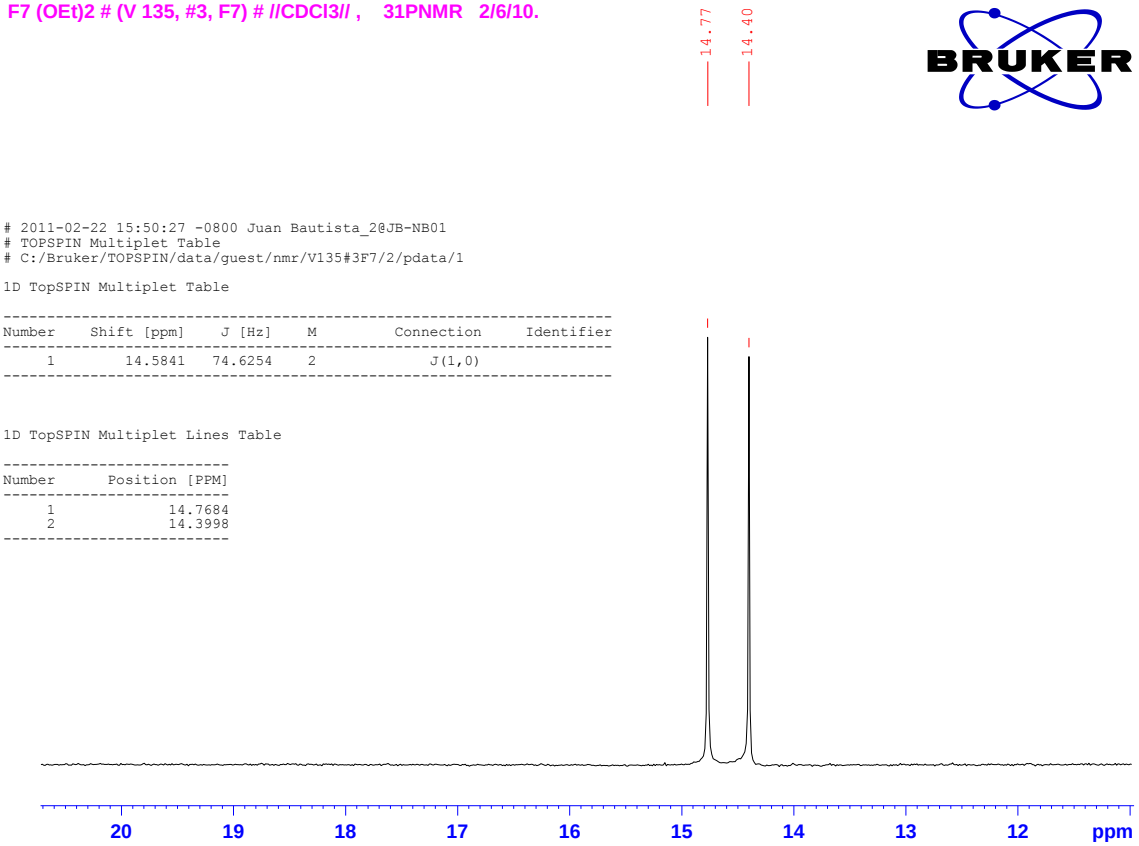

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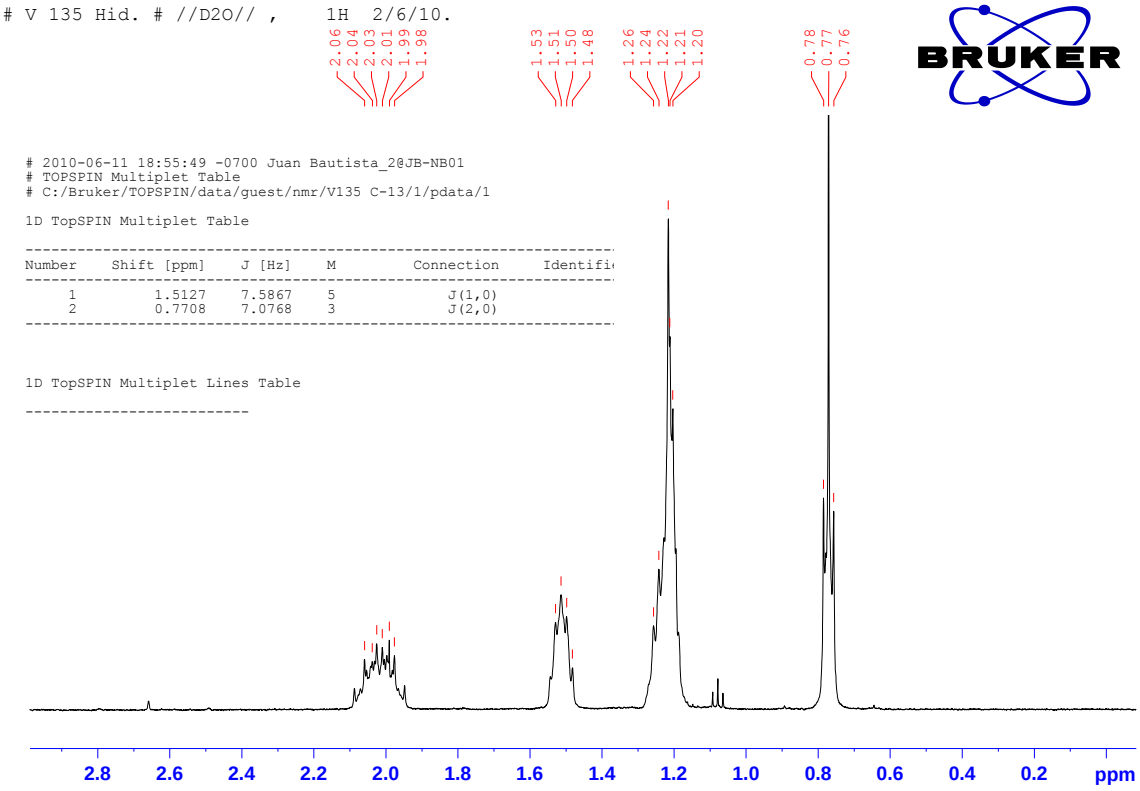

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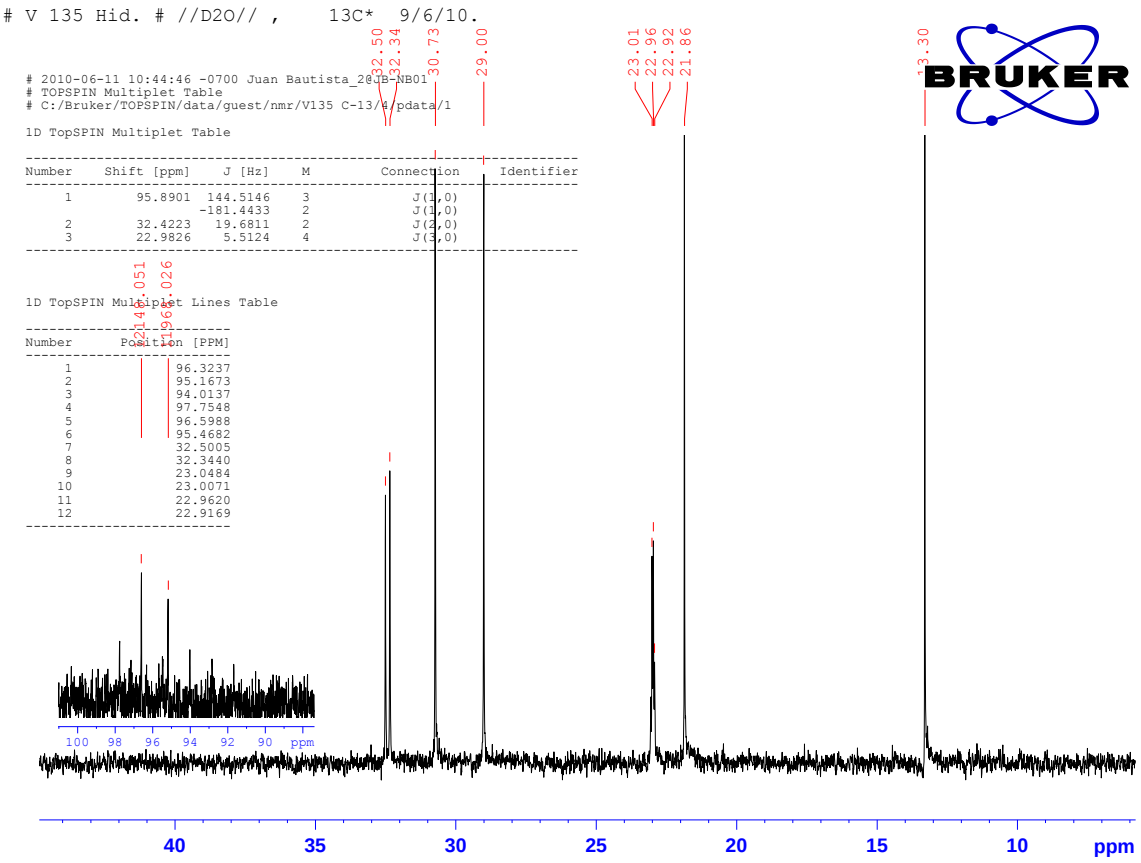

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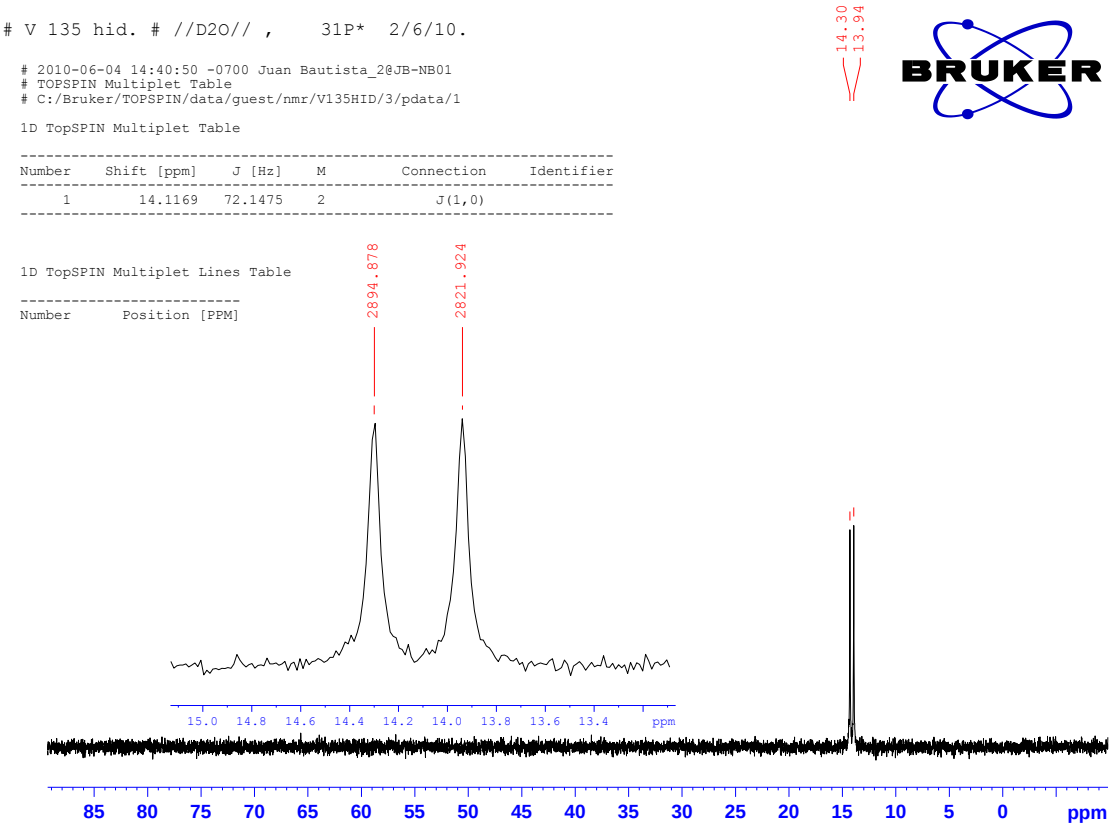

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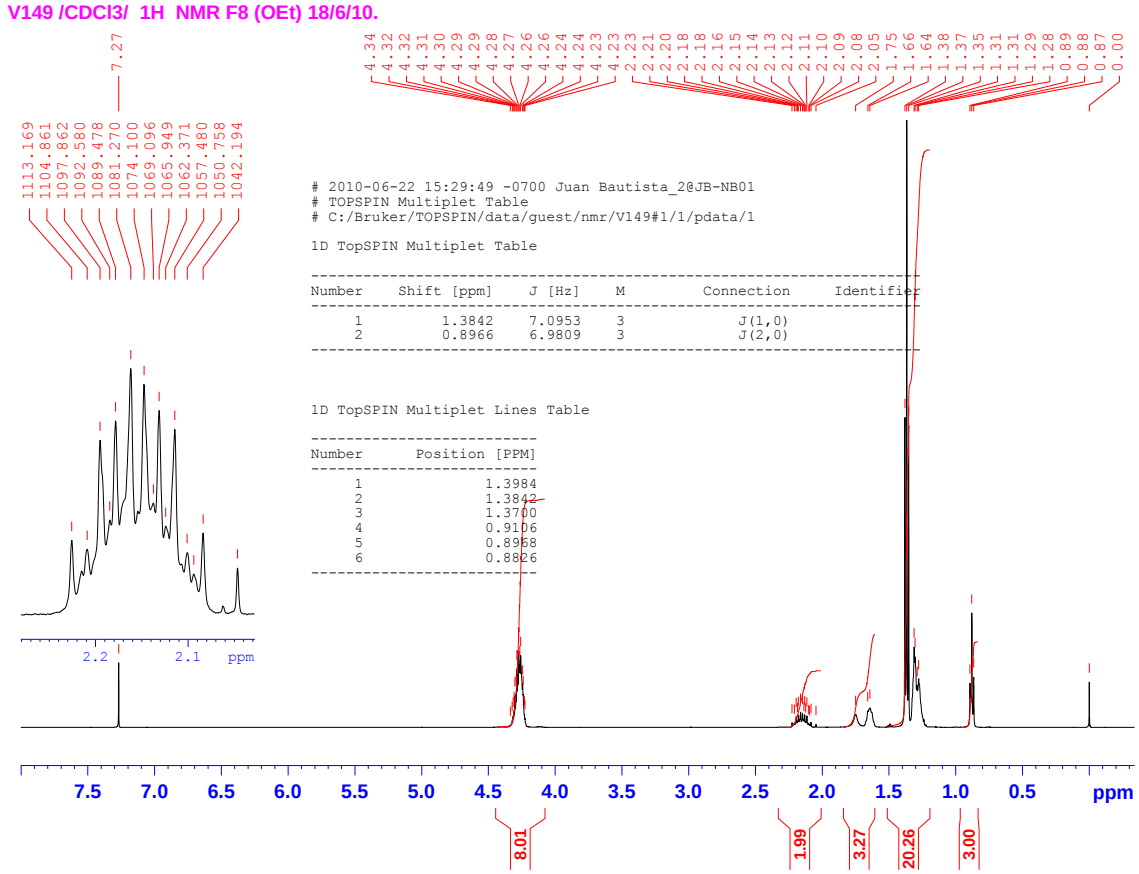

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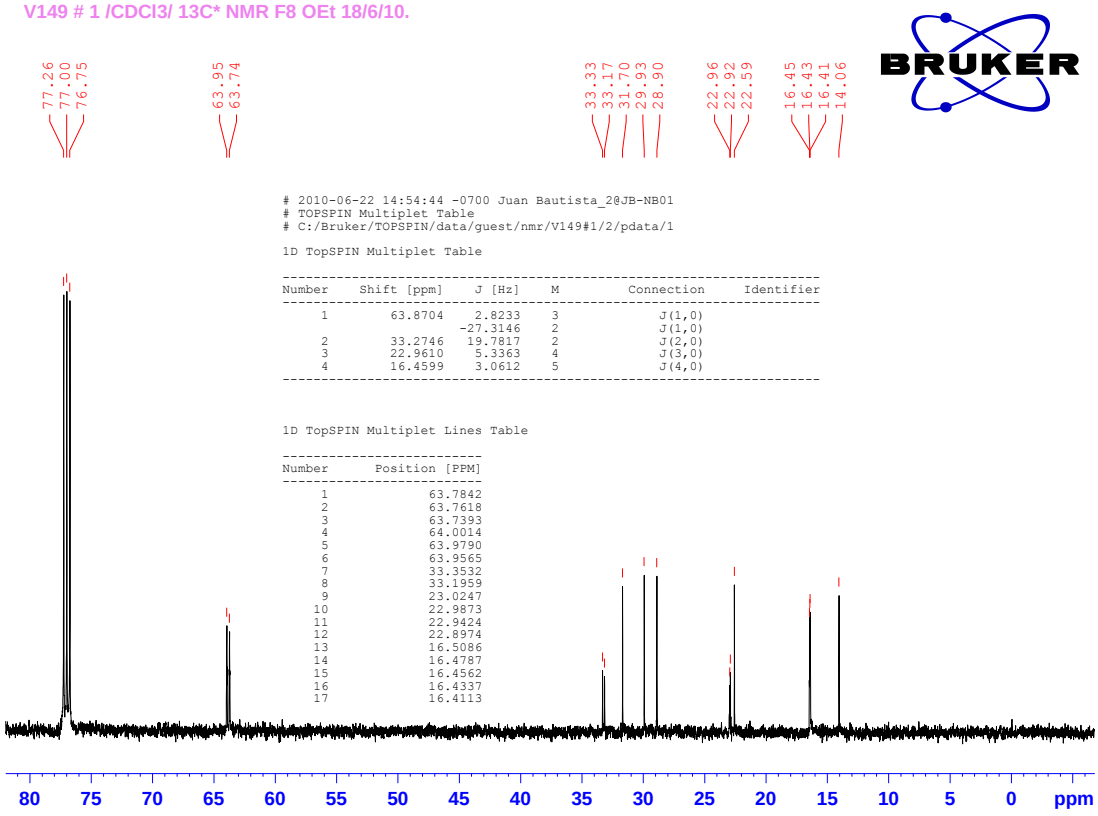

