

# **Supporting Information of**

## **Site-selective Conversion of Azido Groups at Carbonyl $\alpha$ -Positions to Diazo Groups in Di- and Triazido Compounds**

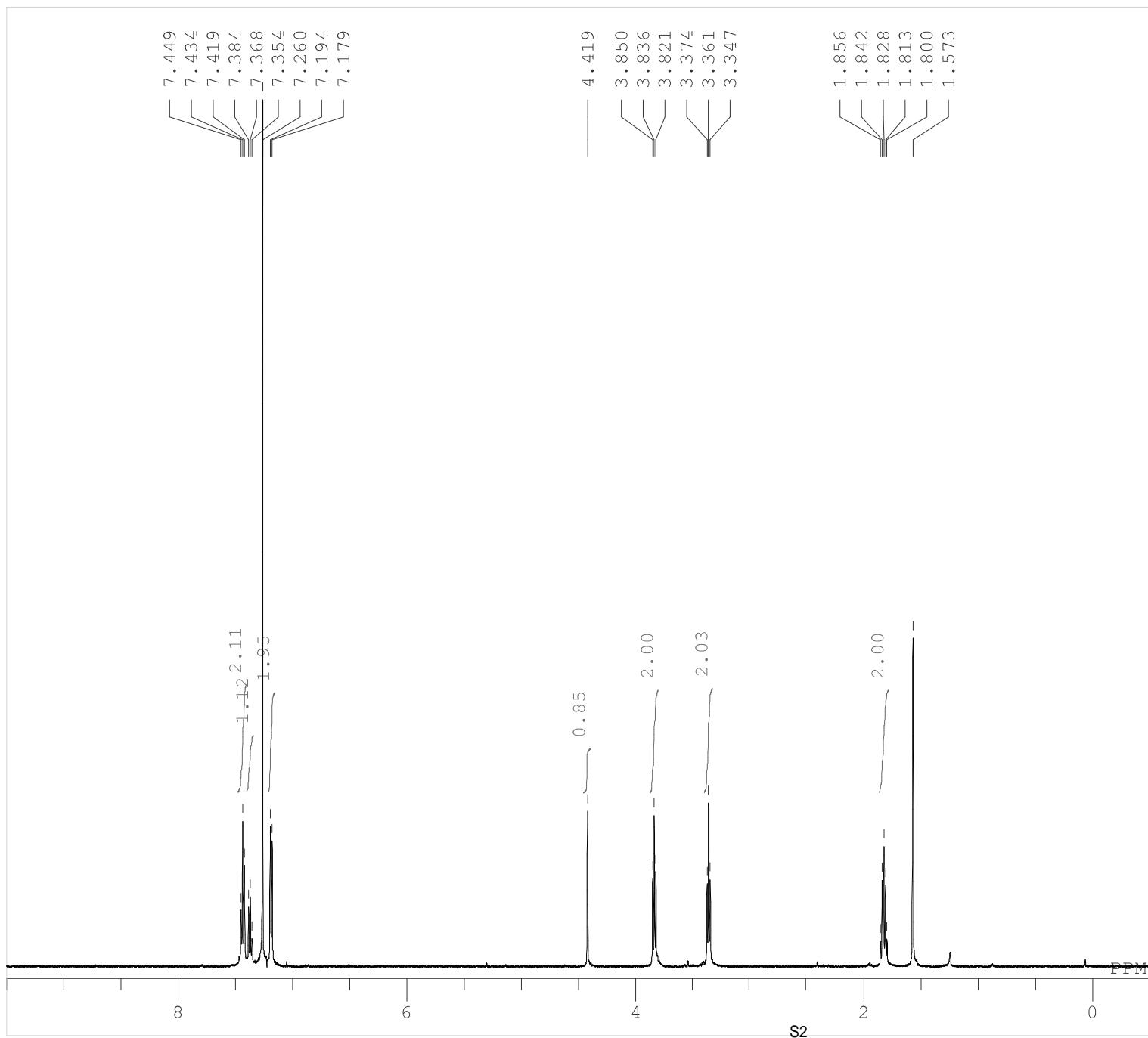
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Tsumoru Morimoto, and Kiyomi Kakiuchi.

Division of Materials Science, Graduate School of Science and Technology,  
Nara Institute of Science and Technology (NAIST)  
8916-5 Takayamacho, Ikoma, Nara 630-0192, Japan

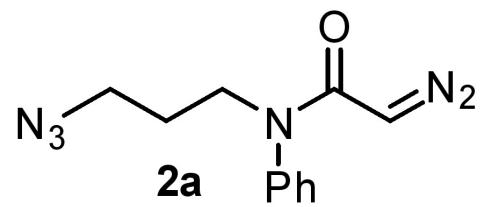
Corresponding author's e-mail: [tanimoto@ms.naist.jp](mailto:tanimoto@ms.naist.jp)

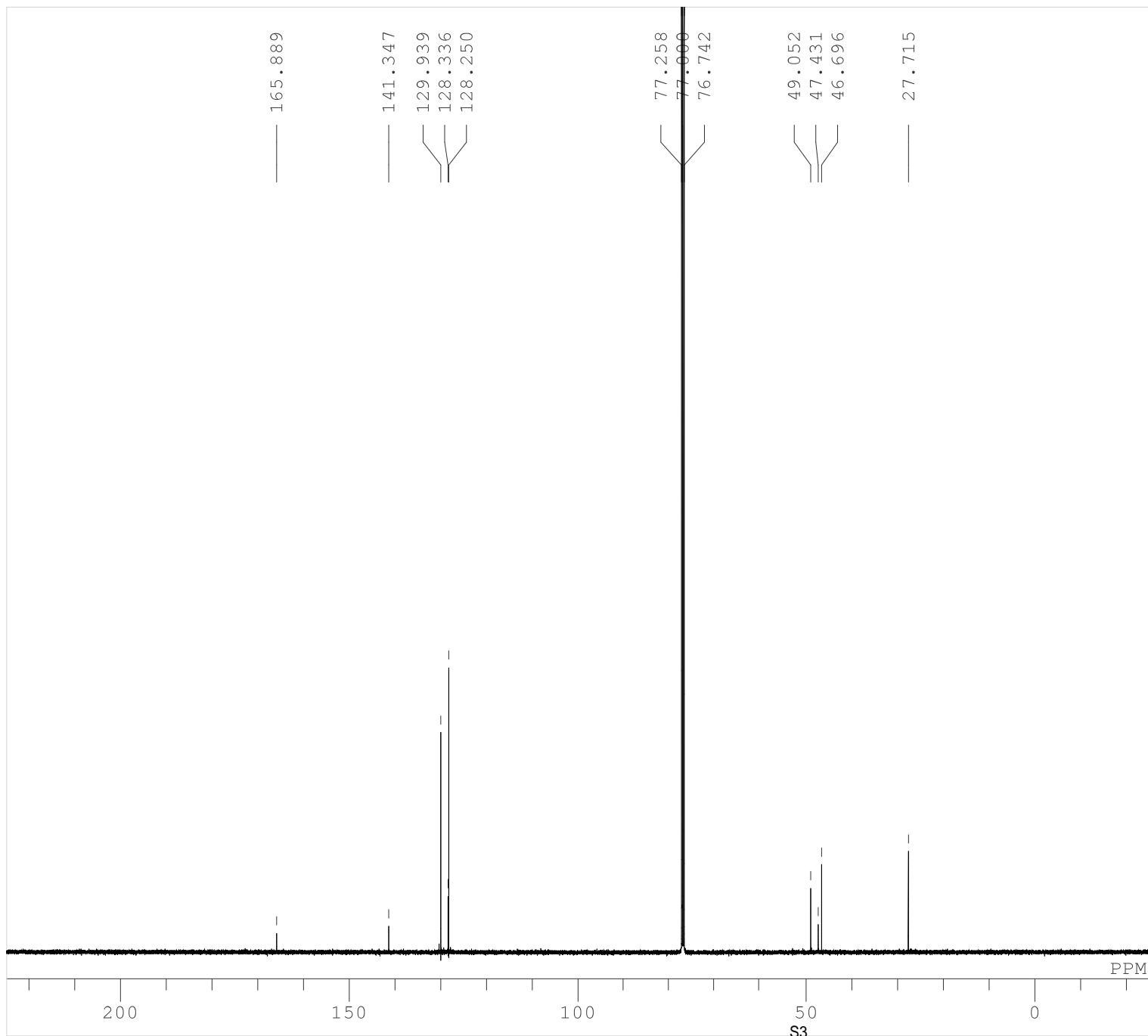
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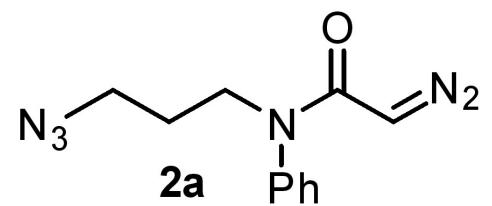


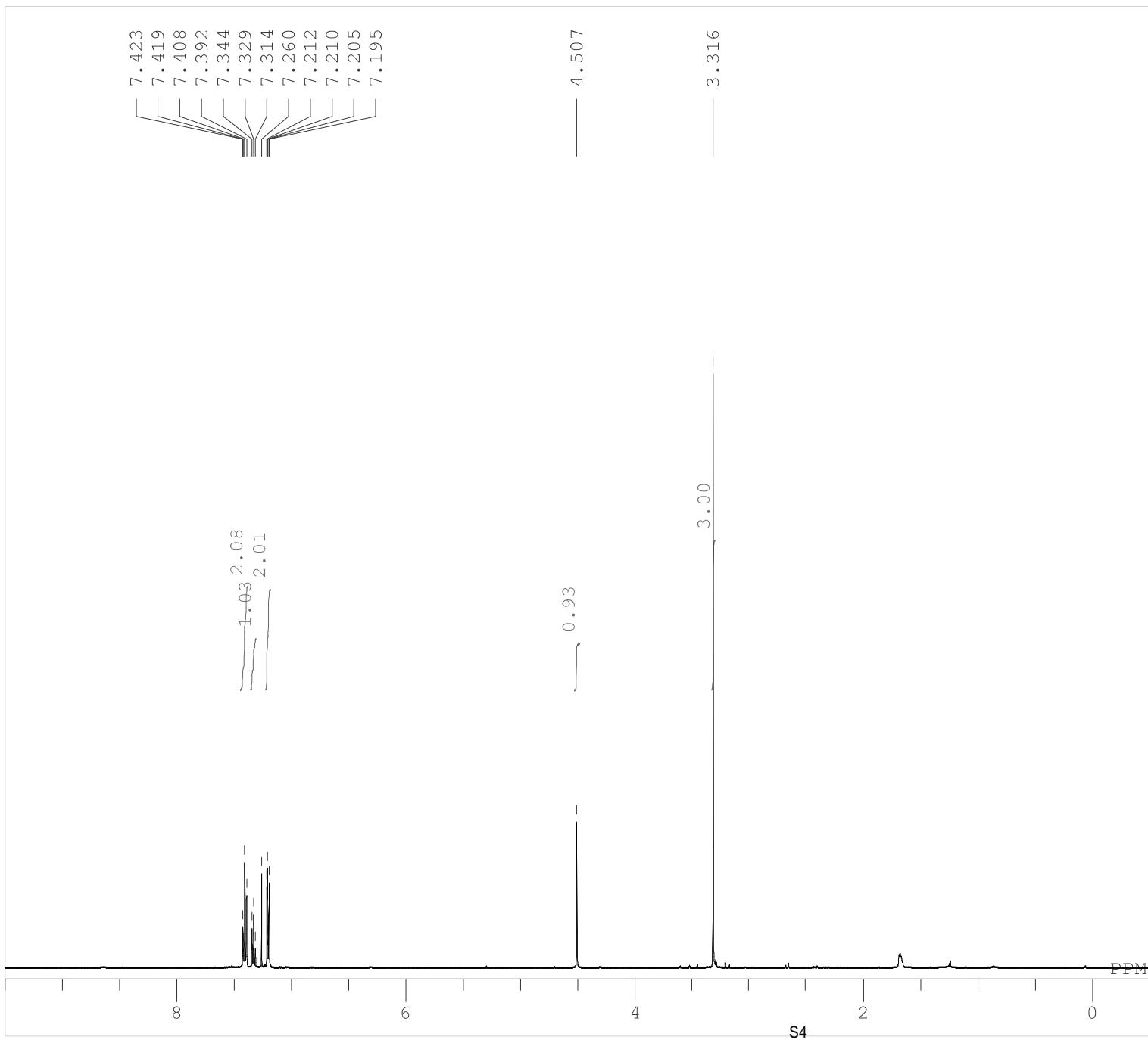
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 PD 5.0000 sec  
 PW1 6.85 usec  
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 CTEMP 14.8 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 48