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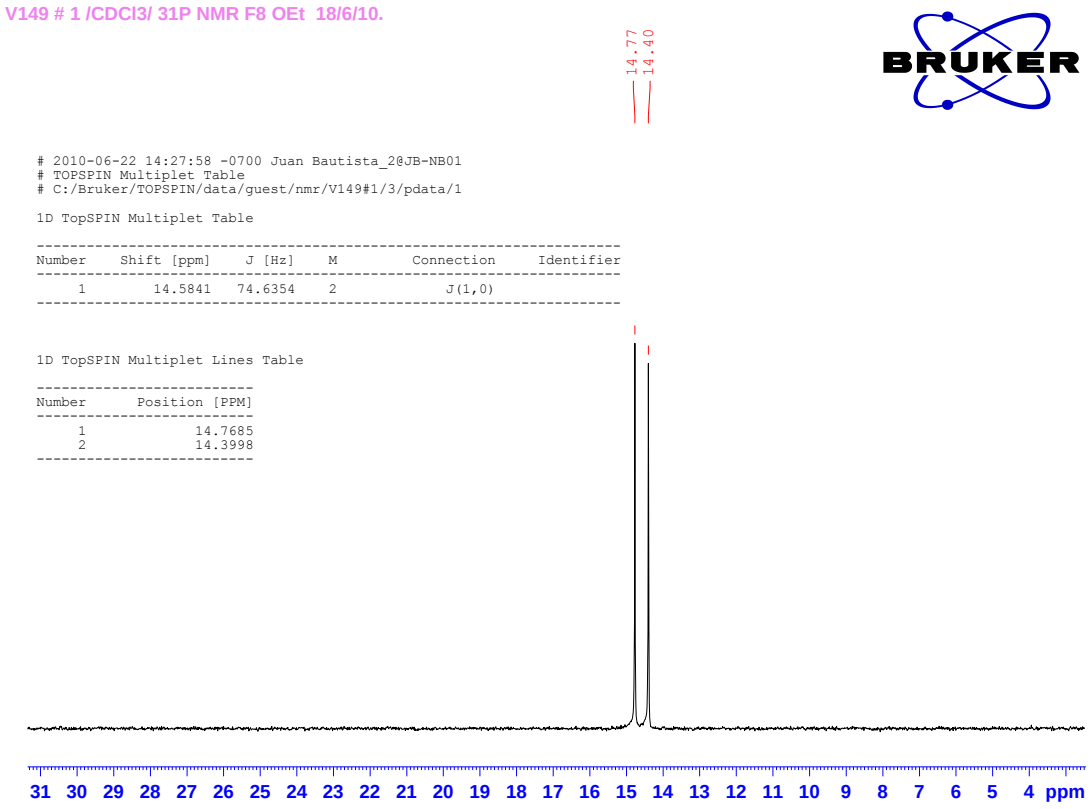

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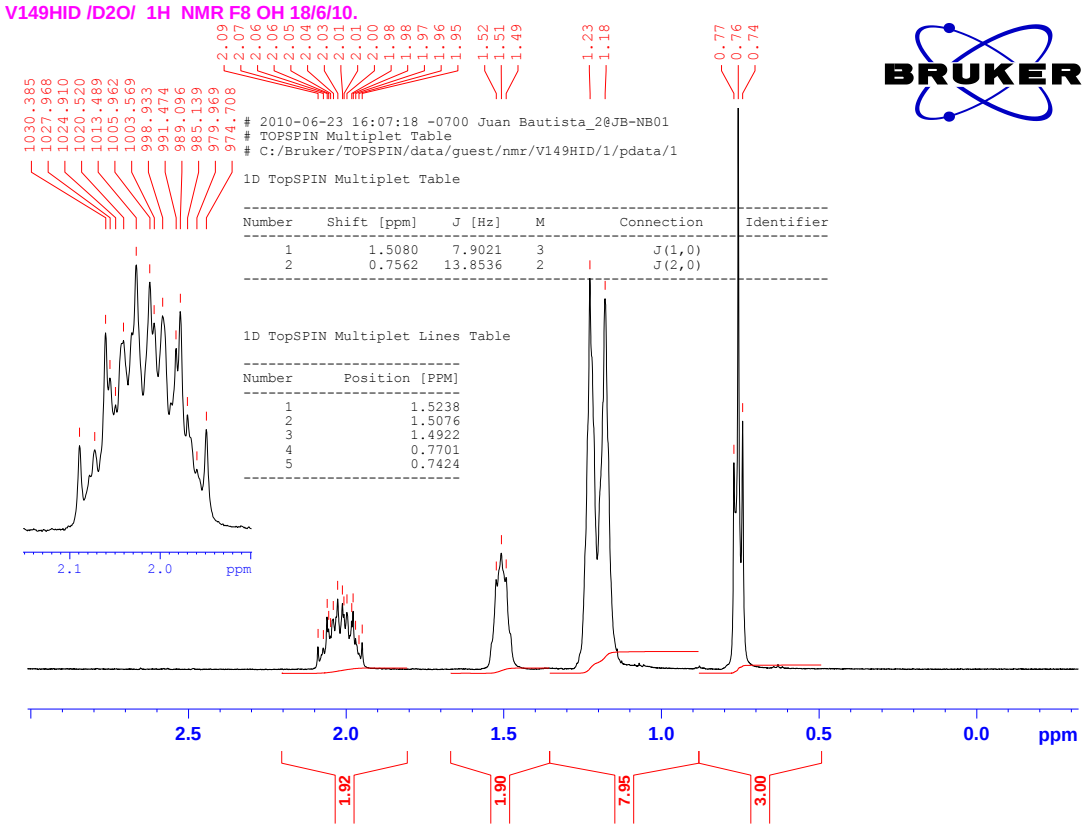

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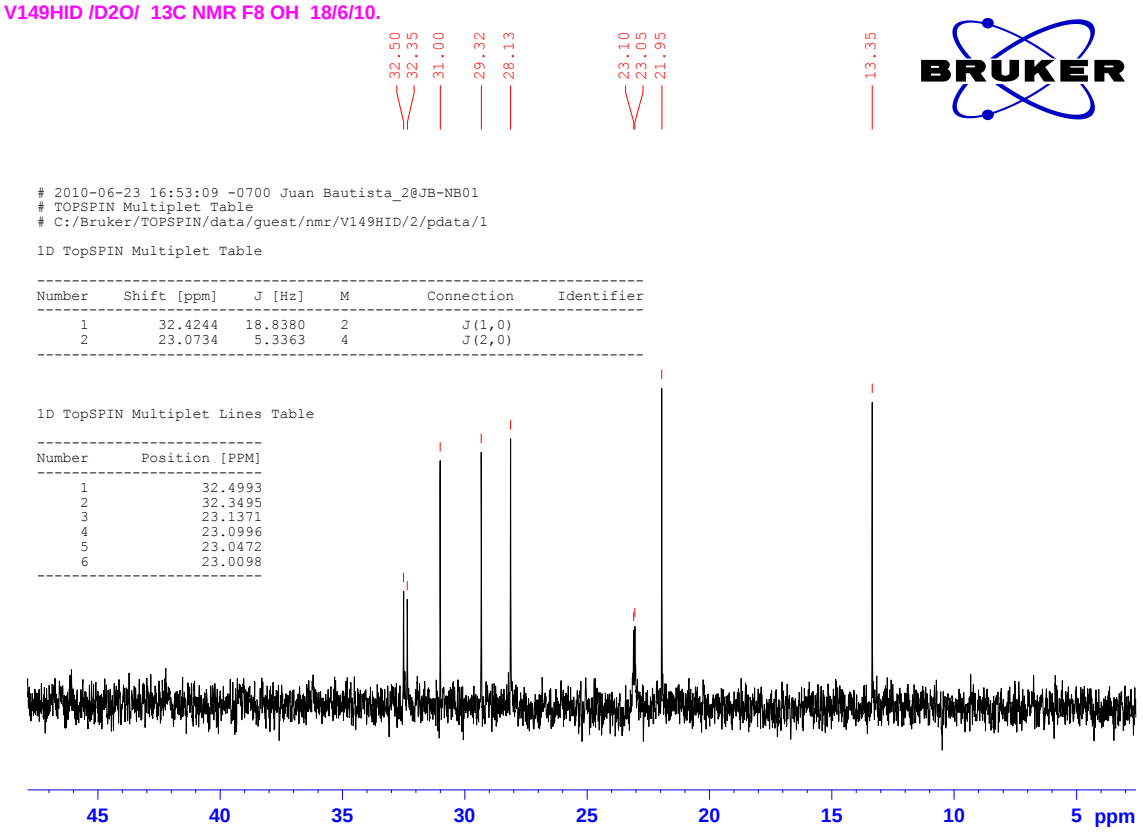

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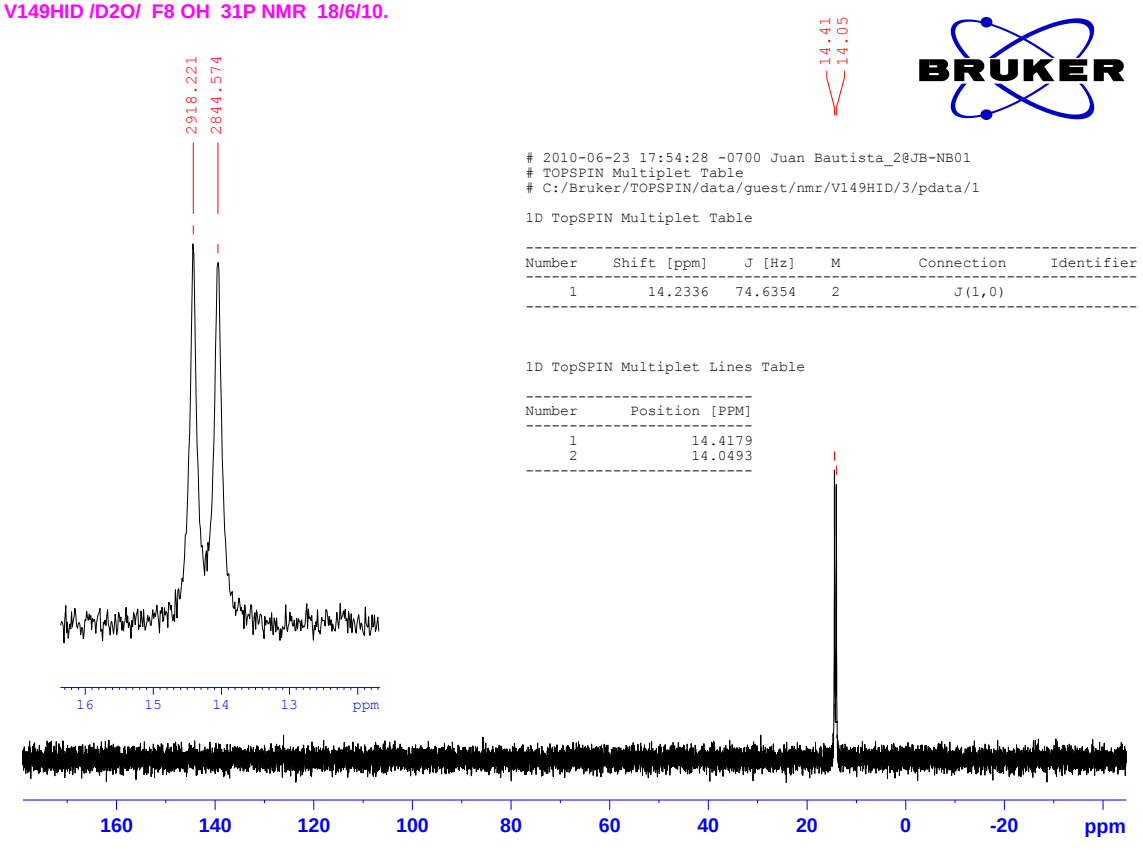

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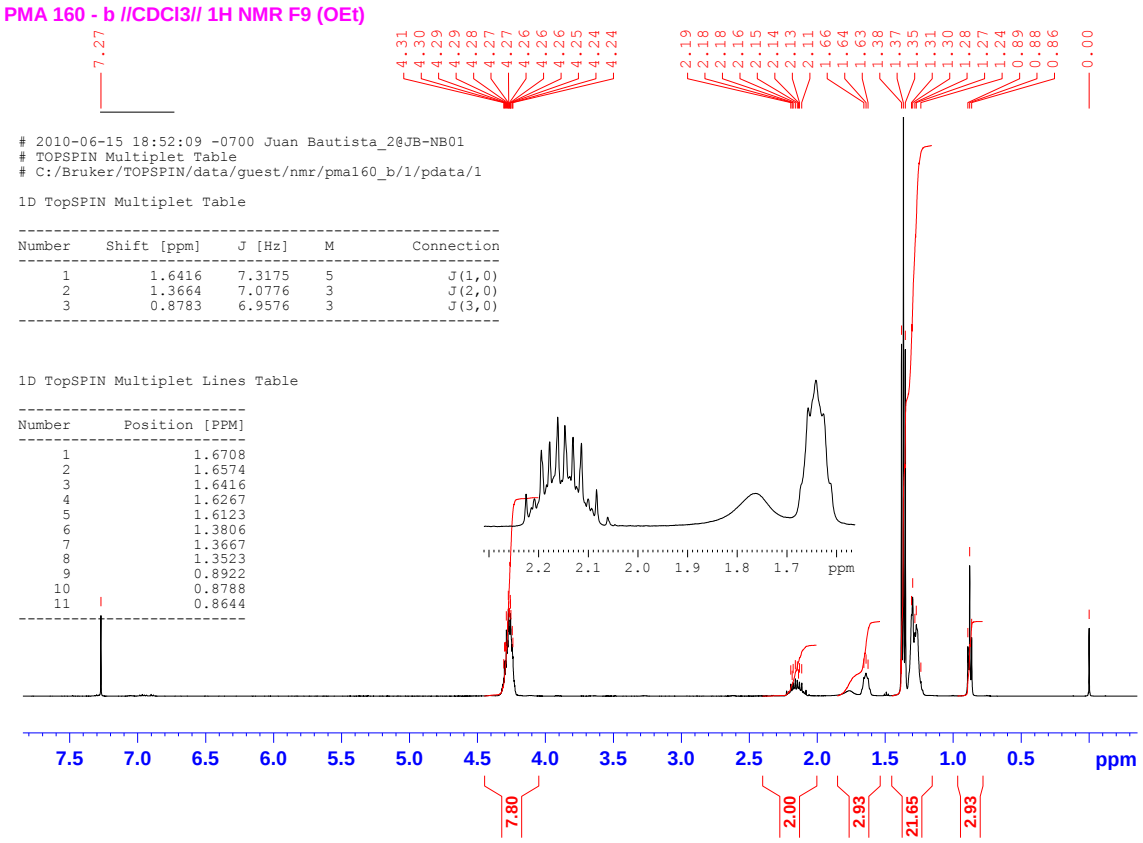

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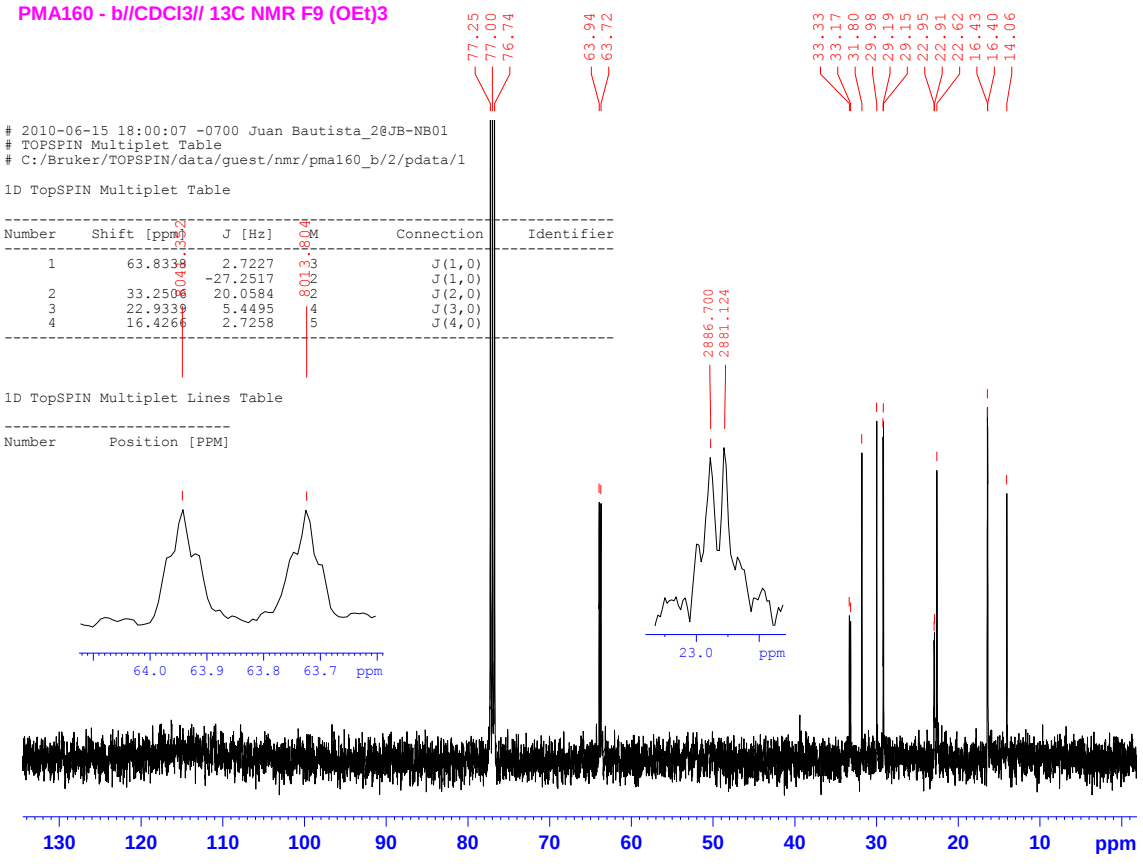

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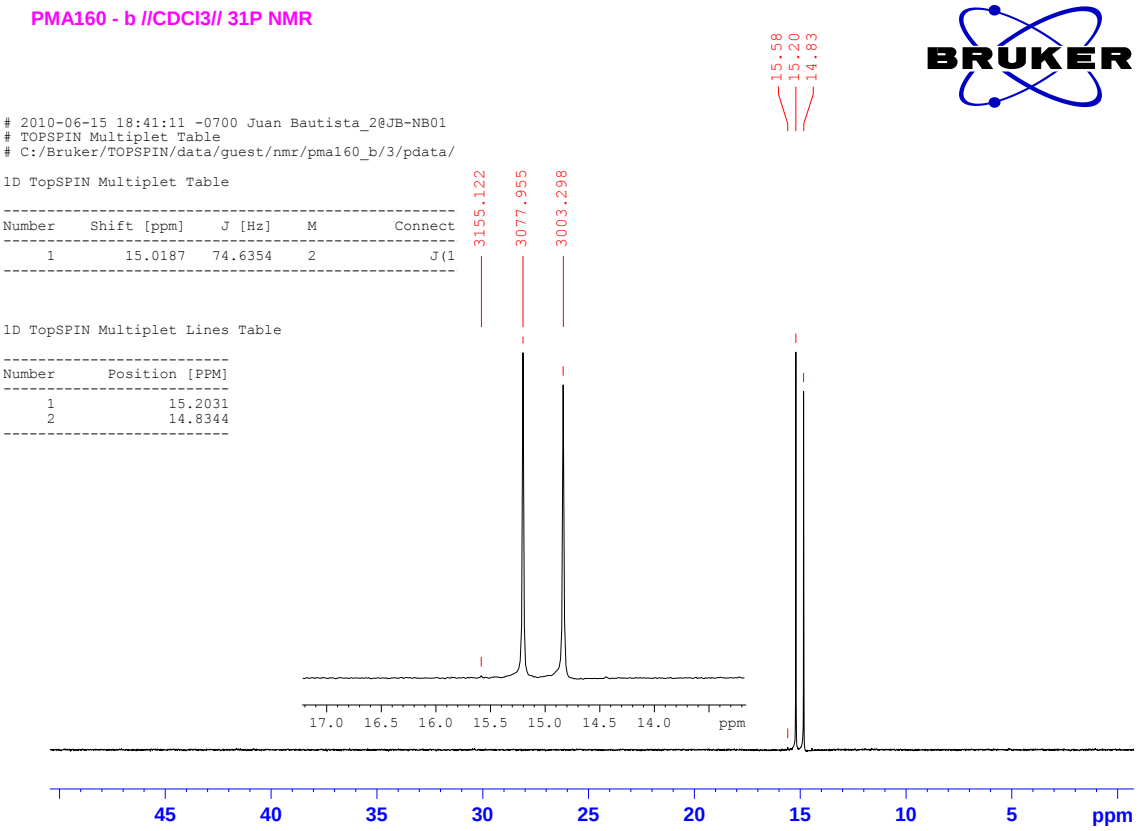

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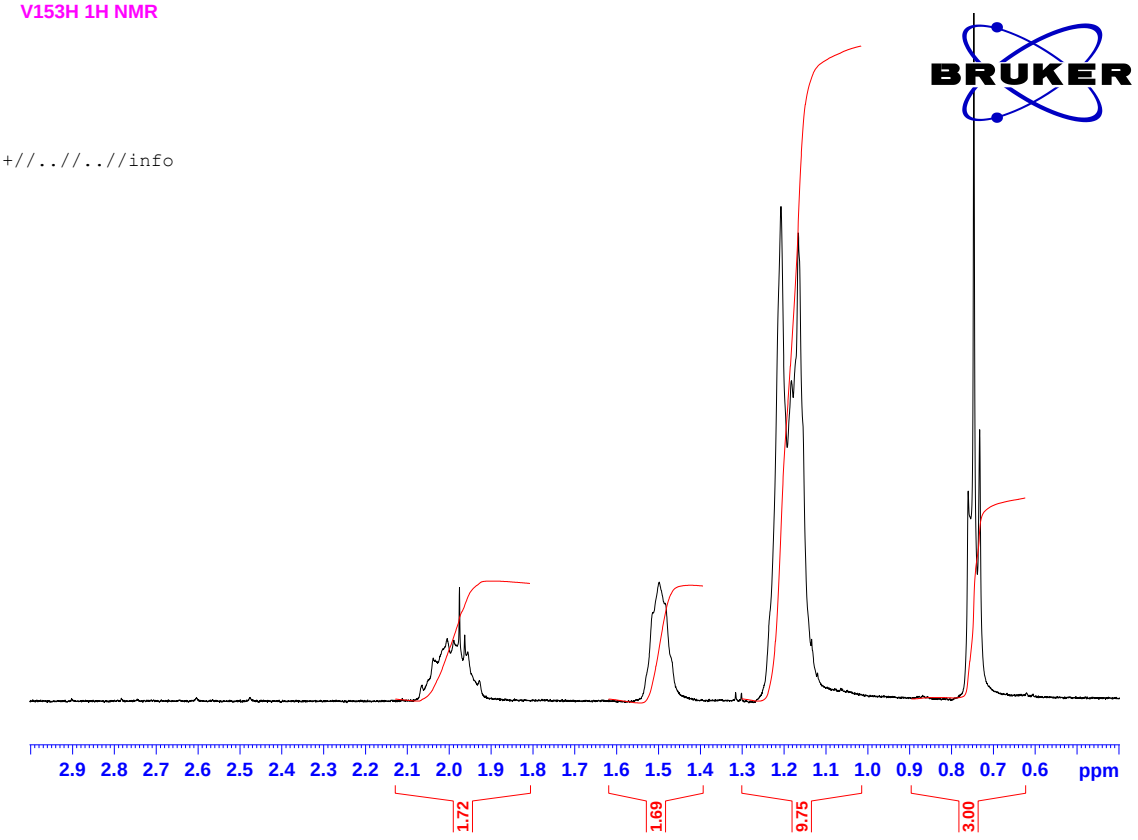

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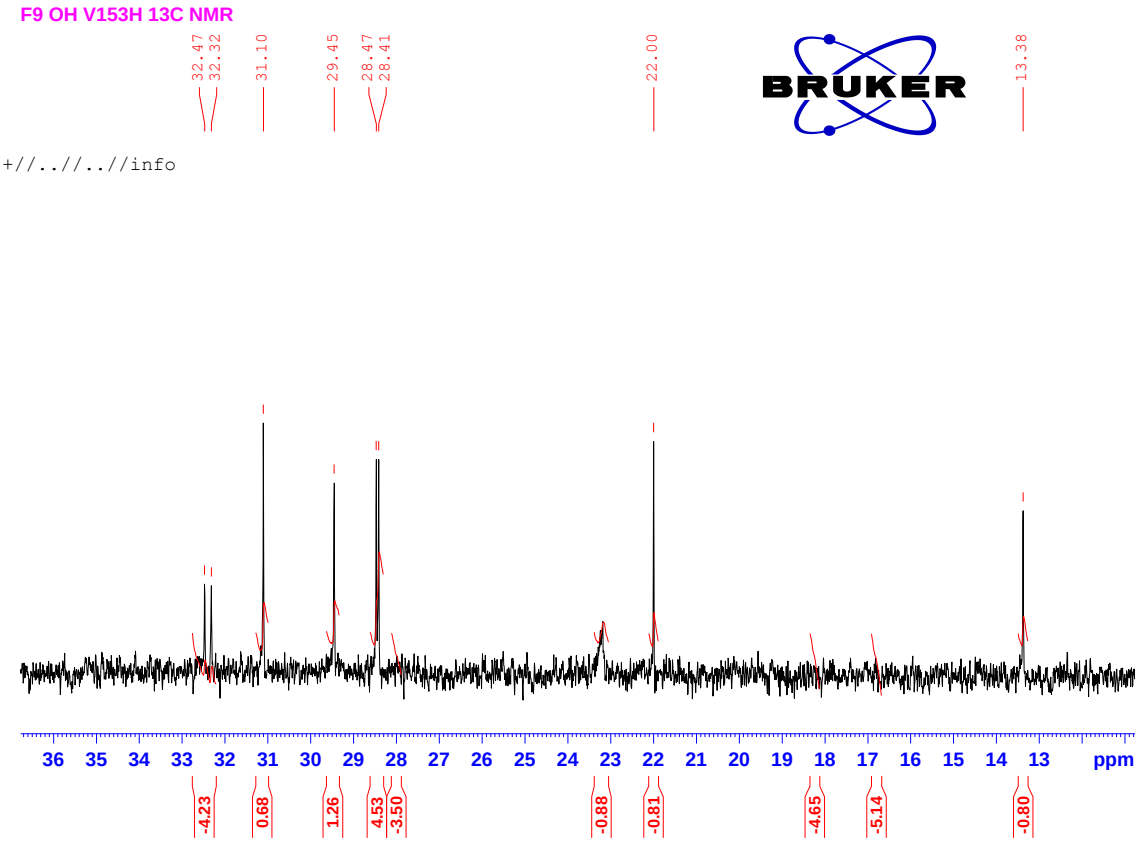

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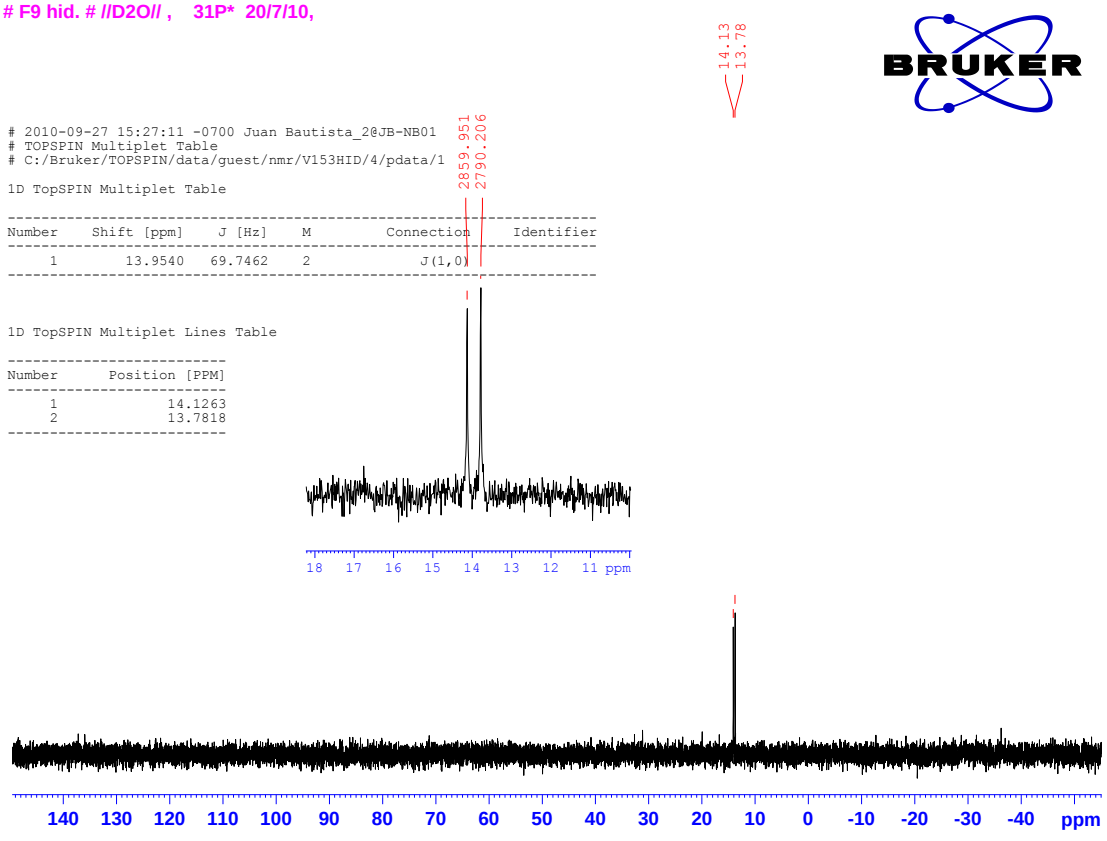

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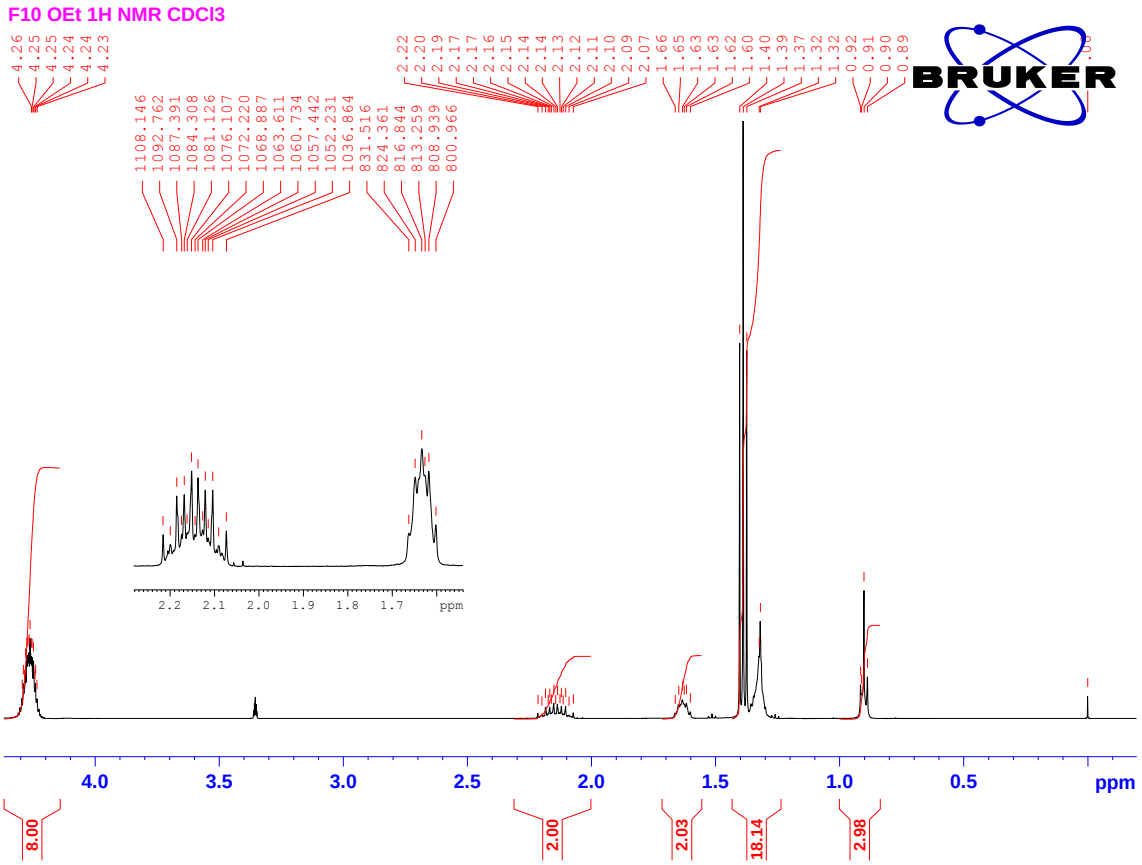