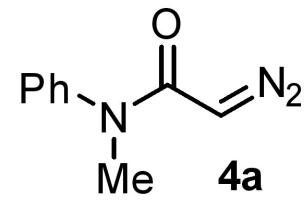


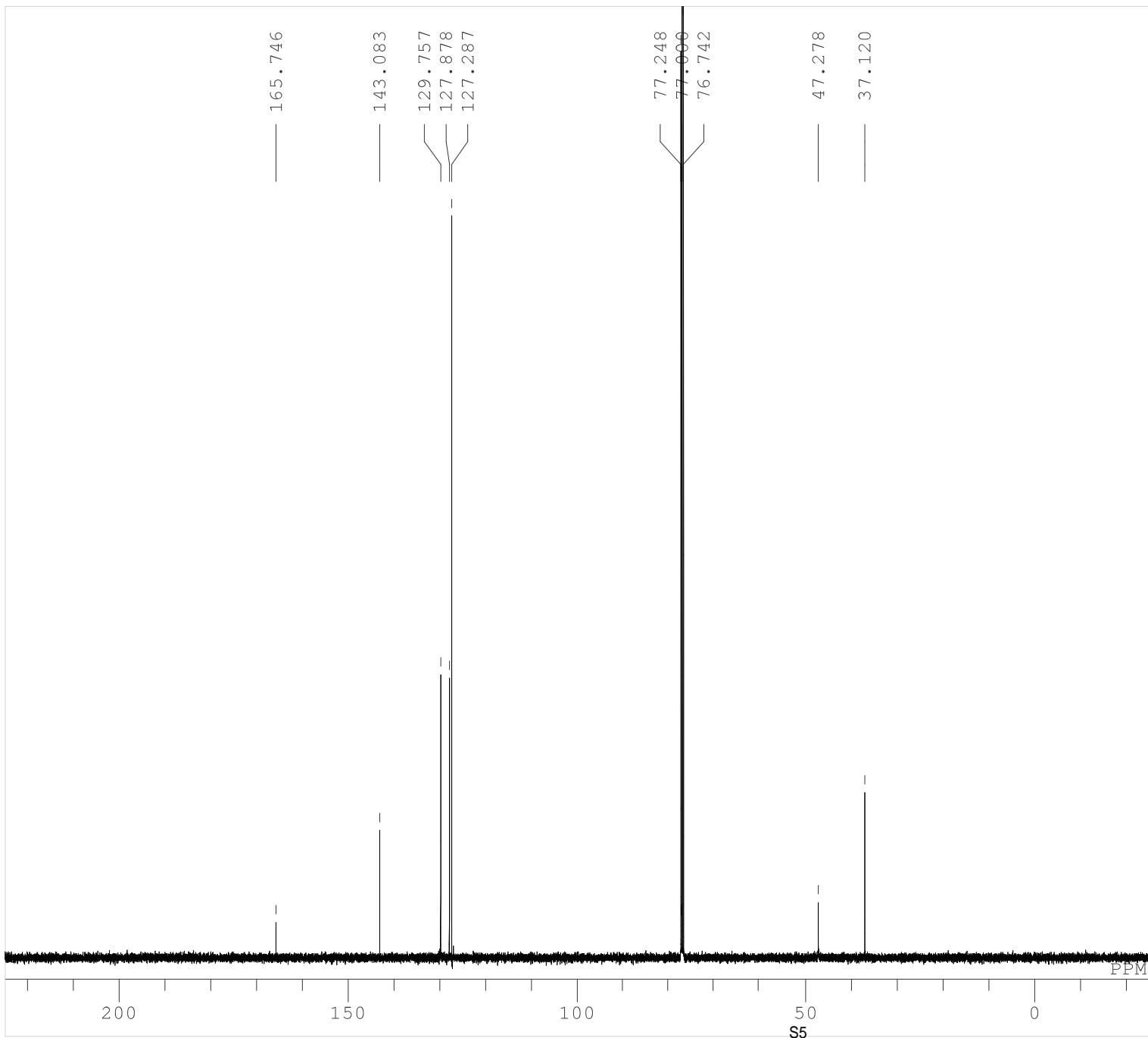
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POINT 26214  
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ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
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RGAIN 60



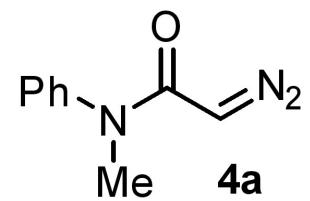


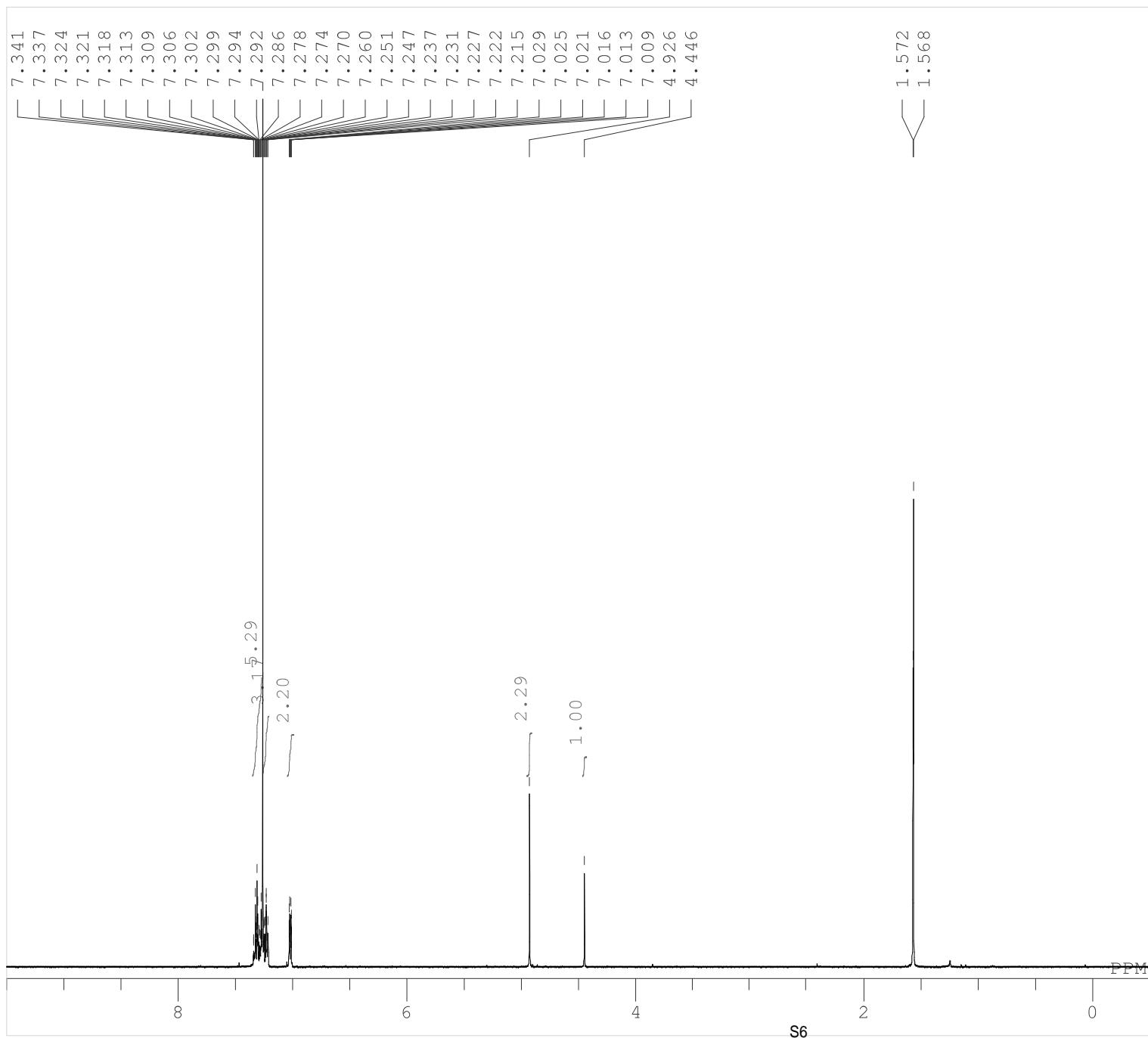
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 PD 5.0000 sec  
 PW1 6.22 usec  
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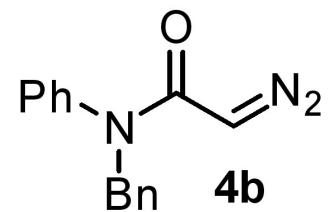