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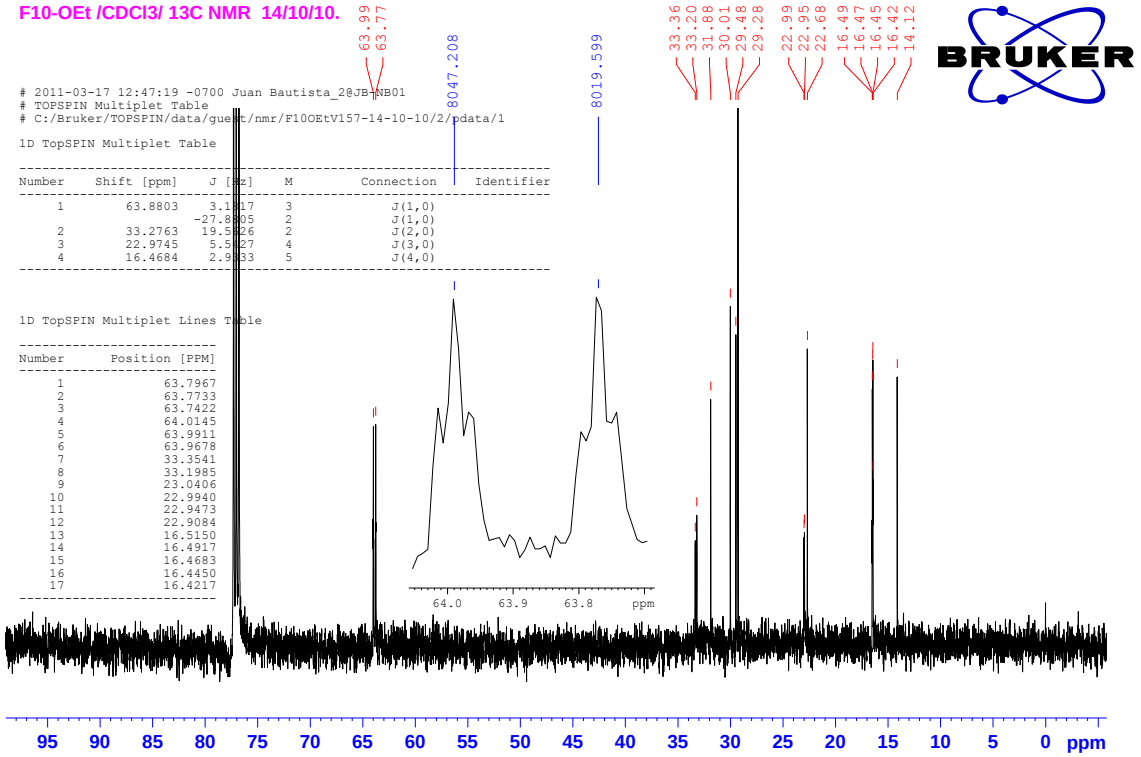

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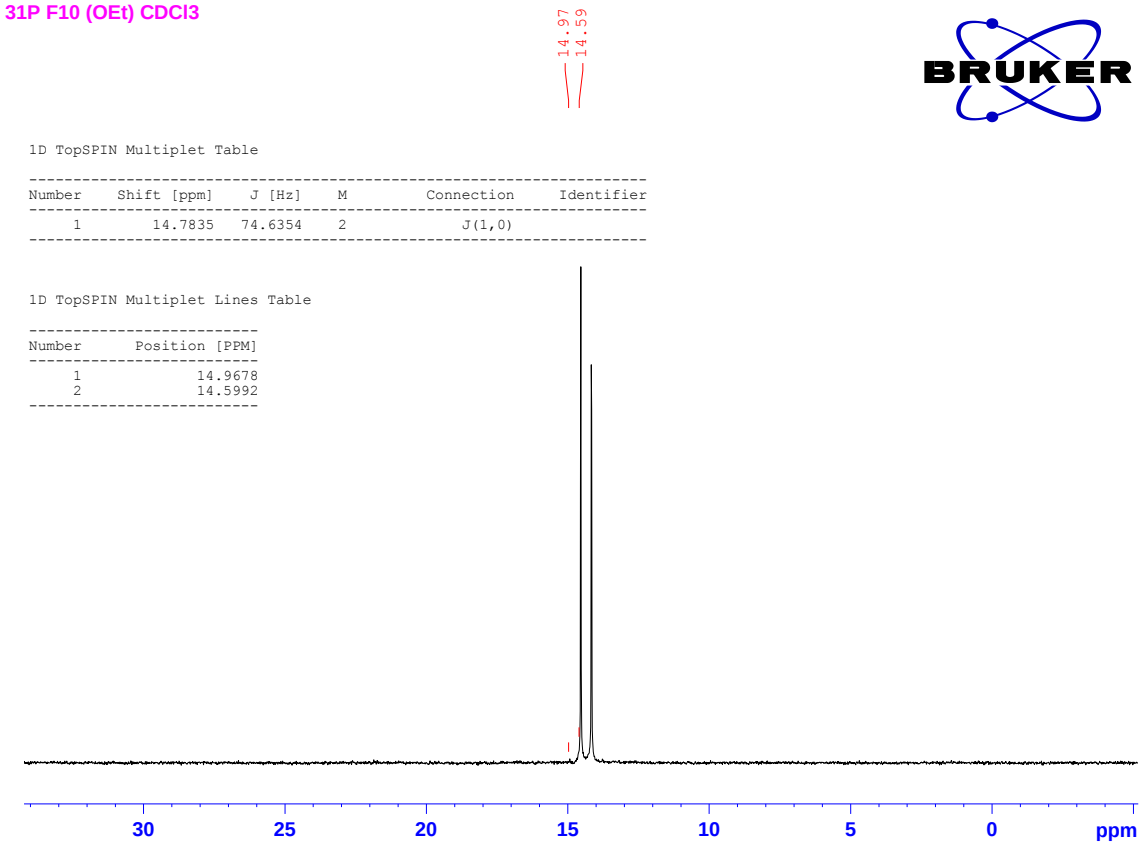

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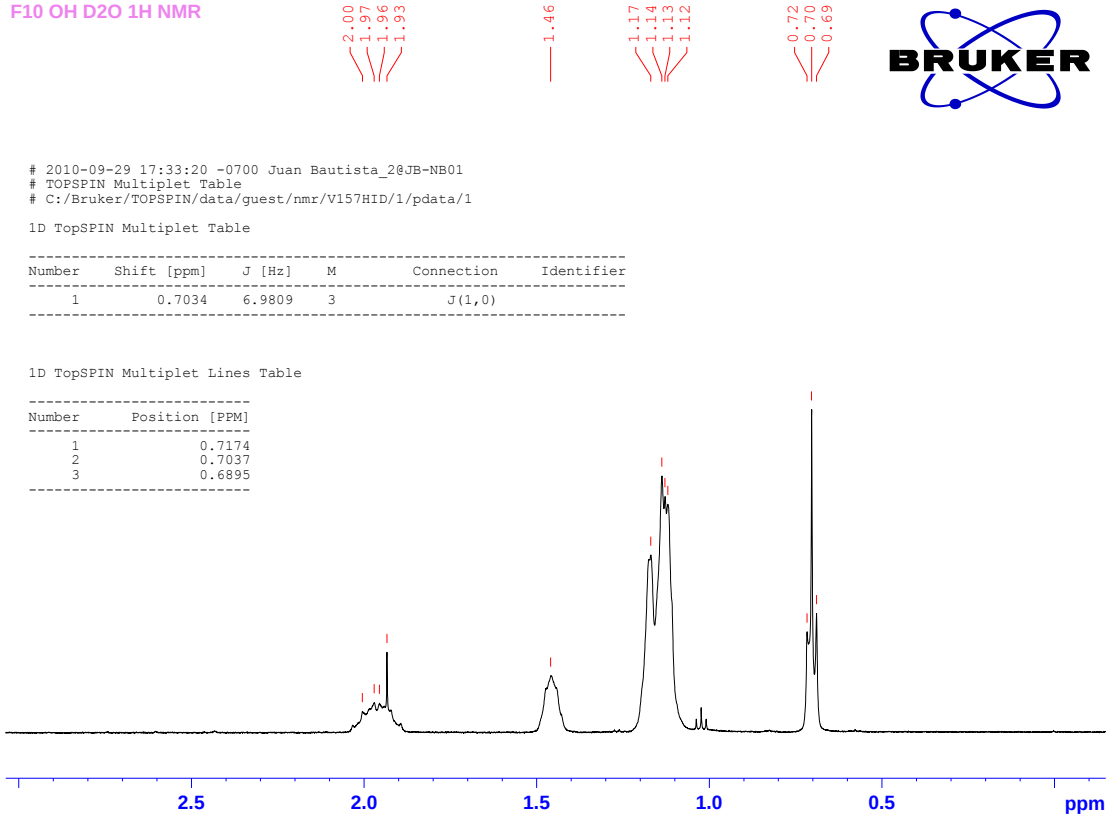
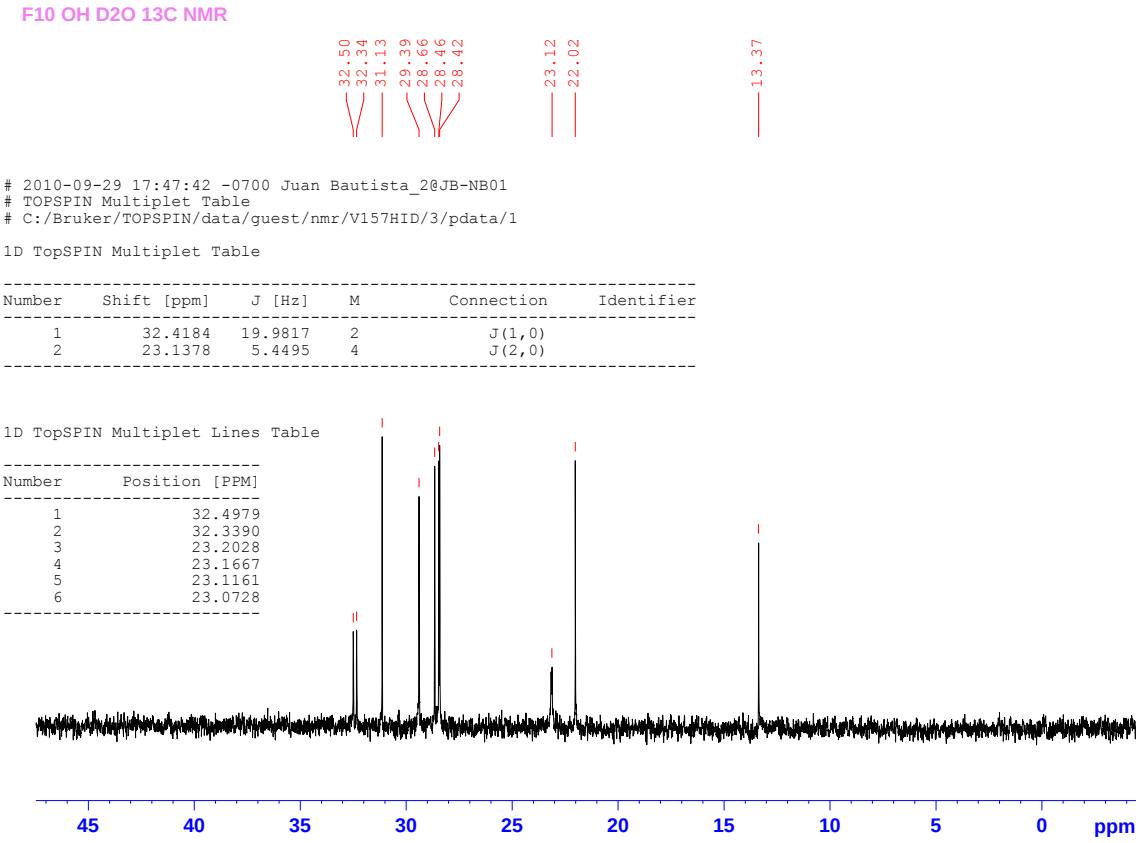
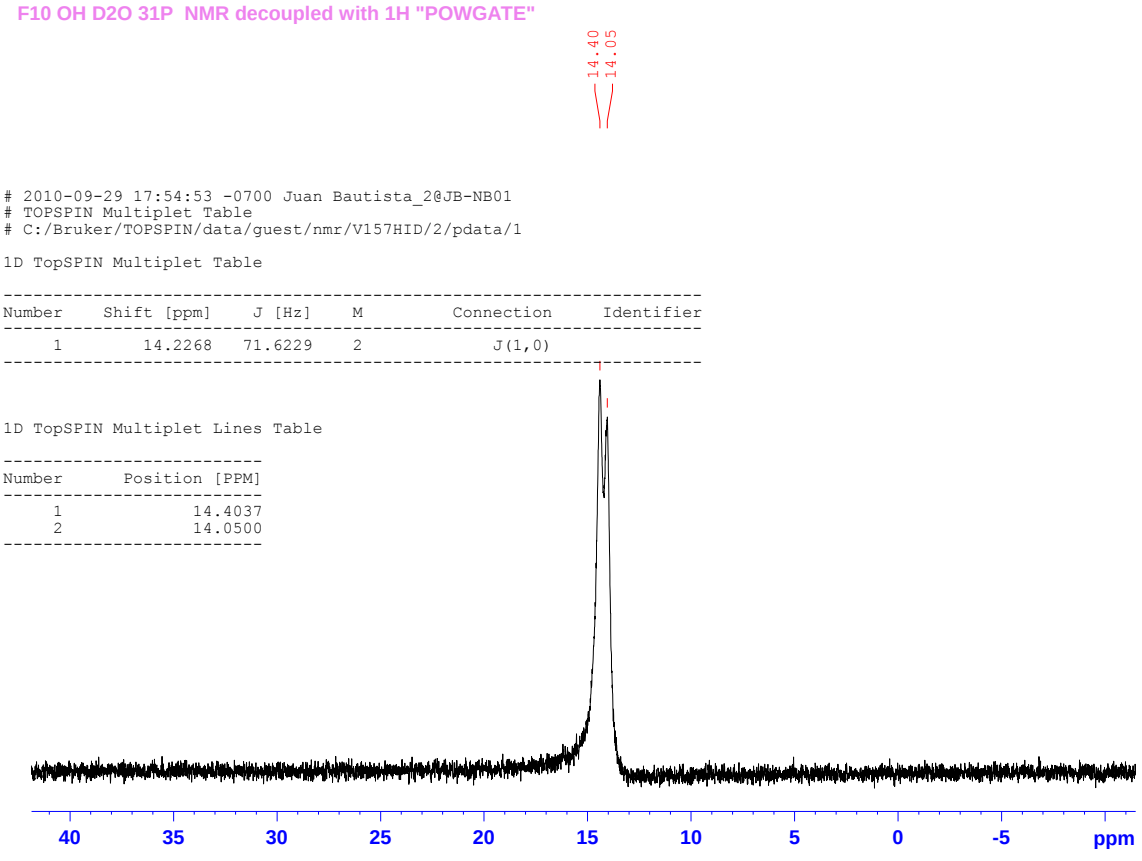


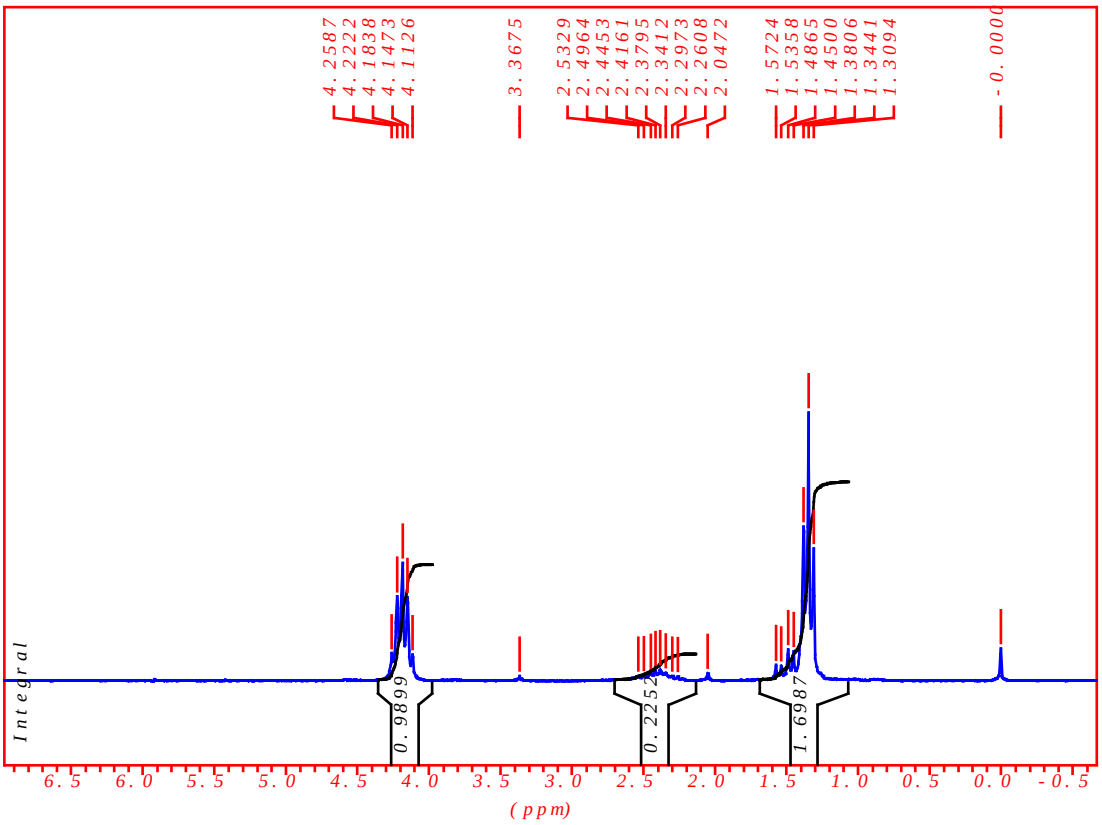
^{1}H NMR spectrum of compound **44**



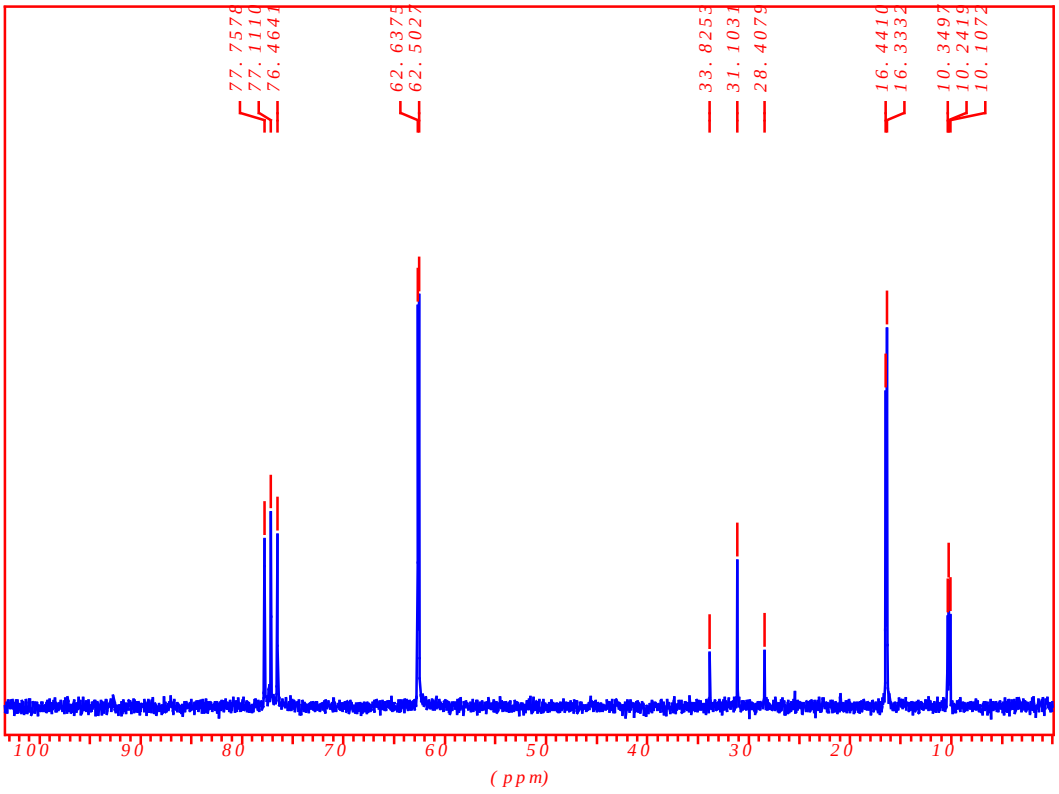
^{13}C NMR spectrum of compound **44**



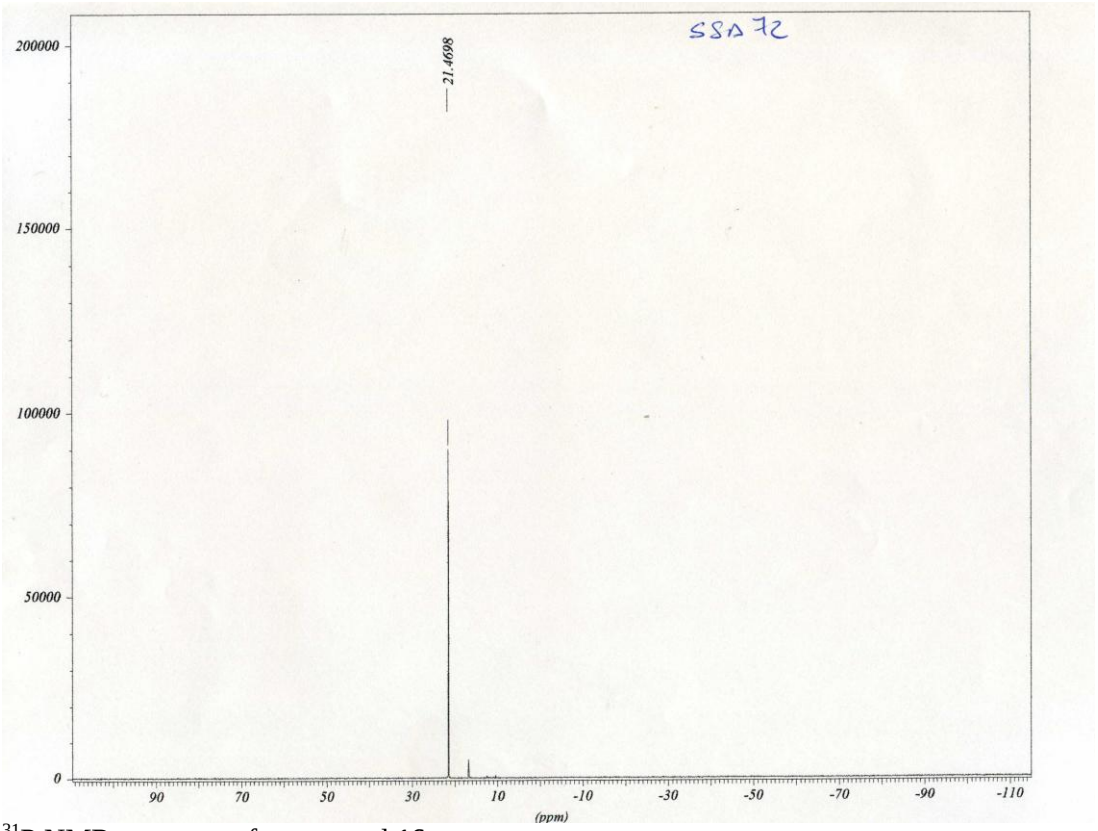
^{31}P NMR spectrum of compound **44**



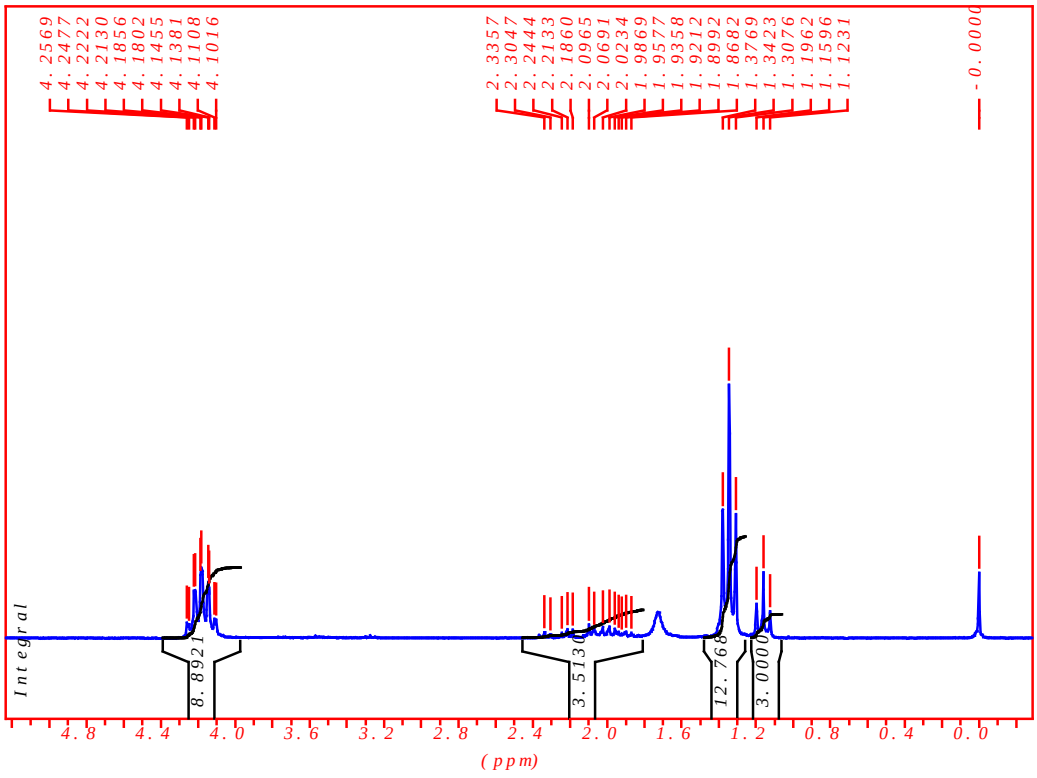
^{1}H NMR Spectrum of compound **16**



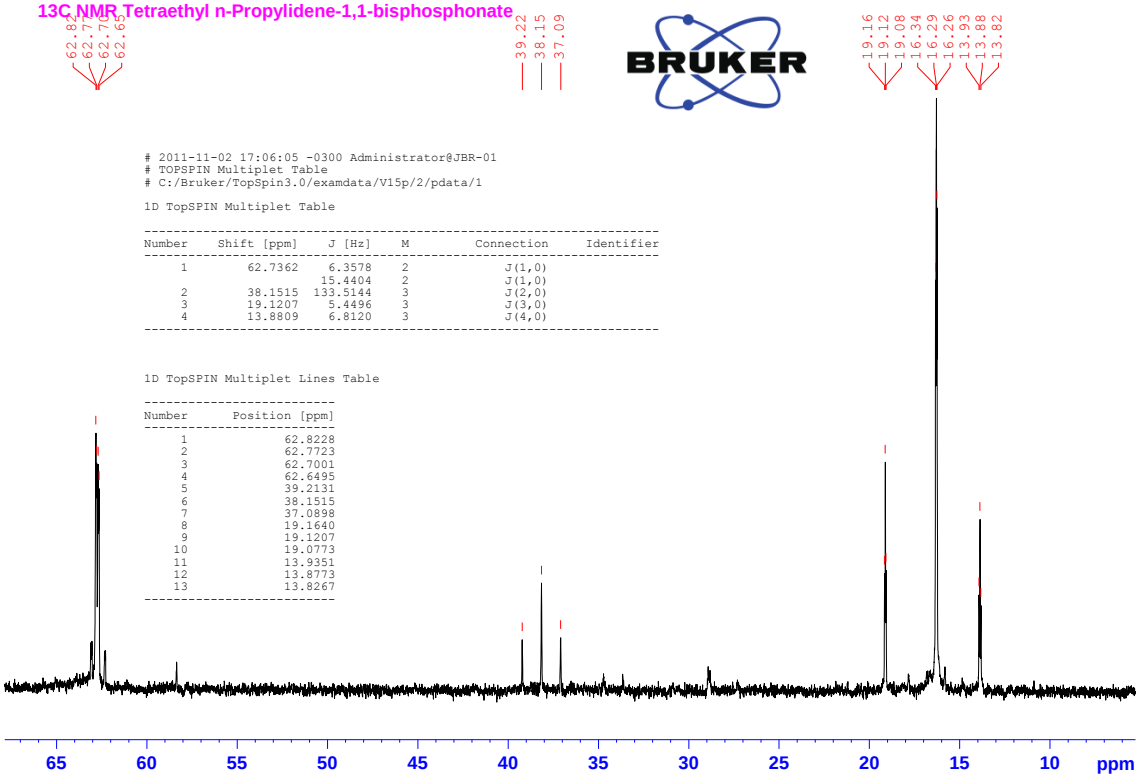
^{13}C NMR Spectrum of compound **16**



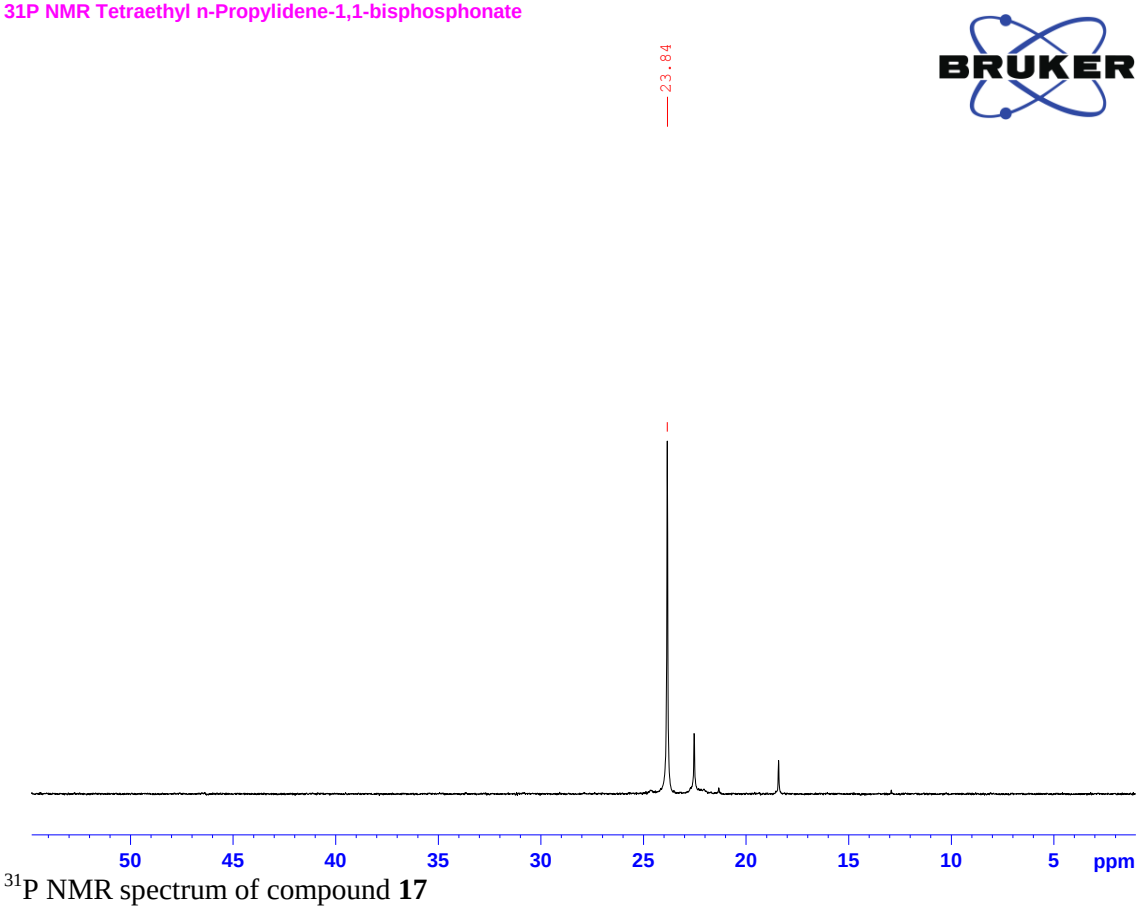
^{31}P NMR spectrum of compound **16**



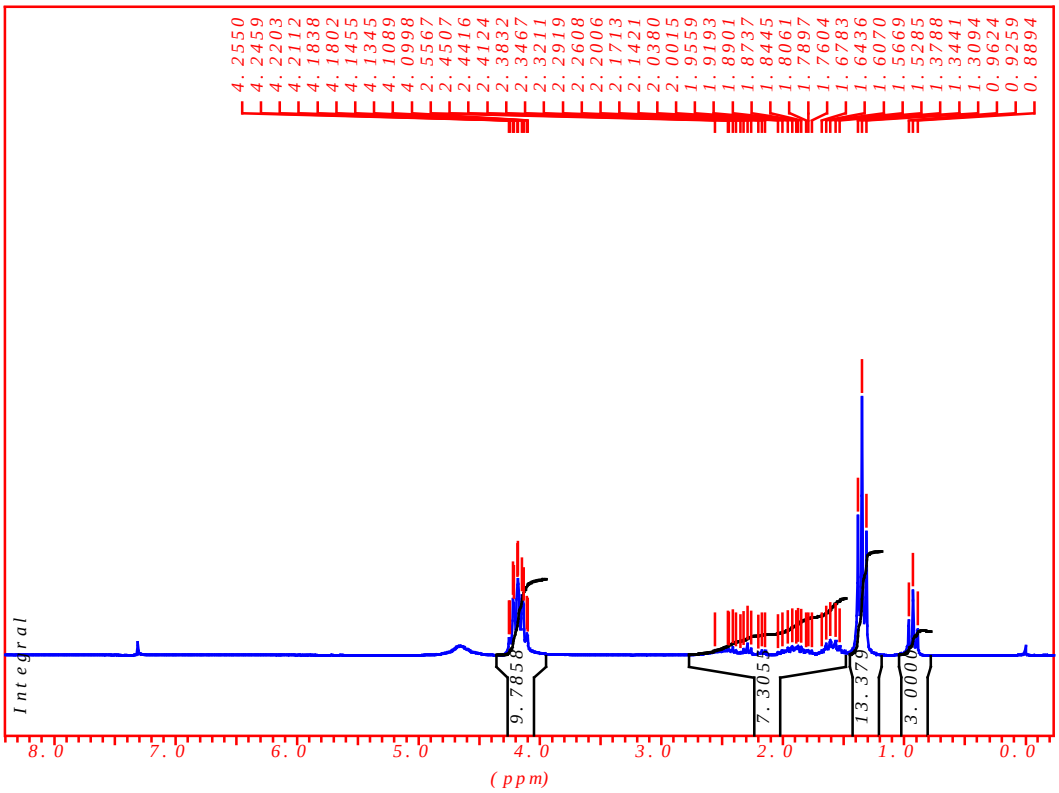
^{1}H NMR Spectrum of compound **17**



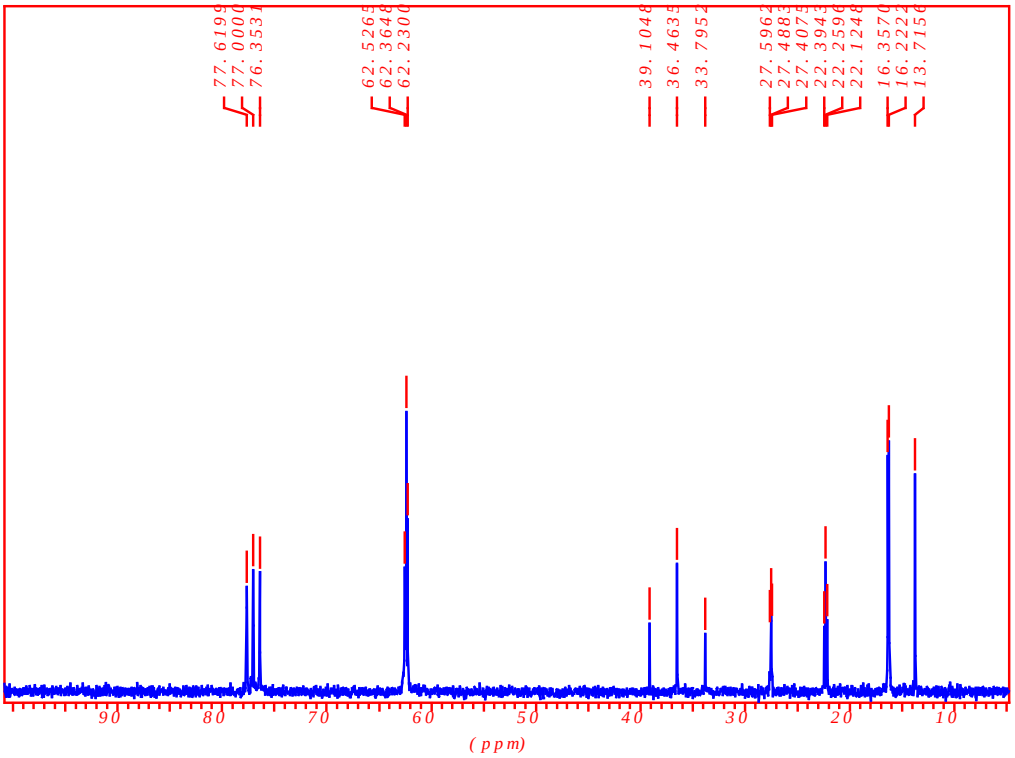