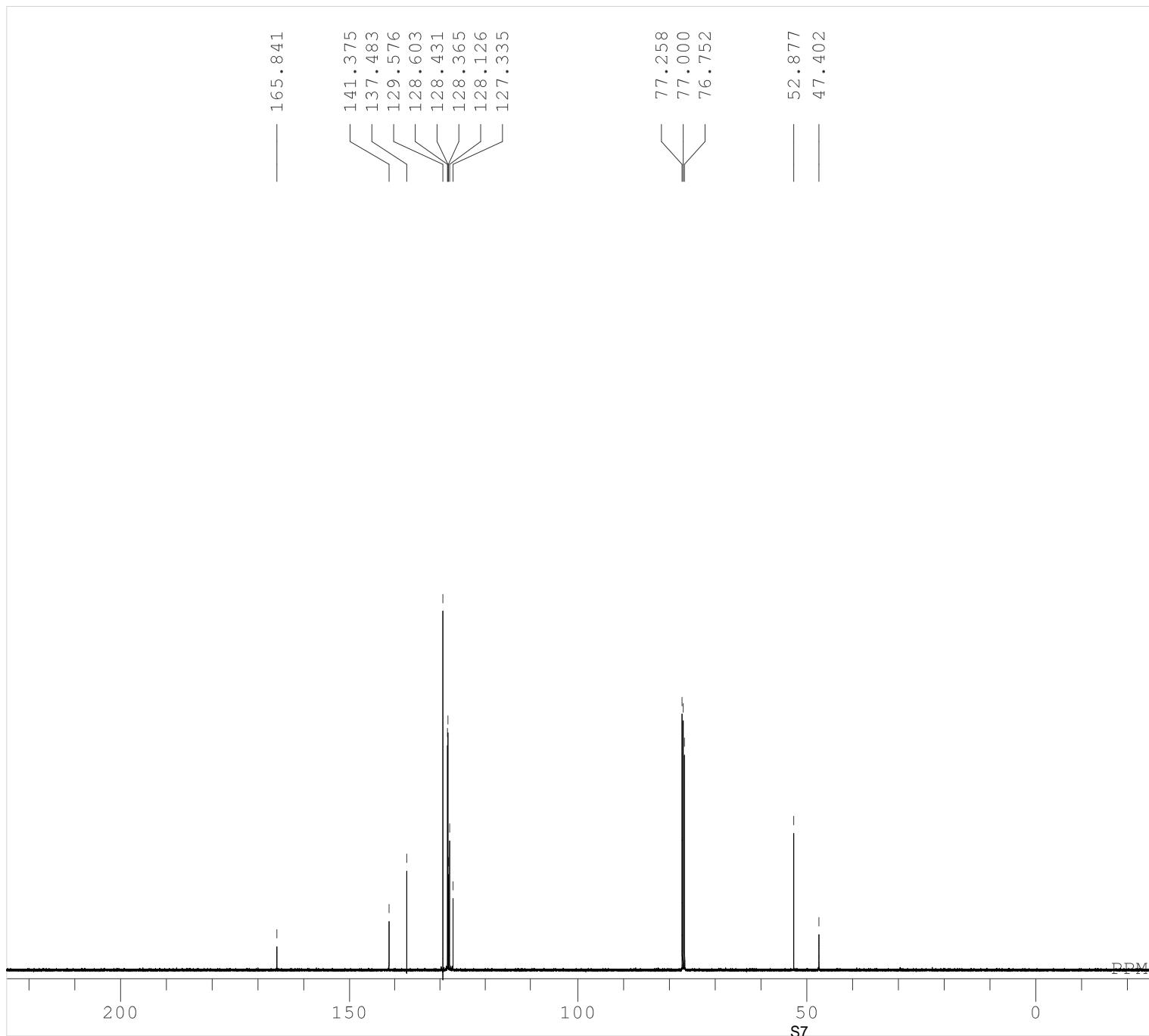
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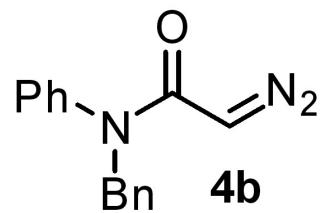


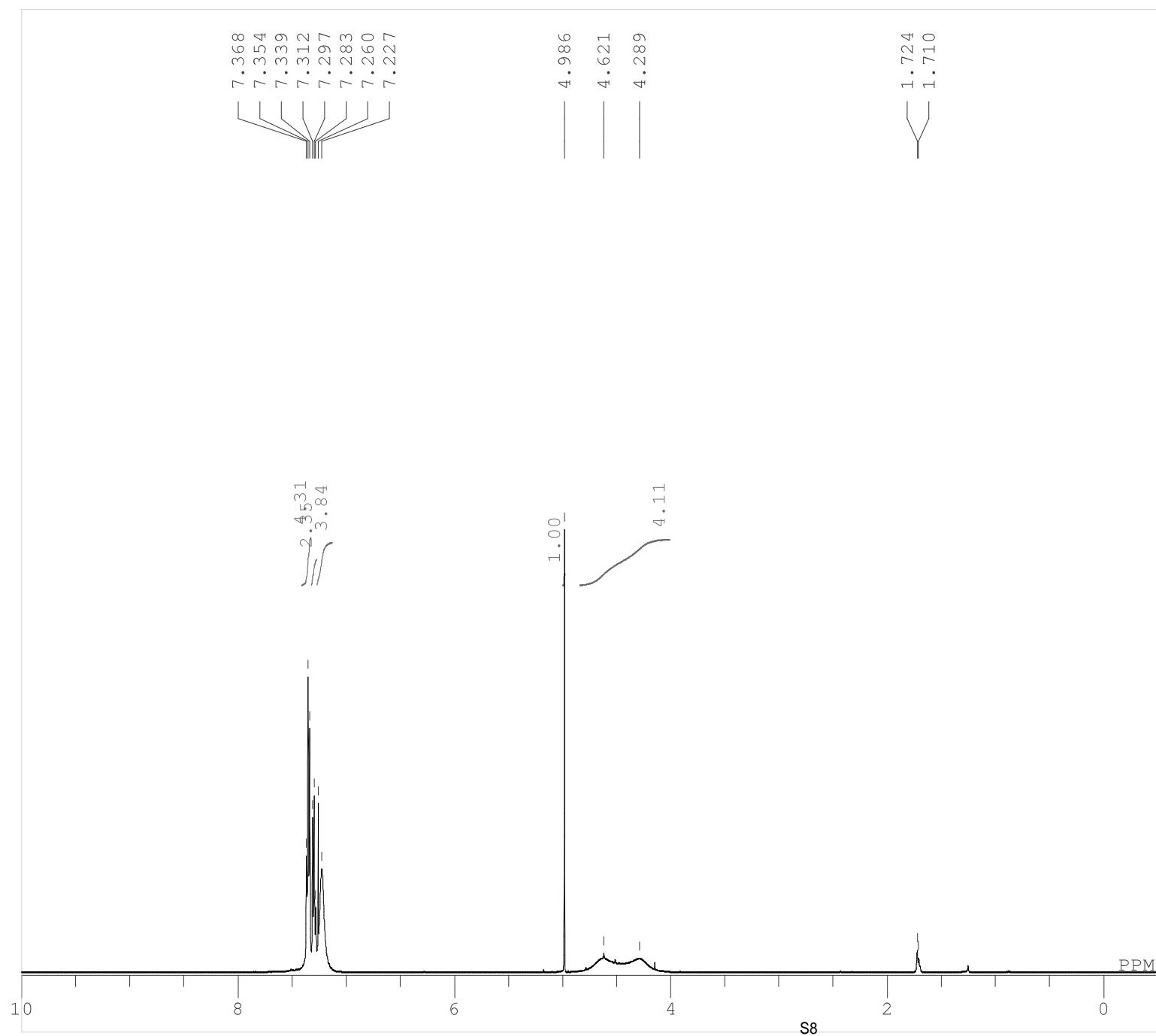
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 PW1 6.85 usec  
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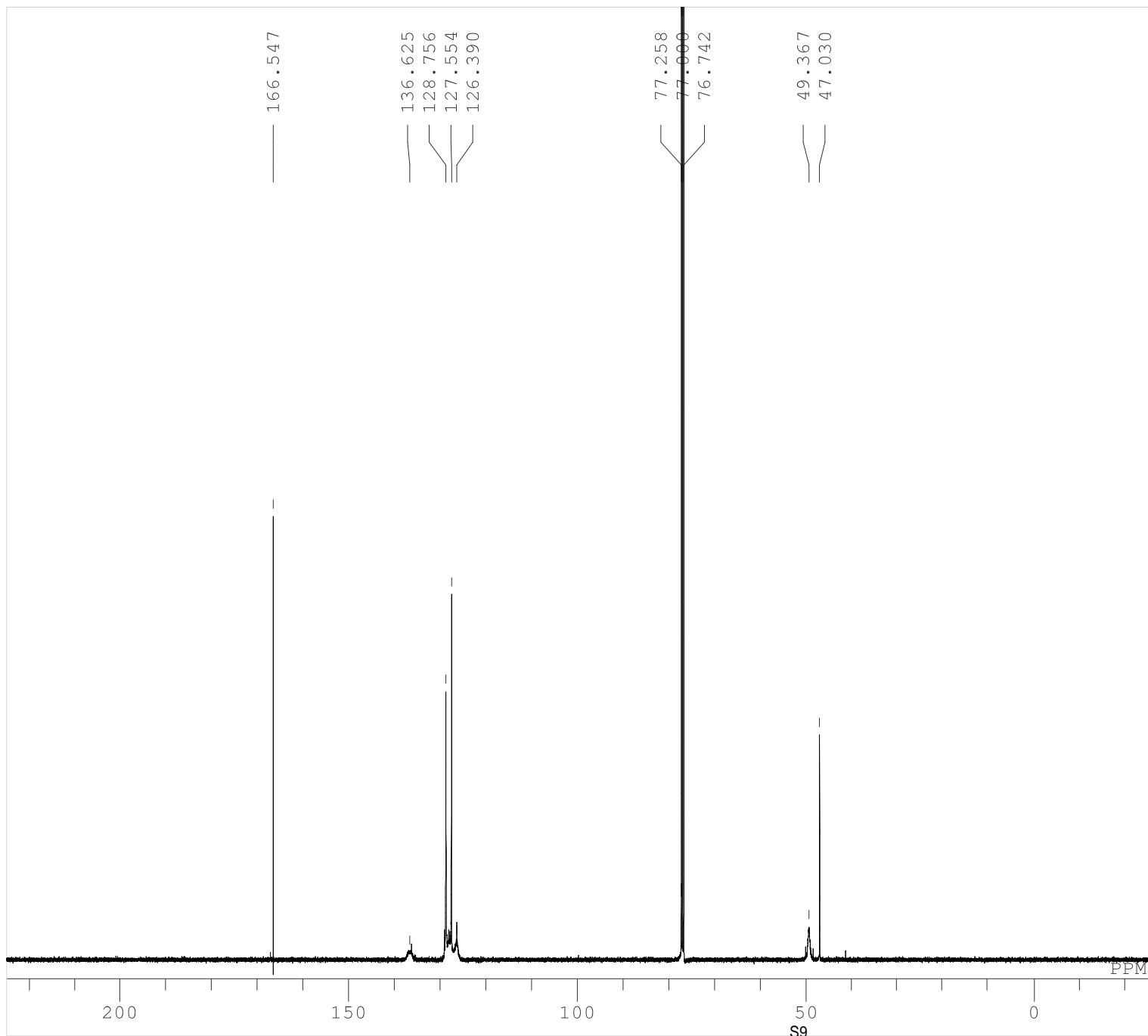