^{13}C NMR Spectrum of compound **17**



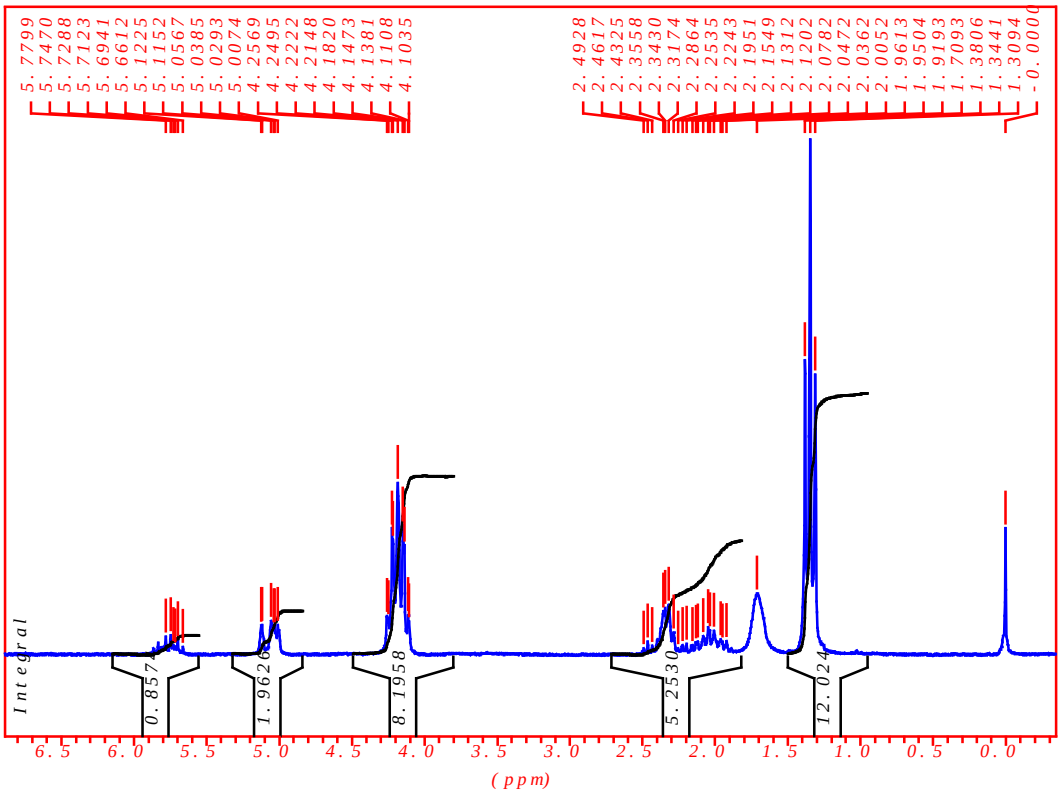
^{31}P NMR spectrum of compound **17**



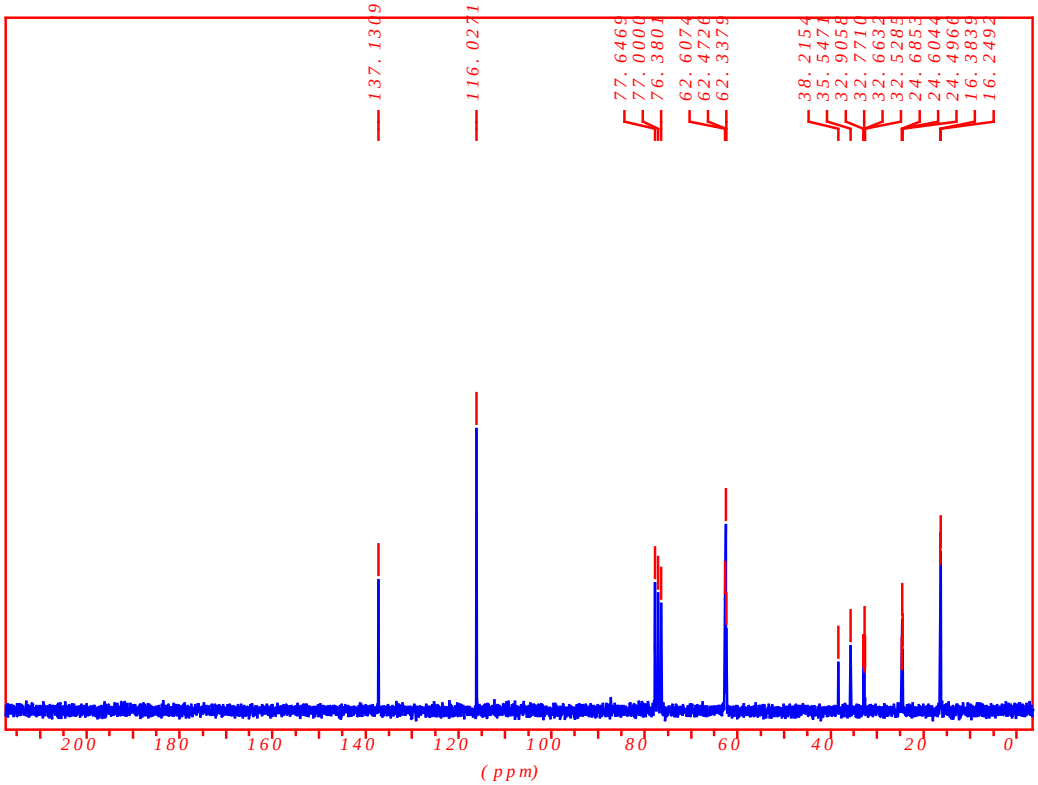
^{1}H NMR Spectrum of compound **18**



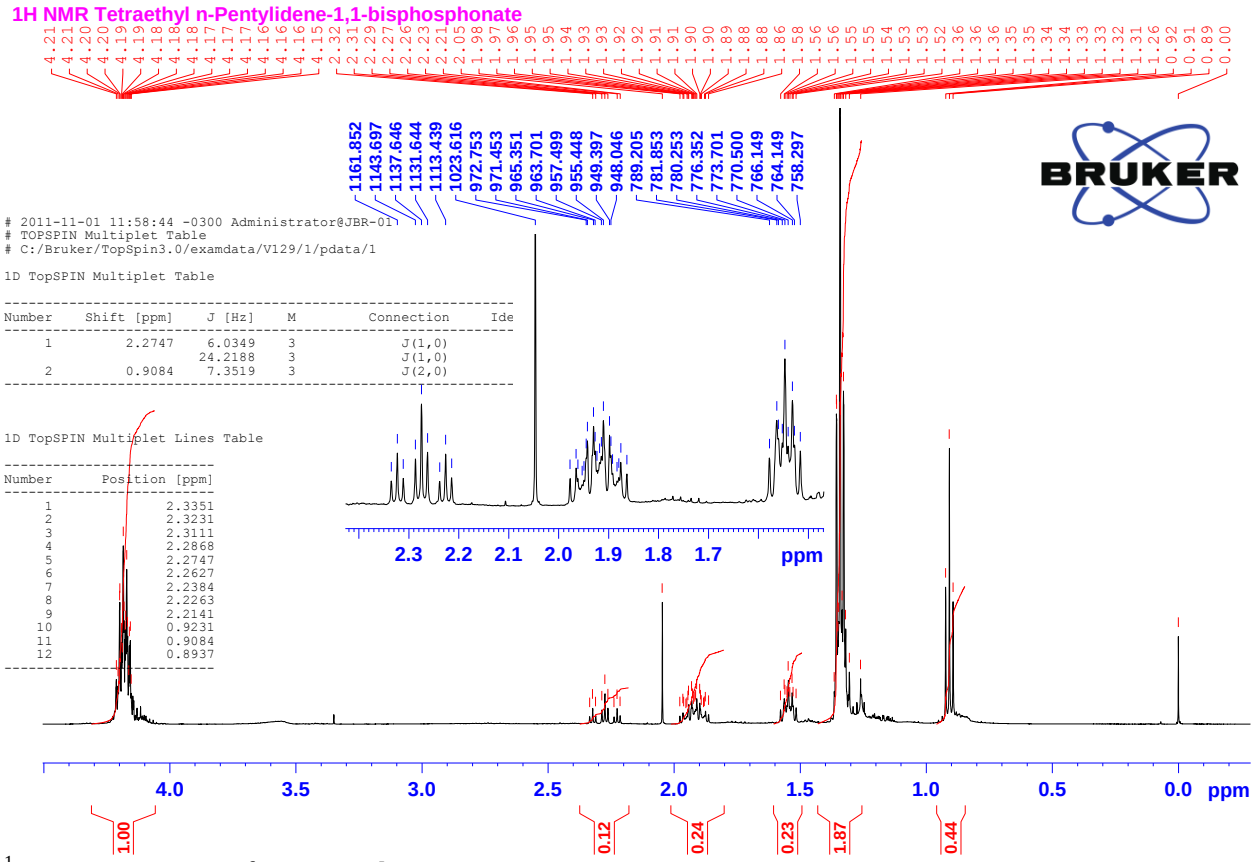
^{13}C NMR Spectrum of compound **18**



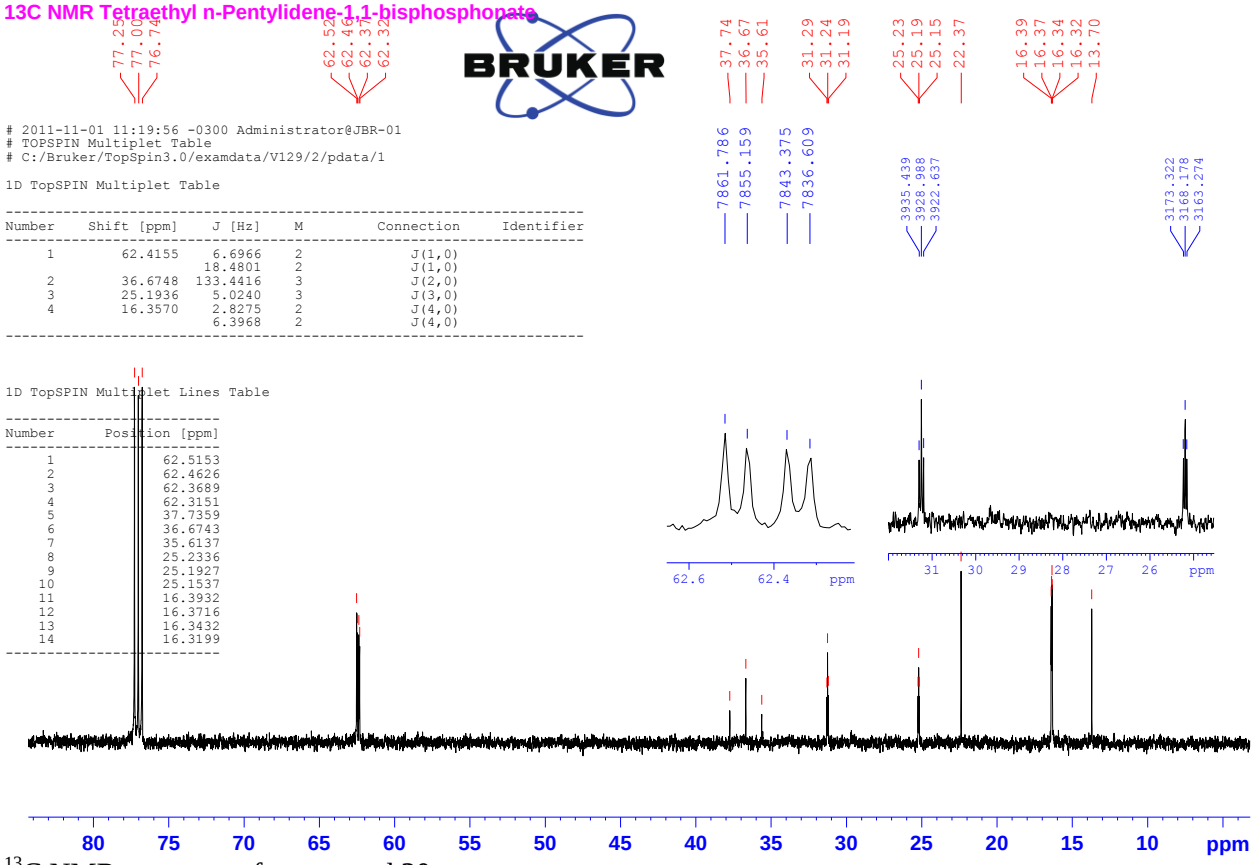
^{1}H NMR Spectrum of compound **19**



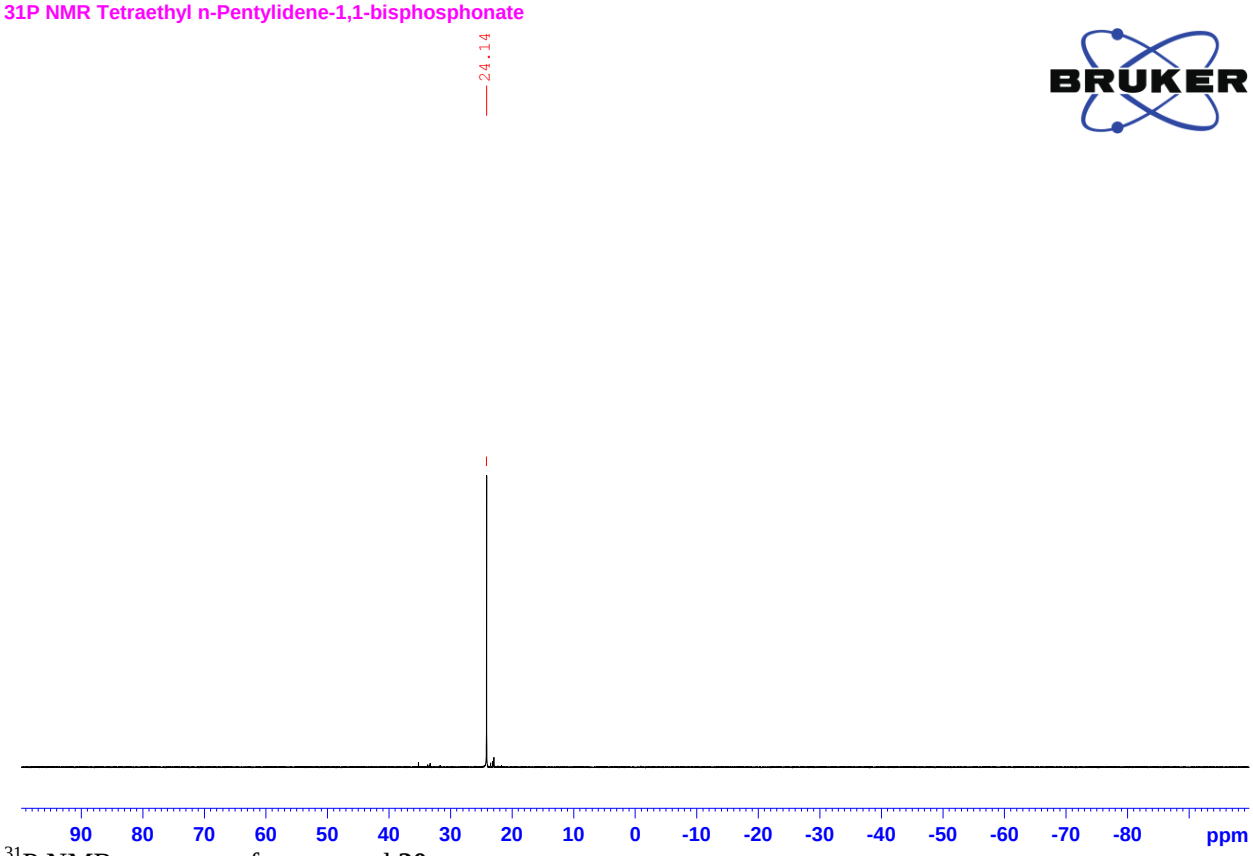
^{13}C NMR Spectrum of compound **19**



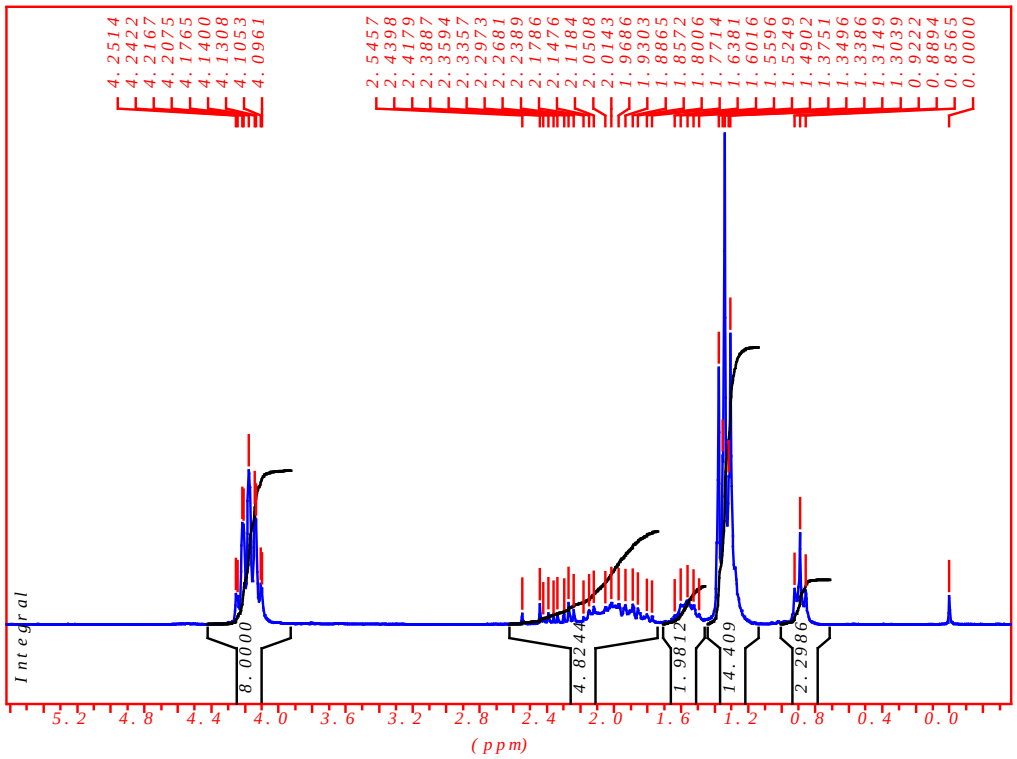
^{1}H NMR spectrum of compound **20**



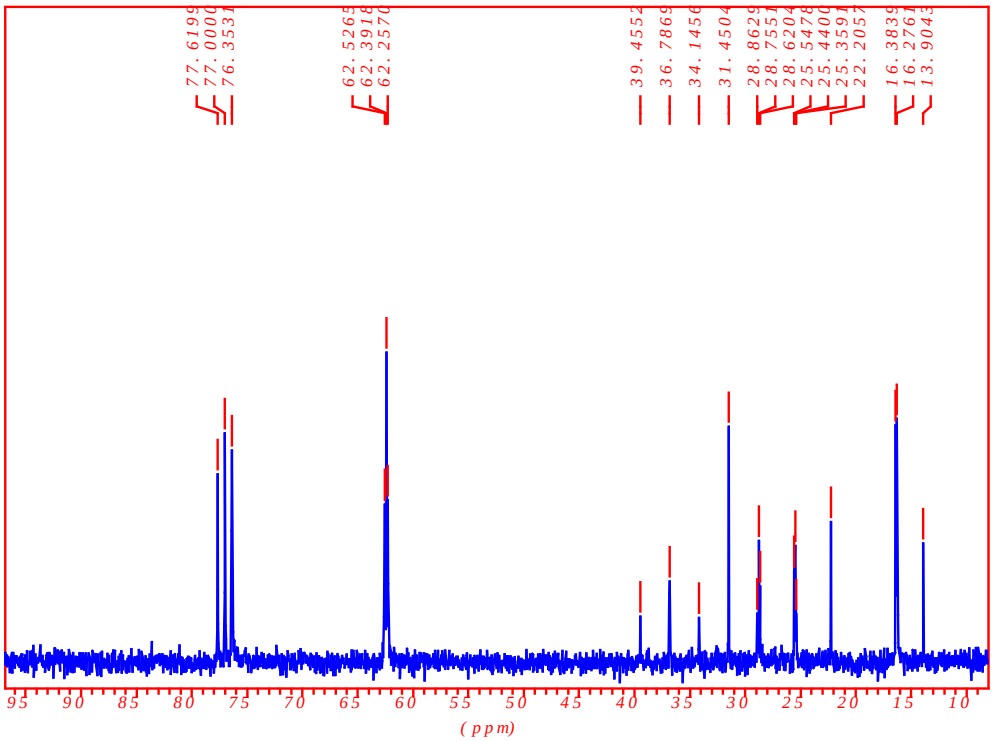
^{13}C NMR spectrum of compound **20**