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 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 1260  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
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 RGAIN 60

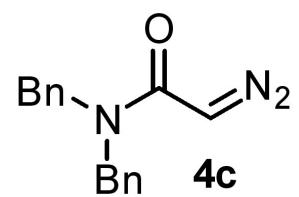


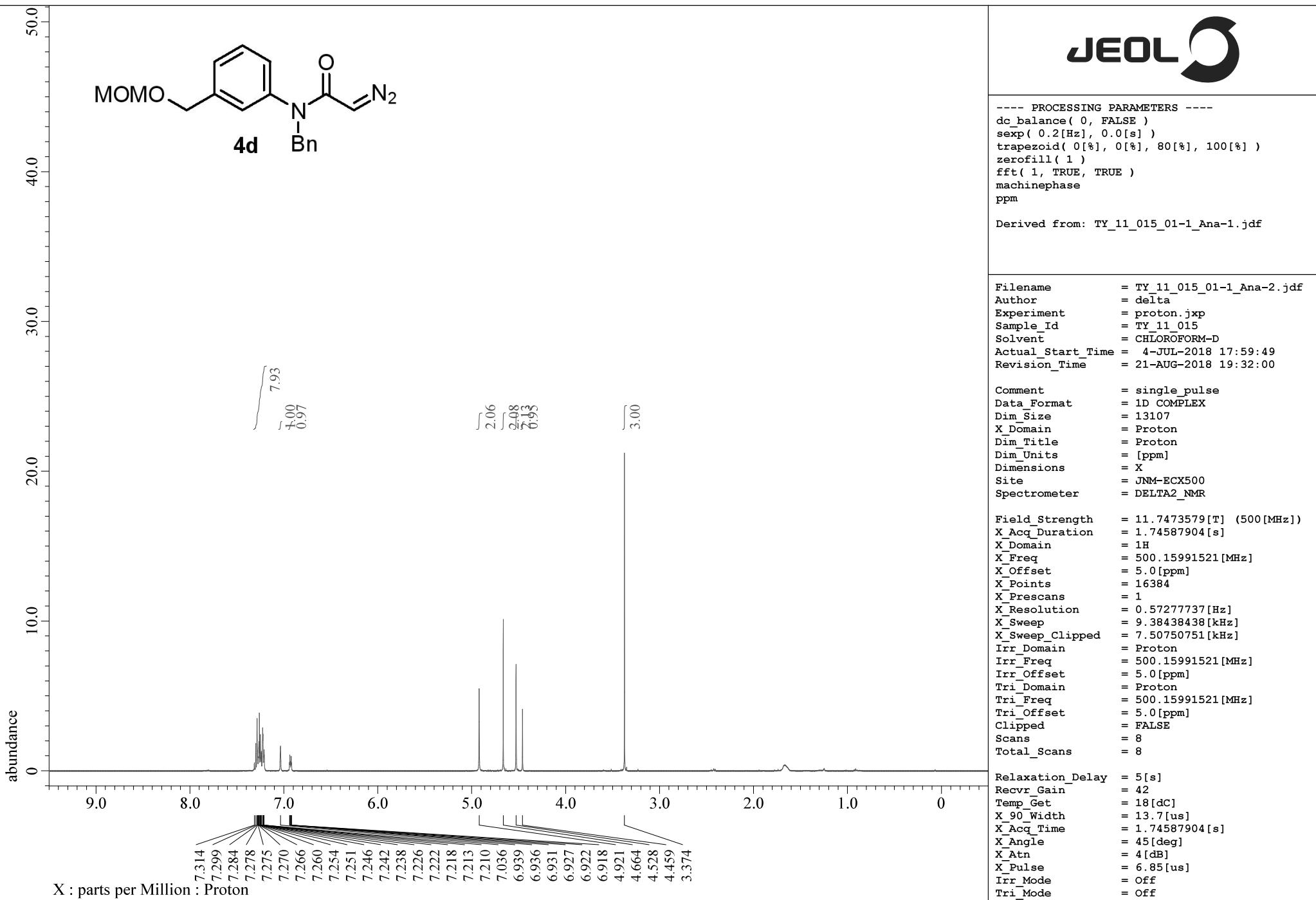


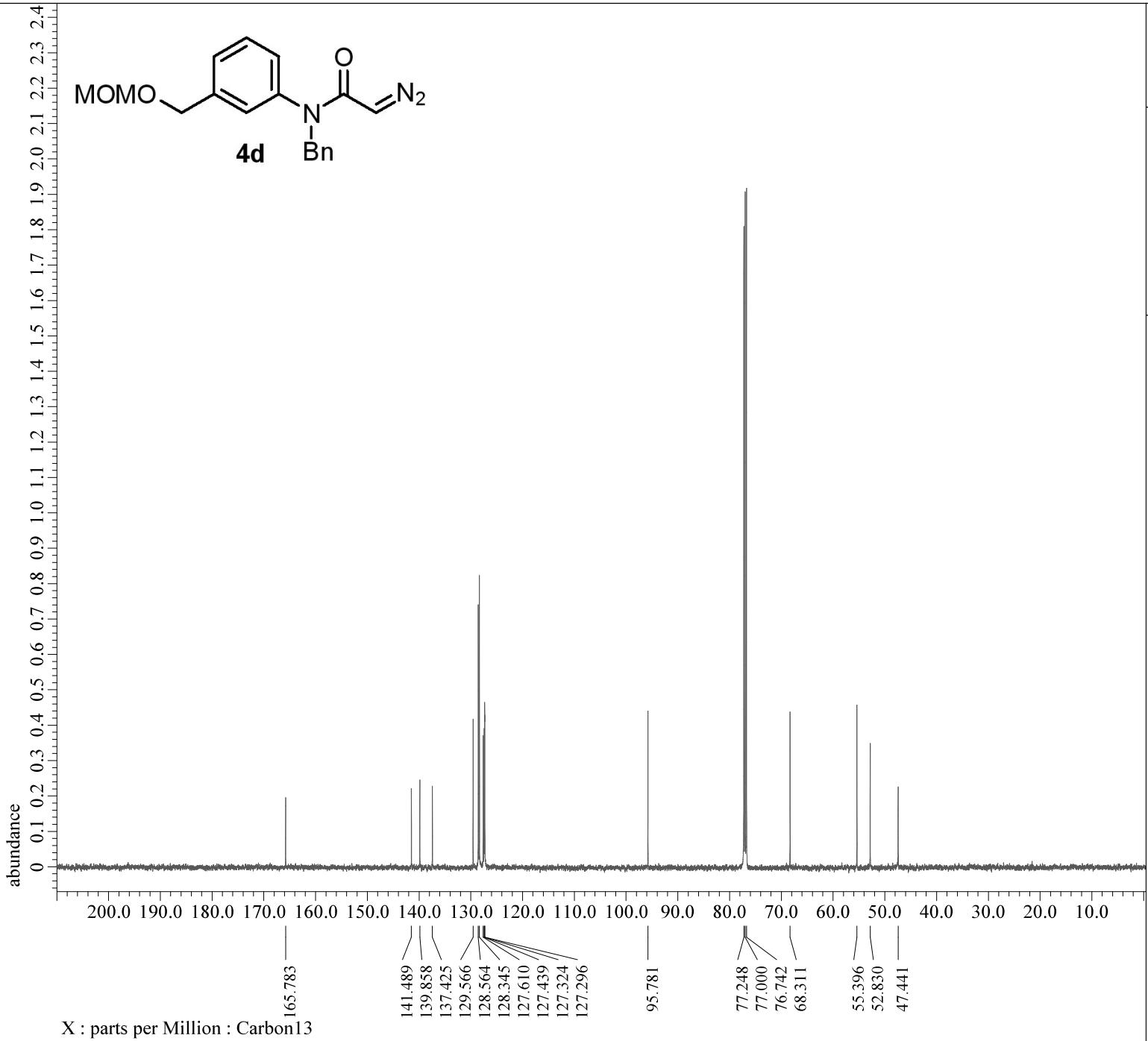
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 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 13.1 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 36



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EXMOD carbon.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 kHz  
OBFIN 4.21 Hz  
POINT 26214  
FREQU 31446.54 Hz  
SCANS 3603  
ACQTM 0.8336 sec  
PD 10.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 13.2 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 60



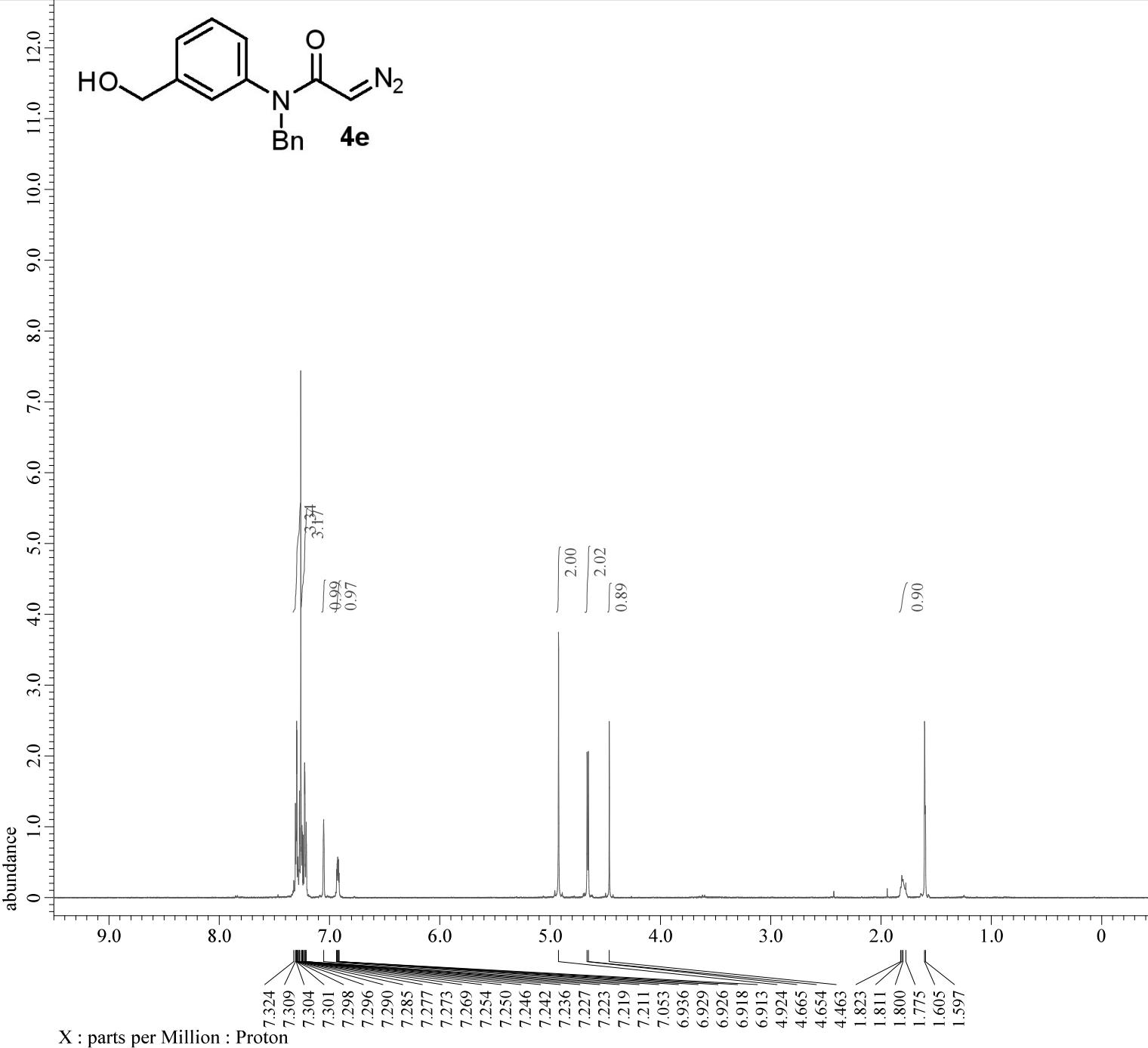
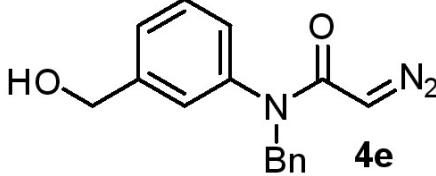




**JEOL**

---- PROCESSING PARAMETERS ----  
dc\_balance( 0, FALSE )  
sexp( 2.0[Hz], 0.0[s] )  
trapezoid( 0[%], 0[%], 80[%], 100[%] )  
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fft( 1, TRUE, TRUE )  
machinephase  
ppm  
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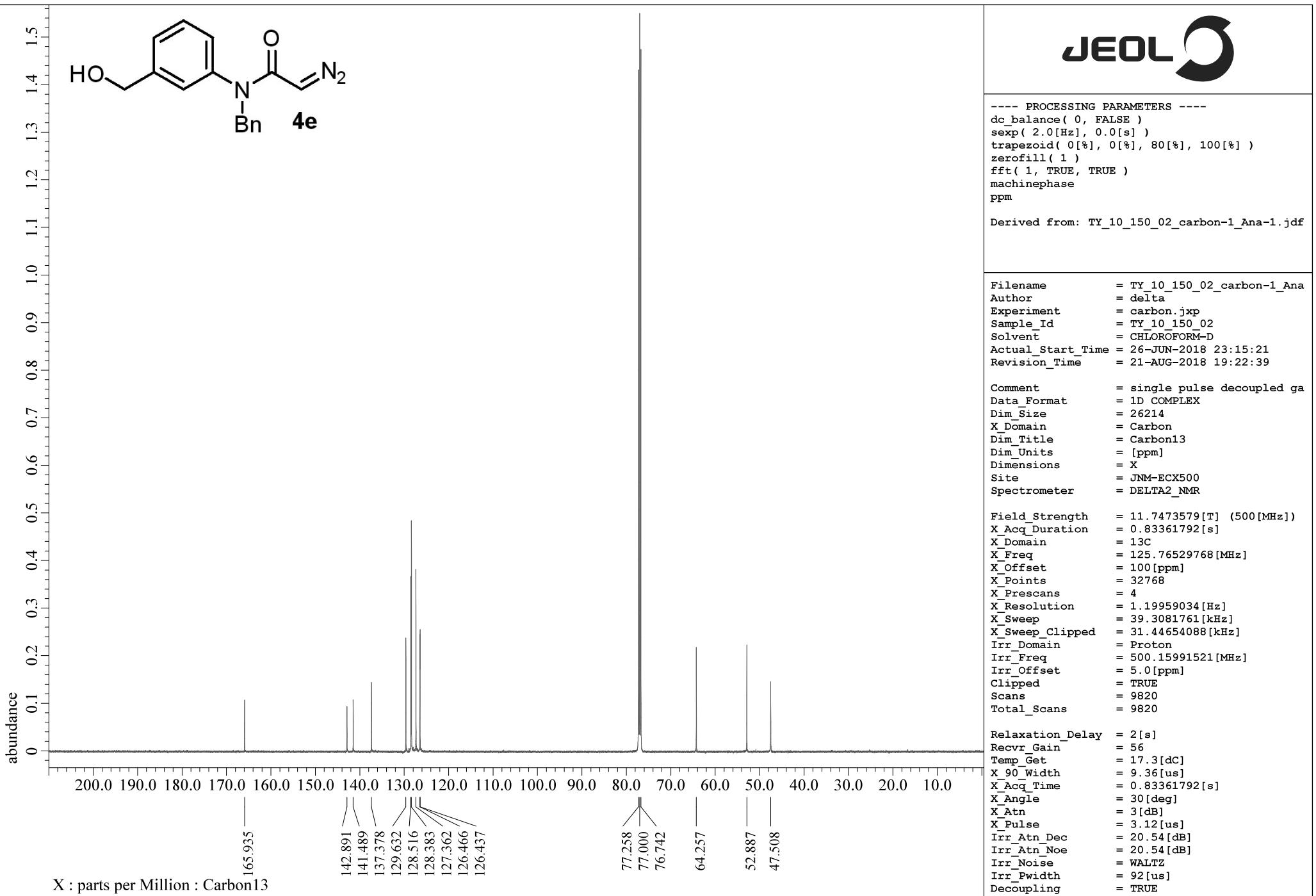
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Author = delta  
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Revision\_Time = 21-AUG-2018 19:32:38  
Comment = single pulse decoupled ga  
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Dim\_Title = Carbon13  
Dim\_Units = [ppm]  
Dimensions = X  
Site = JNM-ECX500  
Spectrometer = DELTA2\_NMR  
Field\_Strength = 11.7473579[T] (500[MHz])  
X\_Acq\_Duration = 0.83361792[s]  
X\_Domain = 13C  
X\_Freq = 125.76529768[MHz]  
X\_Offset = 100[ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 1.19959034[Hz]  
X\_Sweep = 39.3081761[kHz]  
X\_Sweep\_Clipped = 31.44654088[kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 500.15991521[MHz]  
Irr\_Offset = 5.0[ppm]  
Clipped = FALSE  
Scans = 616  
Total\_Scans = 616  
Relaxation\_Delay = 2[s]  
Recv\_Gain = 58  
Temp\_Get = 18.1[dC]  
X\_90\_Width = 9.36[us]  
X\_Acq\_Time = 0.83361792[s]  
X\_Angle = 30[deg]  
X\_Atn = 3[dB]  
X\_Pulse = 3.12[us]  
Irr\_Atn\_Dec = 20.54[dB]  
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Decoupling = TRUE

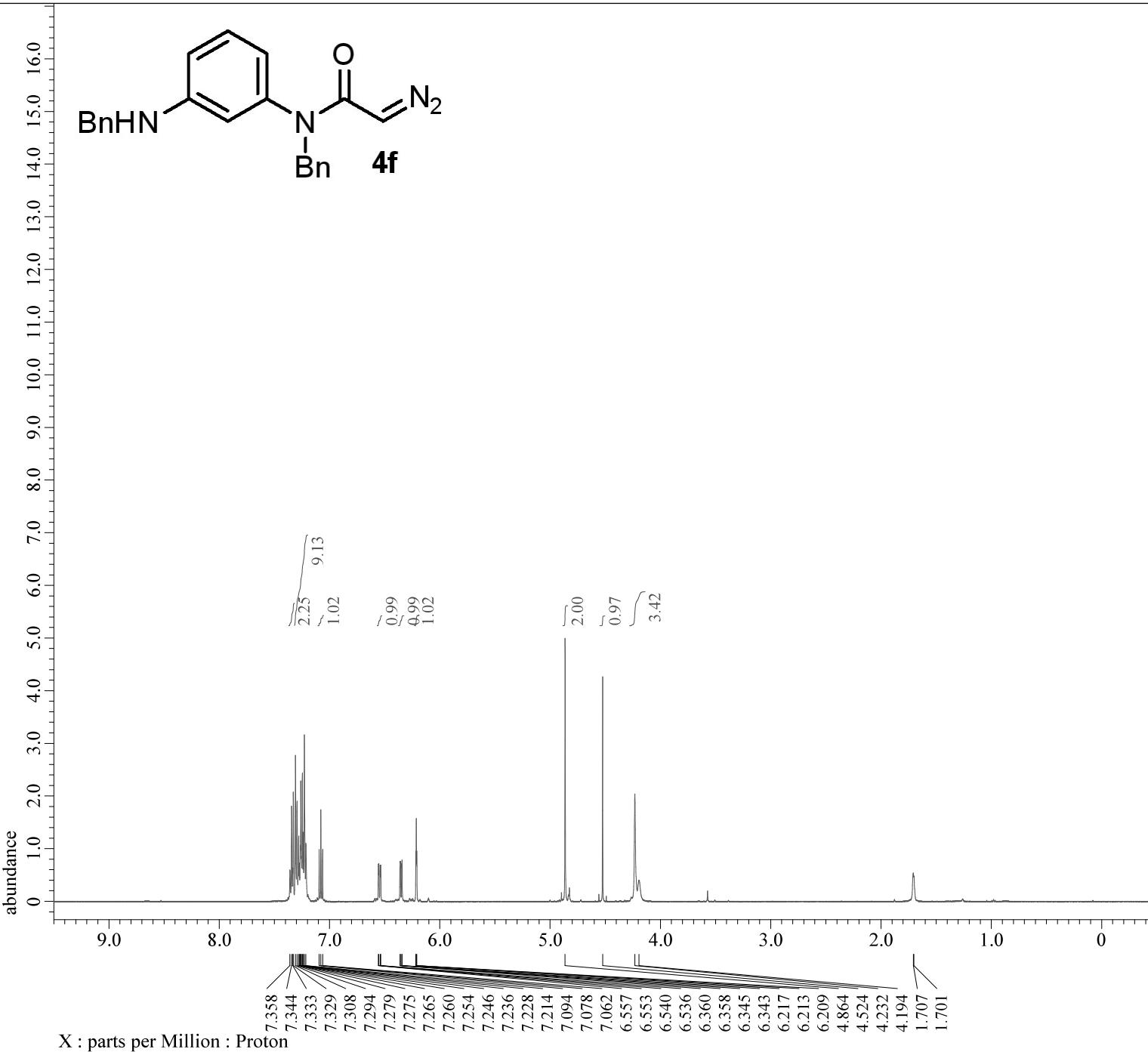
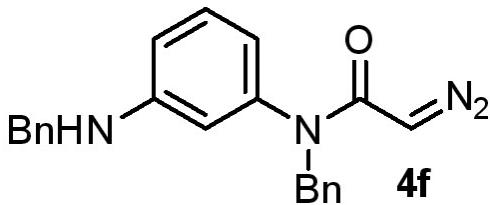