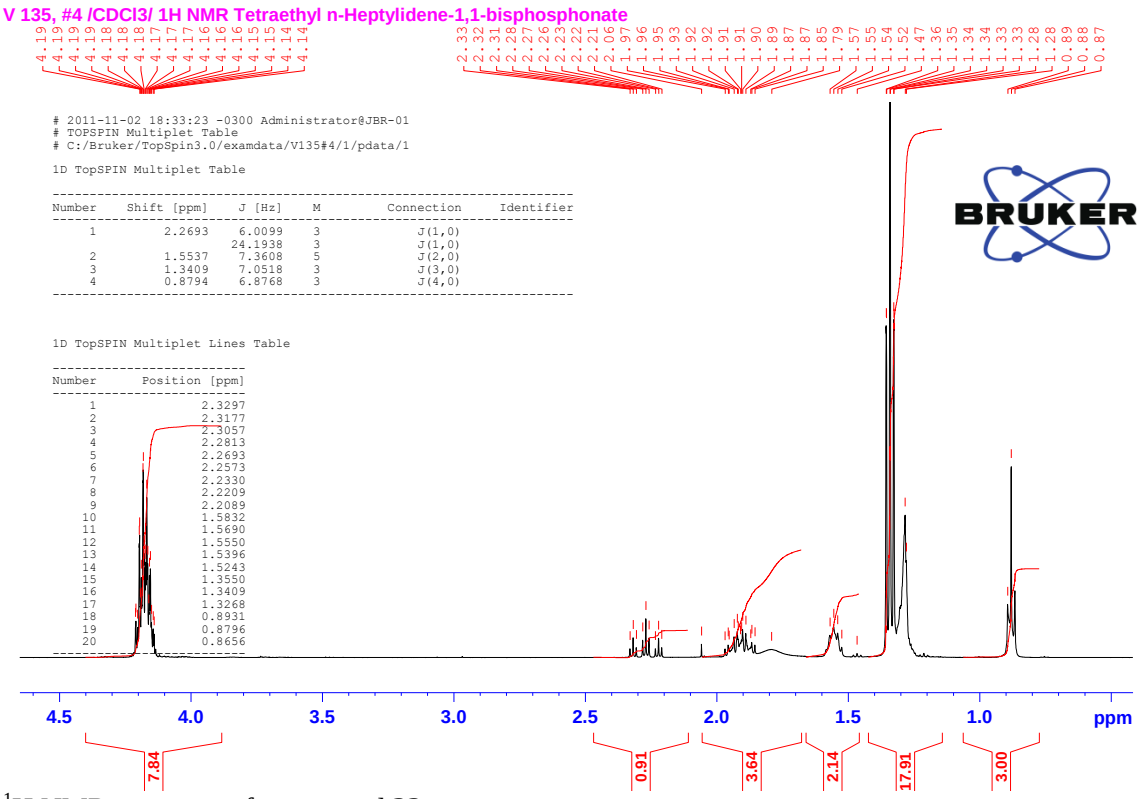
^{31}P NMR spectrum of compound **20**



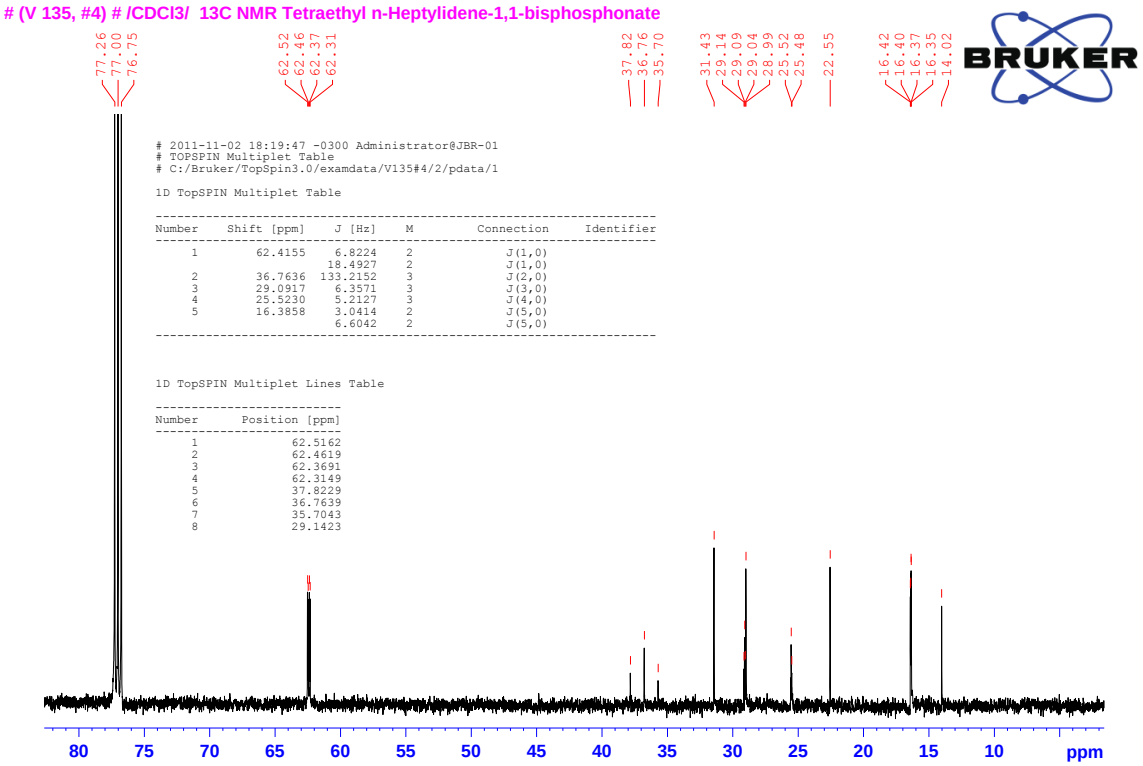
^{1}H NMR Spectrum of compound **21**



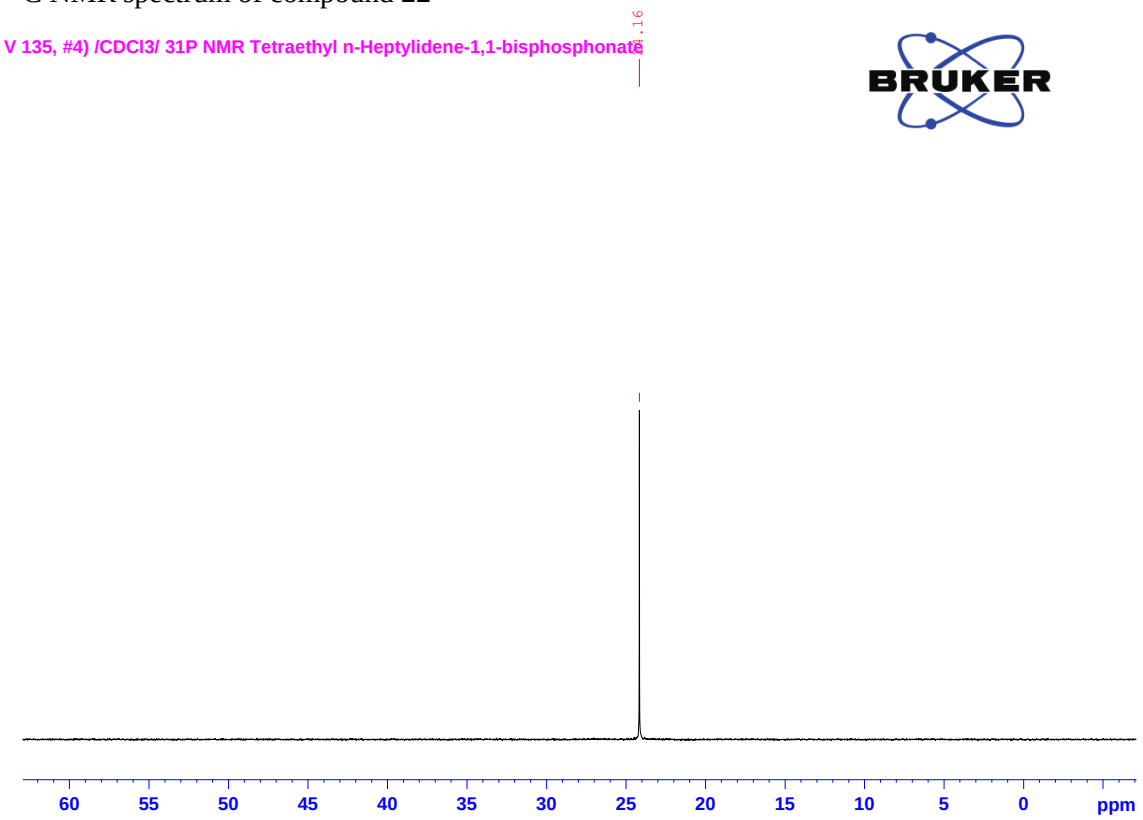
^{13}C NMR Spectrum of compound **21**



^{1}H NMR spectrum of compound **22**

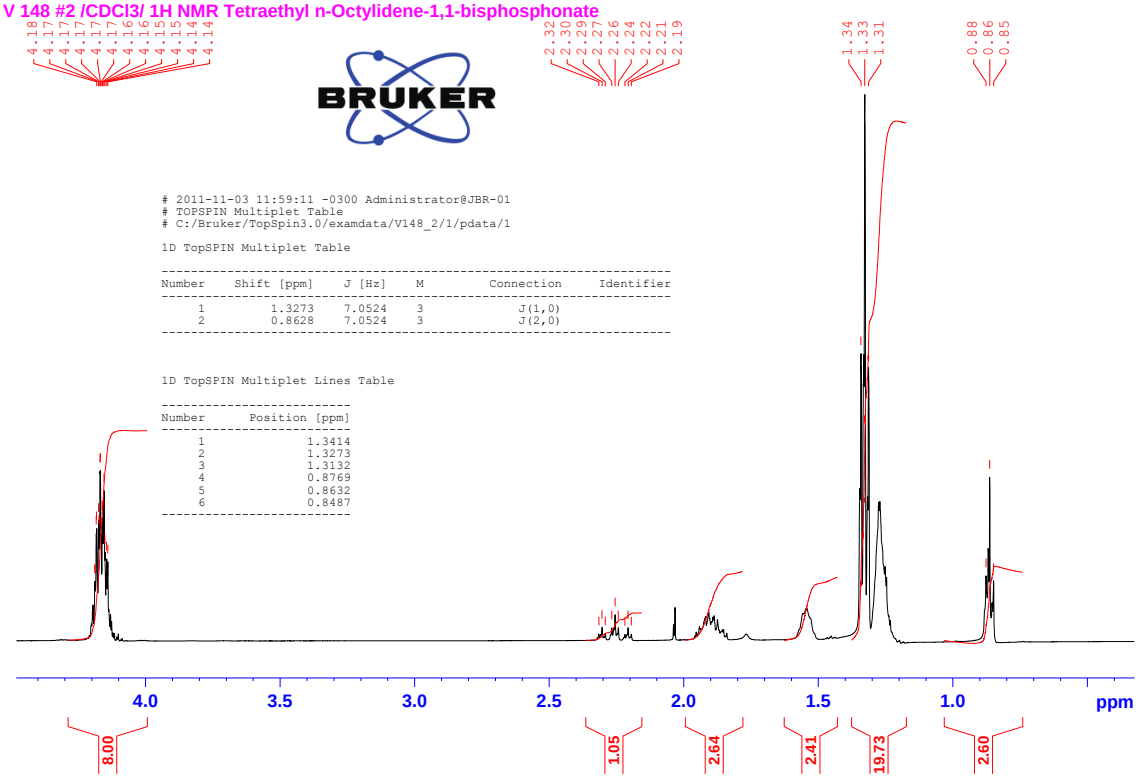


^{13}C NMR spectrum of compound **22**



^{31}P NMR spectrum of compound **22**

V 148 #2 /CDCl3/ 1H NMR Tetraethyl n-Octylidene-1,1-bisphosphonate

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# TOPSPIN Multiplet Table
# C:/Bruker/TopSpin3.0/examdata/V148_2/1/pdata/1