**JEOL**

---- PROCESSING PARAMETERS ----  
dc\_balance( 0, FALSE )  
sexp( 0.2[Hz], 0.0[s] )  
trapezoid( 0[%], 0[%], 80[%], 100[%] )  
zerofill( 1 )  
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machinephase  
ppm  
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Author = delta  
Experiment = proton.jxp  
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Revision\_Time = 21-AUG-2018 19:21:39  
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Dim\_Title = Proton  
Dim\_Units = [ppm]  
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Spectrometer = DELTA2\_NMR  
Field\_Strength = 11.7473579[T] (500[MHz])  
X\_Acq\_Duration = 1.74587904[s]  
X\_Offset = 5.0[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.57277737[Hz]  
X\_Sweep = 9.38438438[kHz]  
X\_Sweep\_Clipped = 7.50750751[kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 500.15991521[MHz]  
Irr\_Offset = 5.0[ppm]  
Tri\_Domain = Proton  
Tri\_Freq = 500.15991521[MHz]  
Tri\_Offset = 5.0[ppm]  
Clipped = FALSE  
Scans = 8  
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Relaxation\_Delay = 5[s]  
Recvr\_Gain = 46  
Temp\_Get = 14.4[dC]  
X\_90\_Width = 13.7[us]  
X\_Acq\_Time = 1.74587904[s]  
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X\_Pulse = 6.85[us]  
Irr\_Mode = Off  
Tri\_Mode = Off

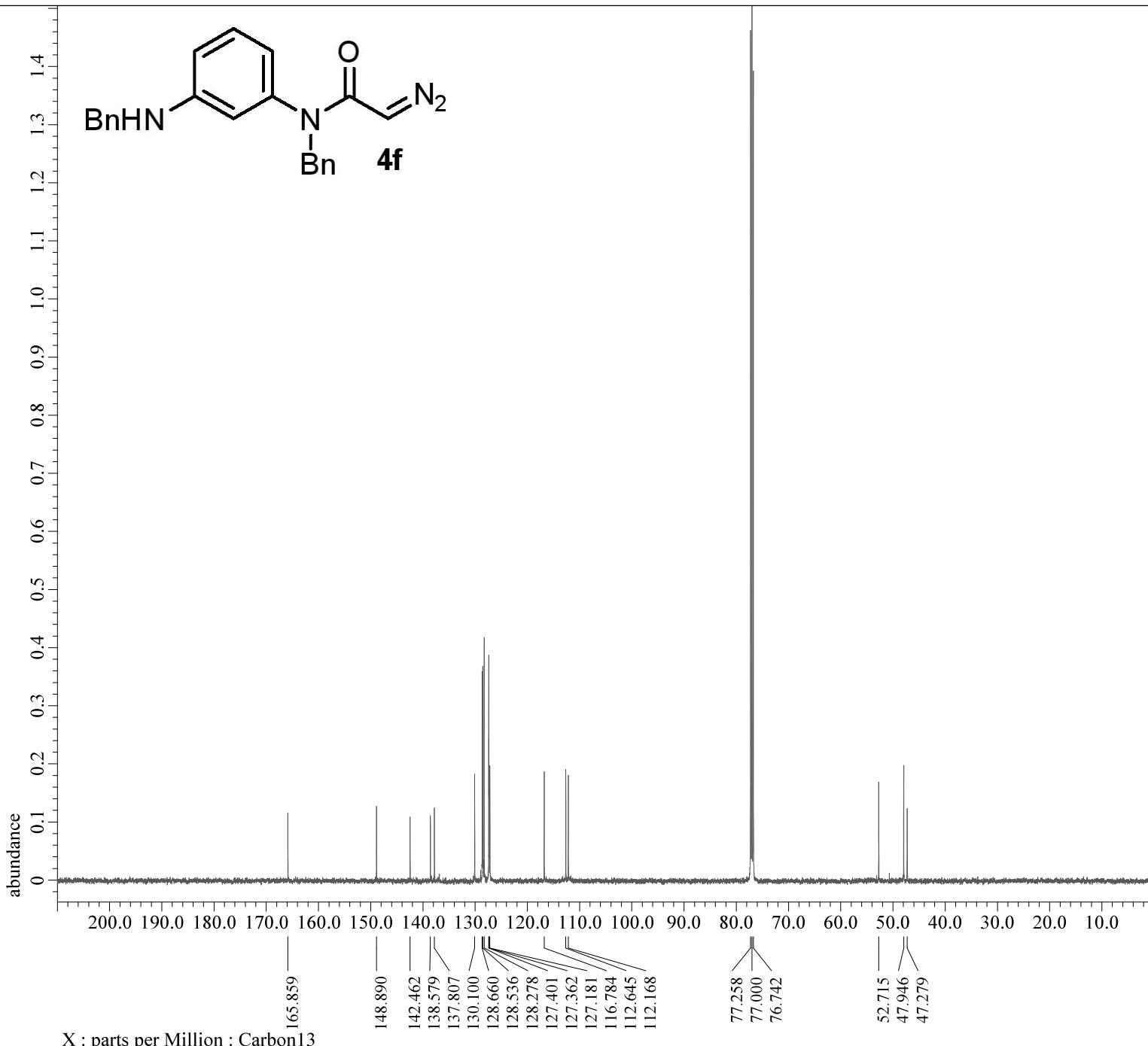
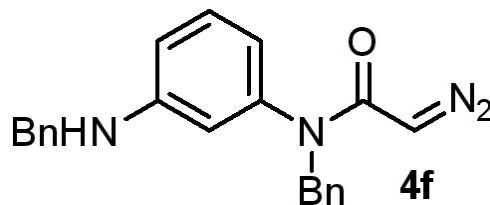




**JEOL**

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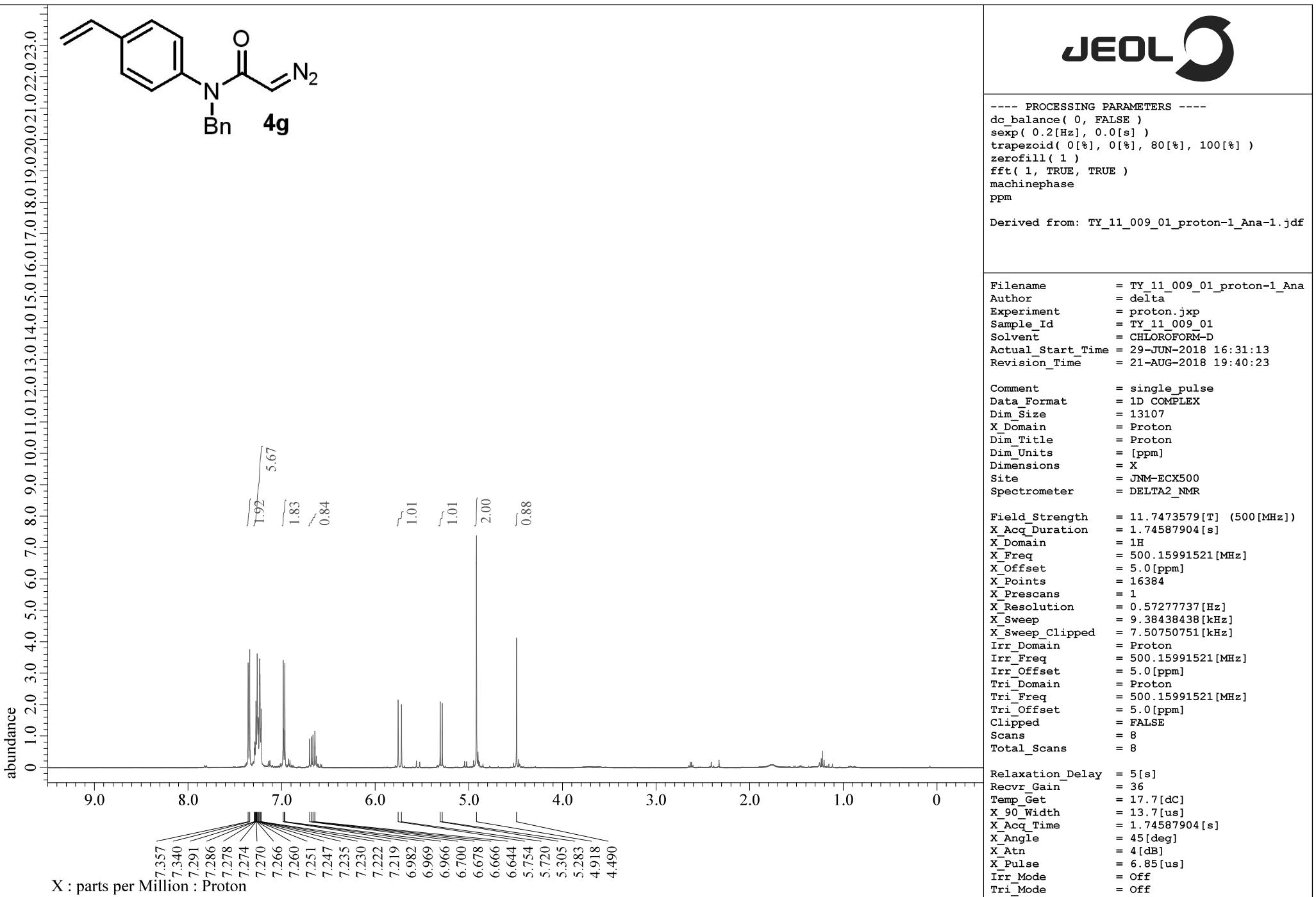
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**X\_Freq** = 500.15991521[MHz]  
**X\_Offset** = 5.0[ppm]  
**X\_Points** = 16384  
**X\_Prescans** = 1  
**X\_Resolution** = 0.57277737[Hz]  
**X\_Sweep** = 9.38438438[kHz]  
**X\_Sweep\_Clipped** = 7.50750751[kHz]  
**Irr\_Domain** = Proton  
**Irr\_Freq** = 500.15991521[MHz]  
**Irr\_Offset** = 5.0[ppm]  
**Tri\_Domain** = Proton  
**Tri\_Freq** = 500.15991521[MHz]  
**Tri\_Offset** = 5.0[ppm]  
**Clipped** = FALSE  
**Scans** = 8  
**Total\_Scans** = 8  
  
**Relaxation\_Delay** = 5[s]  
**Recvr\_Gain** = 34  
**Temp\_Get** = 18[dC]  
**X\_90\_Width** = 13.7[us]  
**X\_Acq\_Time** = 1.74587904[s]  
**X\_Angle** = 45[deg]  
**X\_Atn** = 4[dB]  
**X\_Pulse** = 6.85[us]  
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**Tri\_Mode** = Off

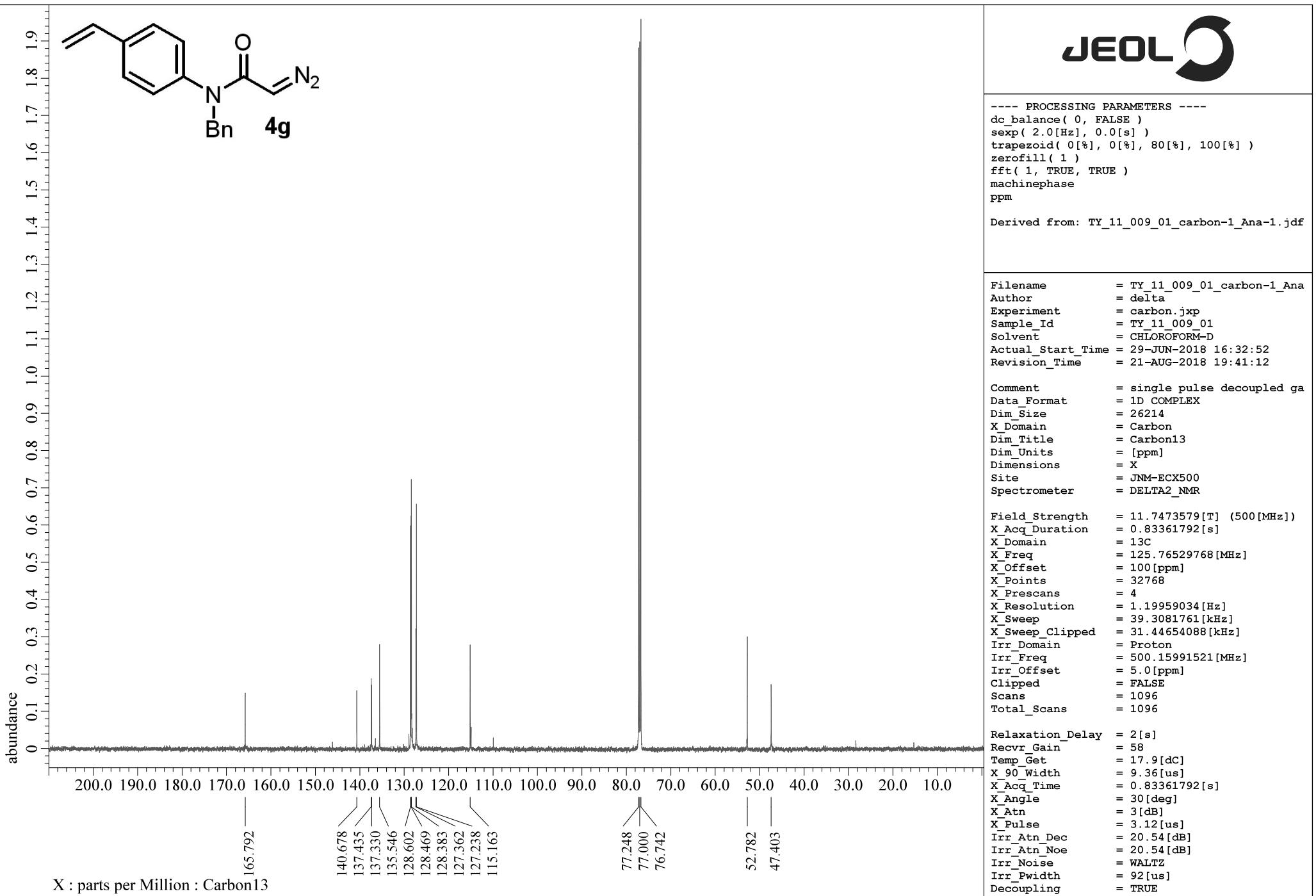


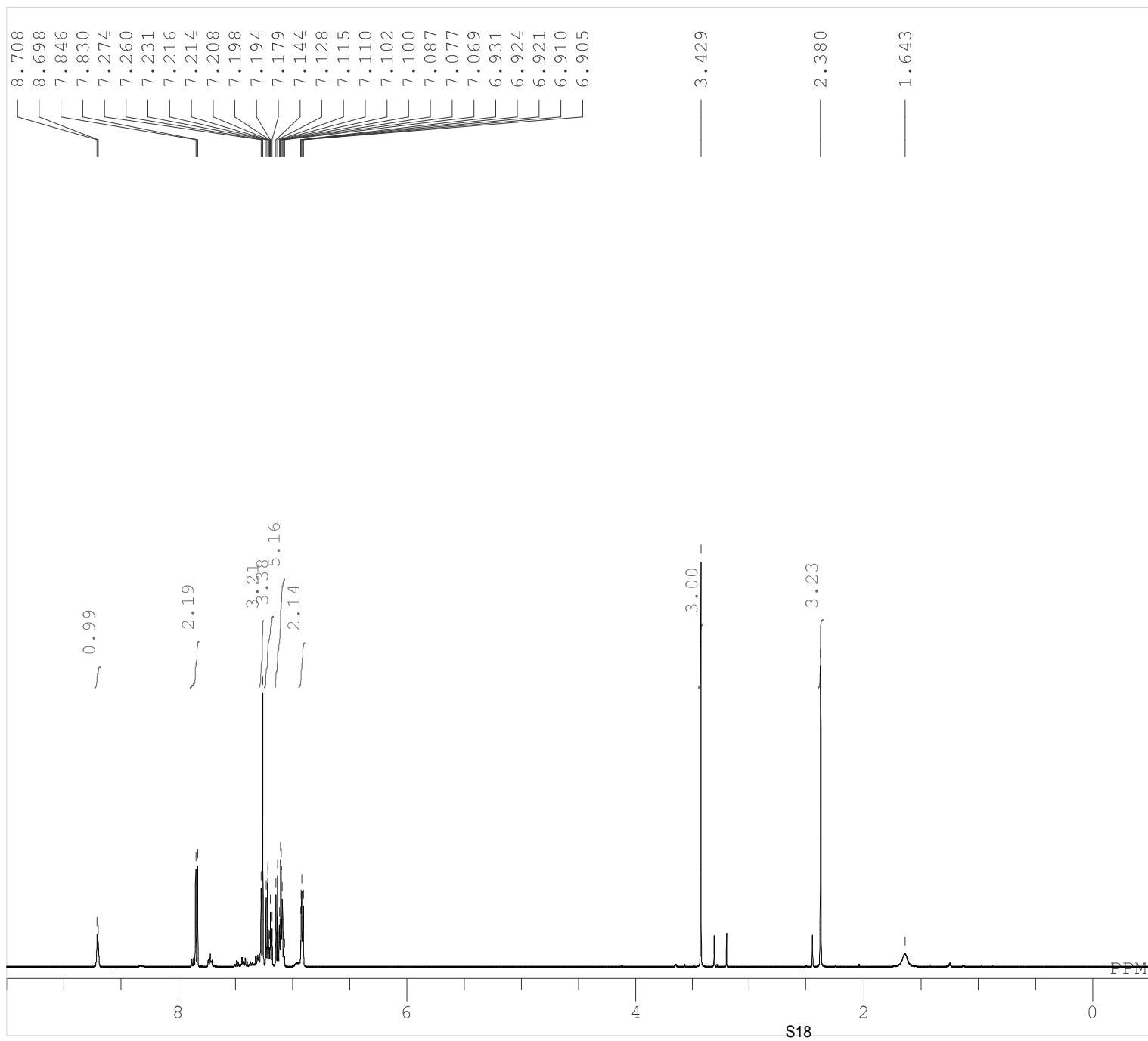
**JEOL**

---- PROCESSING PARAMETERS ----  
dc\_balance( 0, FALSE )  
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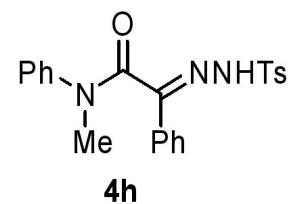
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Revision\_Time = 21-AUG-2018 19:04:29  
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Dim\_Title = Carbon13  
Dim\_Units = [ppm]  
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Spectrometer = DELTA2\_NMR  
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X\_Freq = 125.76529768[MHz]  
X\_Offset = 100[ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 1.19959034[Hz]  
X\_Sweep = 39.3081761[kHz]  
X\_Sweep\_Clipped = 31.44654088[kHz]  
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Irr\_Freq = 500.15991521[MHz]  
Irr\_Offset = 5.0[ppm]  
Clipped = FALSE  
Scans = 1260  
Total\_Scans = 1260  
Relaxation\_Delay = 2[s]  
Recv\_Gain = 56  
Temp\_Get = 18.2[dC]  
X\_90\_Width = 9.36[us]  
X\_Acq\_Time = 0.83361792[s]  
X\_Angle = 30[deg]  
X\_Atn = 3[dB]  
X\_Pulse = 3.12[us]  
Irr\_Atn\_Dec = 20.54[dB]  
Irr\_Atn\_Noe = 20.54[dB]  
Irr\_Noise = WALTZ  
Irr\_Pwidth = 92[us]  
Decoupling = TRUE