1D TopSPIN Multiplet Table

-------------------------------------------------------------------------------
Number    Shift [ppm]    J [Hz]    M         Connection     Identifier
-------------------------------------------------------------------------------
     1         1.3273    7.0524    3             J(1,0)
     2         0.8628    7.0524    3             J(2,0)
-------------------------------------------------------------------------------


1D TopSPIN Multiplet Lines Table

-------------------------
Number      Position [ppm]
-------------------------
     1             1.3414
     2             1.3273
     3             1.3132
     4             0.8769
     5             0.8632
     6             0.8487
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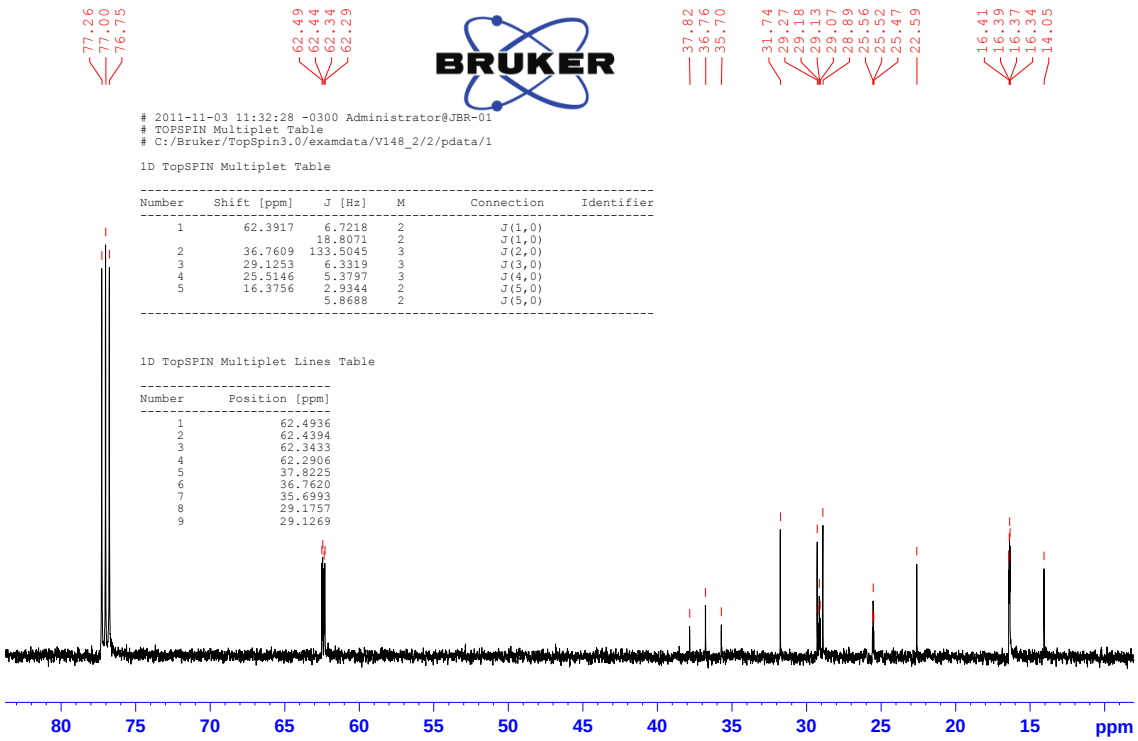
V 148 #2)/CDCl3/ 13C NMR Tetraethyl n-Octylidene-1,1-bisphosphonate

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# 2011-11-03 11:32:28 -0300 Administrator@JBR-01
# TOPSPIN Multiplet Table
# C:/Bruker/TopSpin3.0/examdata/V148_2/2/pdata/1

1D TopSPIN Multiplet Table

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-------------------------------------------------------------------------------
     1        62.3917    6.7218    2             J(1,0)
                        18.8071    2             J(1,0)
     2        36.7609  133.5045    3             J(2,0)
     3        29.1253    6.3319    3             J(3,0)
     4        25.5146    5.3797    3             J(4,0)
     5        16.3756    2.9344    2             J(5,0)
                         5.8688    2             J(5,0)
-------------------------------------------------------------------------------


1D TopSPIN Multiplet Lines Table

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     2             62.4394
     3             62.3433
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     5             37.8225
     6             36.7620
     7             35.6993
     8             29.1757
     9             29.1269
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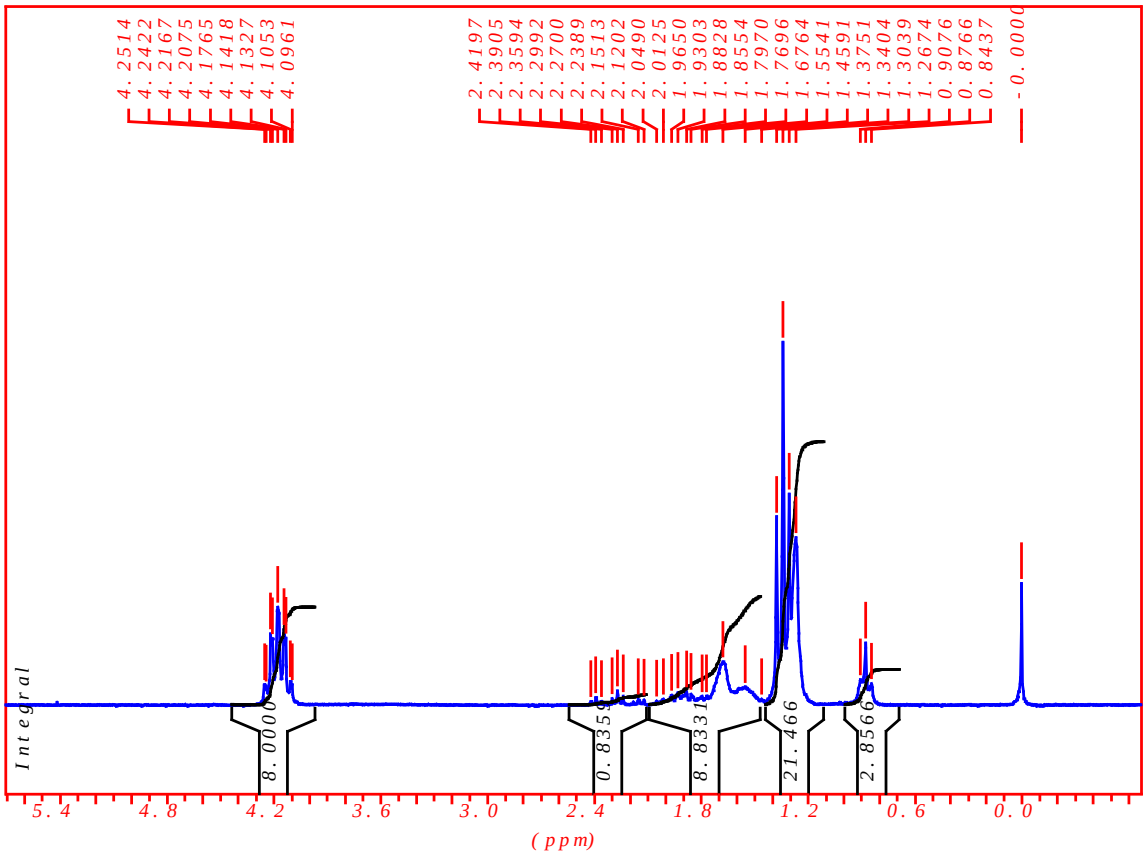
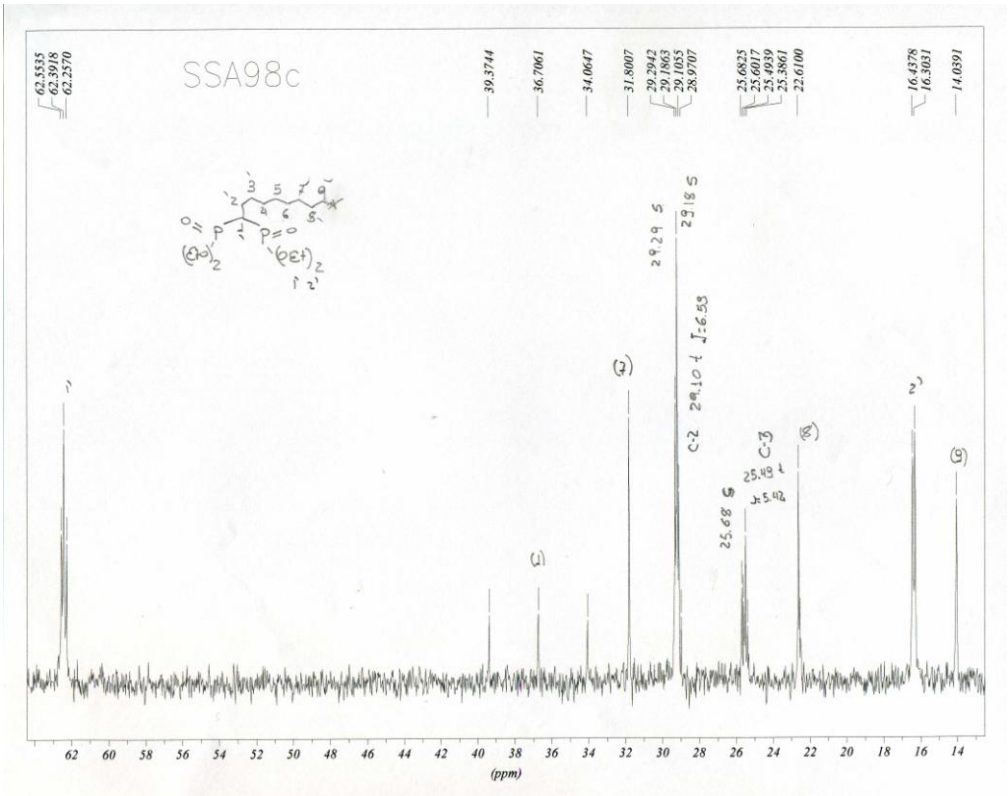
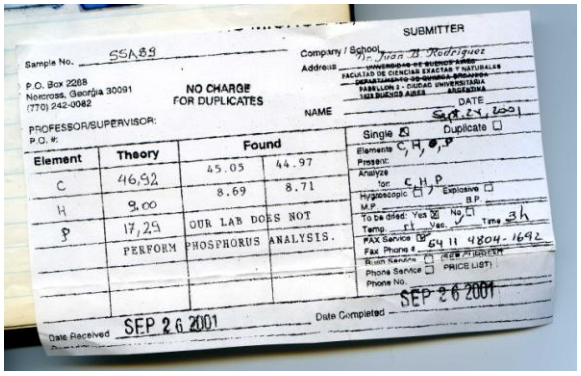


^{1}H NMR Spectrum of compound **24**



^{13}C NMR spectrum of compound **24**



SUBMITTER

Sample No. SSA89

Company / School Dr. Juan B. Rodriguez

Address UNIVERSIDAD DE BUENOS AIRES FACULTAD DE CIENCIAS EXACTAS Y NATURALES DEPARTAMENTO DE QUIMICA ORGANICA PABELLON 2 - CIUDAD UNIVERSITARIA 1428 BUENOS AIRES ARGENTINA

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

NO CHARGE FOR DUPLICATES

NAME

DATE Sept. 24, 2001

PROFESSOR/SUPERVISOR:

P.O. #:

Element	Theory	Found	
C	46.92	45.05	44.97
H	8.00	8.69	8.71
P	17.29	OUR LAB DOES NOT	
	PERFORM	PHOSPHORUS ANALYSIS.	

Single ☒ Duplicate ☐

Elements Present: C, H, O, P

Analyze for: C, H, P

Hygroscopic ☐ Explosive ☐

M.P. B.P.

To be dried: Yes ☒ No ☐

Temp. ☐ Vac. ☐ Time 3h

FAX Service ☒ 54 11 4804-1692

Fax Phone # Rush Service ☐ (SEE CURRENT PRICE LIST)

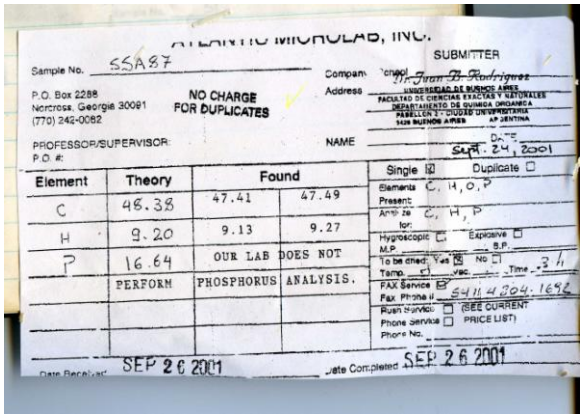
Phone Service ☐

Phone No.

Date Received SEP 26 2001 Date Completed SEP 26 2001

Remarks:

Anal. Compond **21**



SUBMITTER

Sample No. SSA87

Company / School Dr. Juan B. Rodriguez

Address UNIVERSIDAD DE BUENOS AIRES FACULTAD DE CIENCIAS EXACTAS Y NATURALES DEPARTAMENTO DE QUIMICA ORGANICA PABELLON 2 - CIUDAD UNIVERSITARIA 1428 BUENOS AIRES ARGENTINA

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

NO CHARGE FOR DUPLICATES

NAME

DATE Sept. 24, 2001

PROFESSOR/SUPERVISOR:

P.O. #:

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

Single ☒ Duplicate ☐

Elements Present: C, H, O, P

Analyze for: C, H, P

Hygroscopic ☐ Explosive ☐

M.P. B.P.

To be dried: Yes ☒ No ☐

Temp. ☐ Vac. ☐ Time 3 h

FAX Service ☒ 54 11 4804-1692

Fax Phone # Rush Service ☐ (SEE CURRENT PRICE LIST)

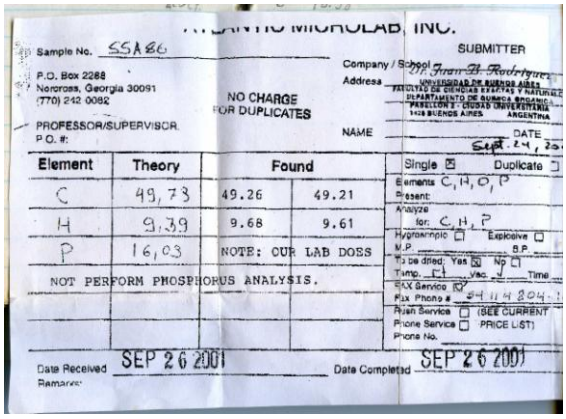
Phone Service ☐

Phone No.

Date Received SEP 26 2001 Date Completed SEP 26 2001

Remarks:

Anal. Compound **22**.



SUBMITTER

Sample No. SSA86

Company / School Dr. Juan B. Rodriguez

Address UNIVERSIDAD DE BUENOS AIRES FACULTAD DE CIENCIAS EXACTAS Y NATURALES DEPARTAMENTO DE QUIMICA ORGANICA PABELLON 2 - CIUDAD UNIVERSITARIA 1428 BUENOS AIRES ARGENTINA

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

NO CHARGE FOR DUPLICATES

NAME

DATE Sept. 24, 2001

PROFESSOR/SUPERVISOR

P.O. #:

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 Present: C, H, O, P

Analyze for: C, H, P

Hygroscopic ☐ Explosive ☐

M.P. B.P.

To be dried: Yes ☒ No ☐

Temp. ☐ Vac. ☐ Time

FAX Service ☒ 54 11 4804-1

Fax Phone # Rush Service ☐ (SEE CURRENT PRICE LIST)

Phone Service ☐

Phone No.

Date Received SEP 26 2001 Date Completed SEP 26 2001

Remarks:

Anal Compound **23**.