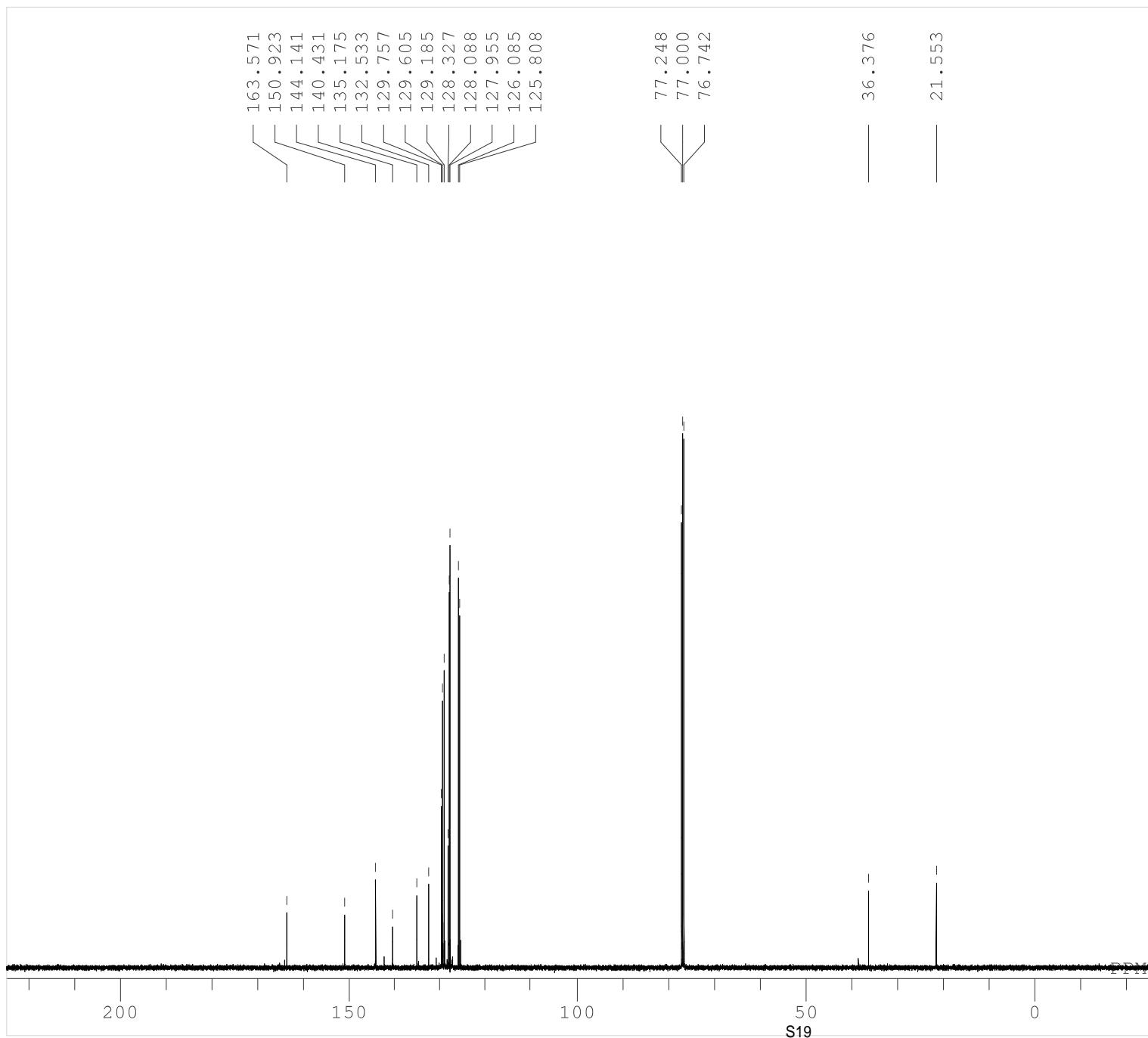




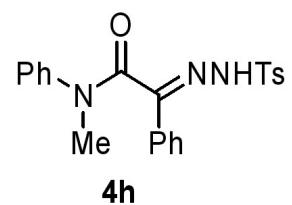


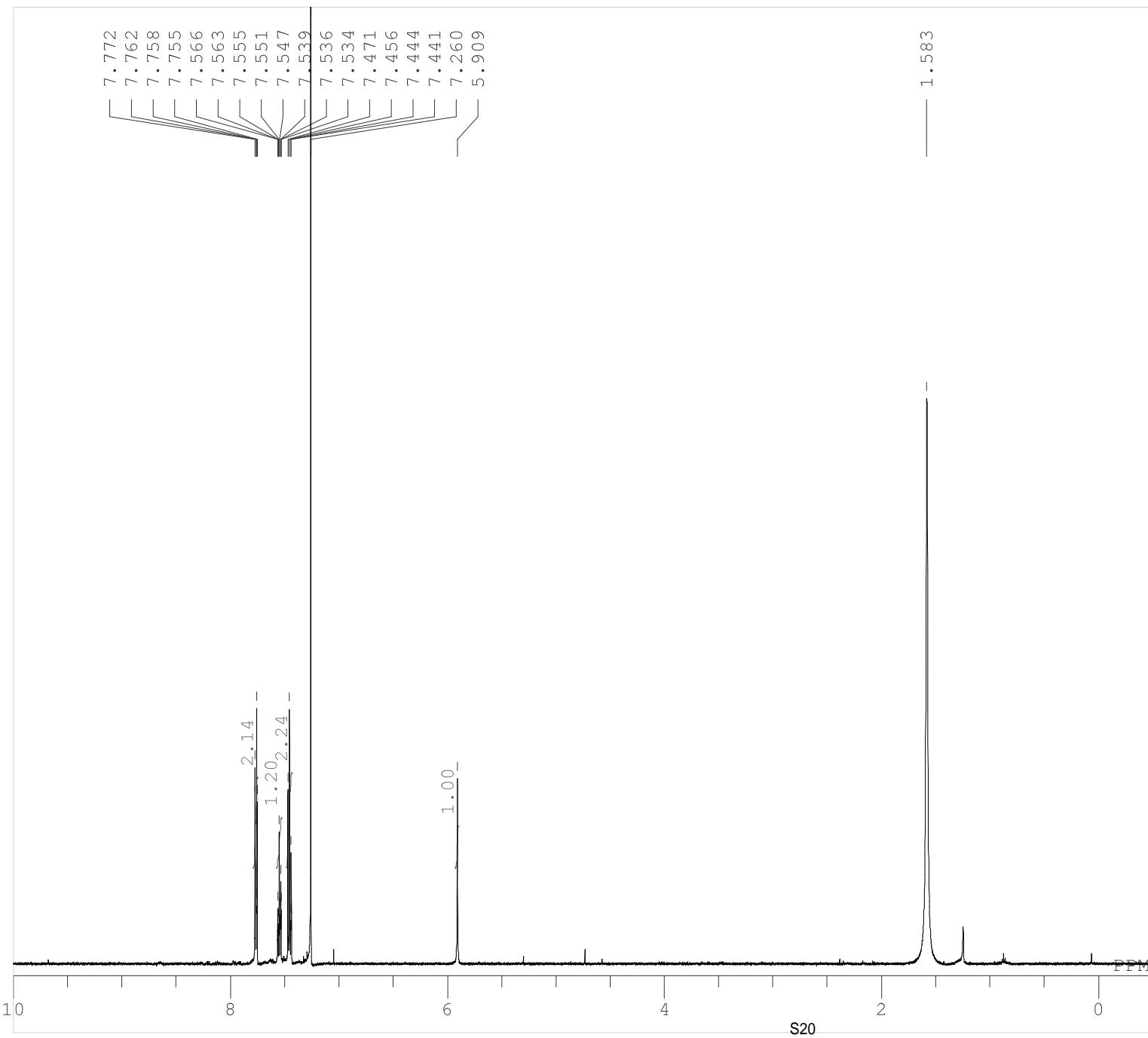
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 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
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 CTEMP 17.6 c  
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 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 40



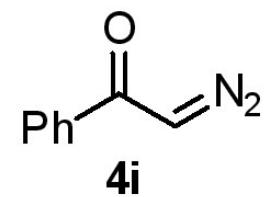


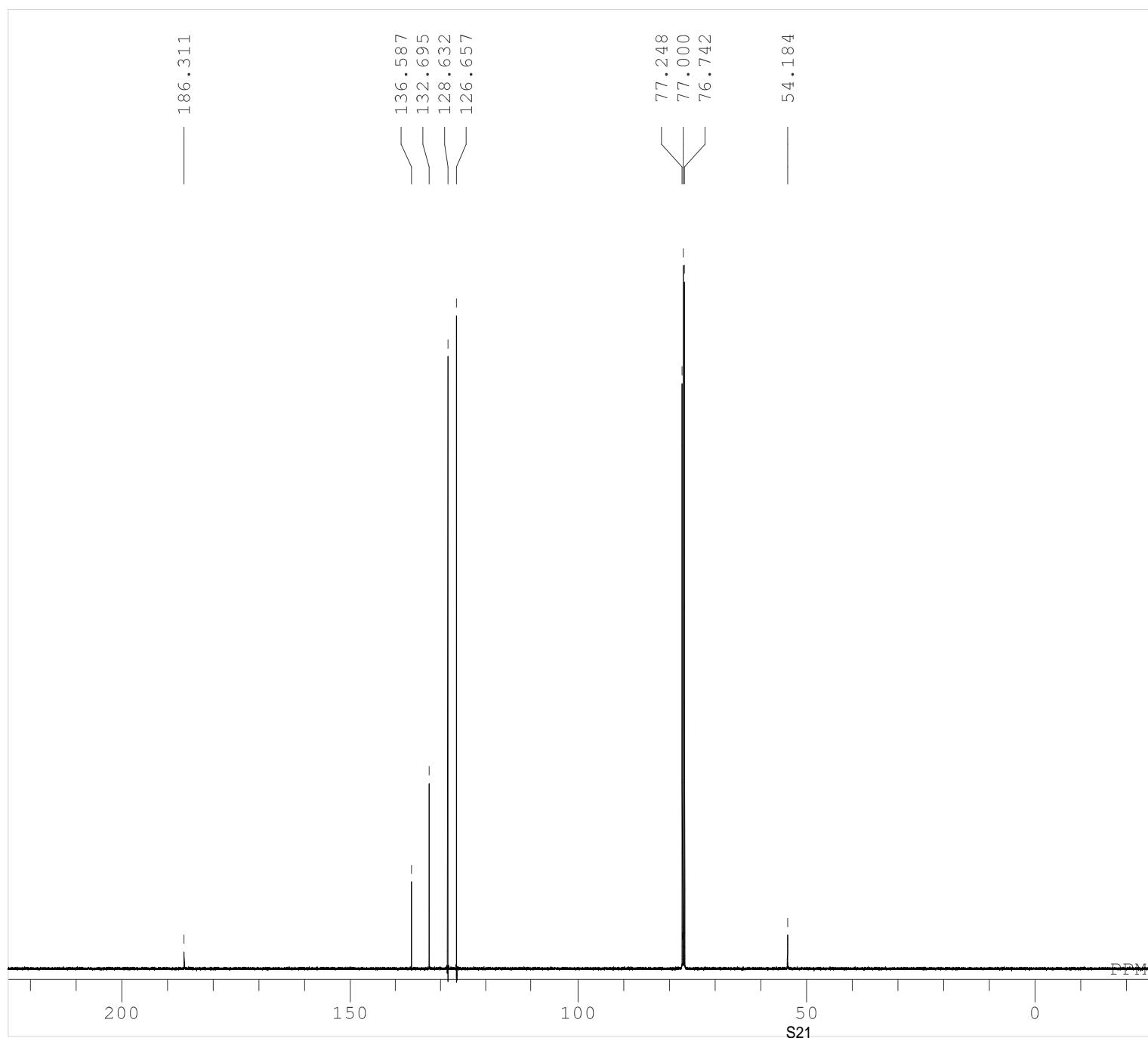
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 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 1260  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 19.2 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60



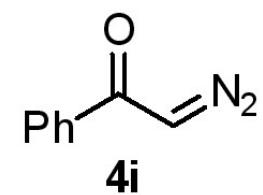


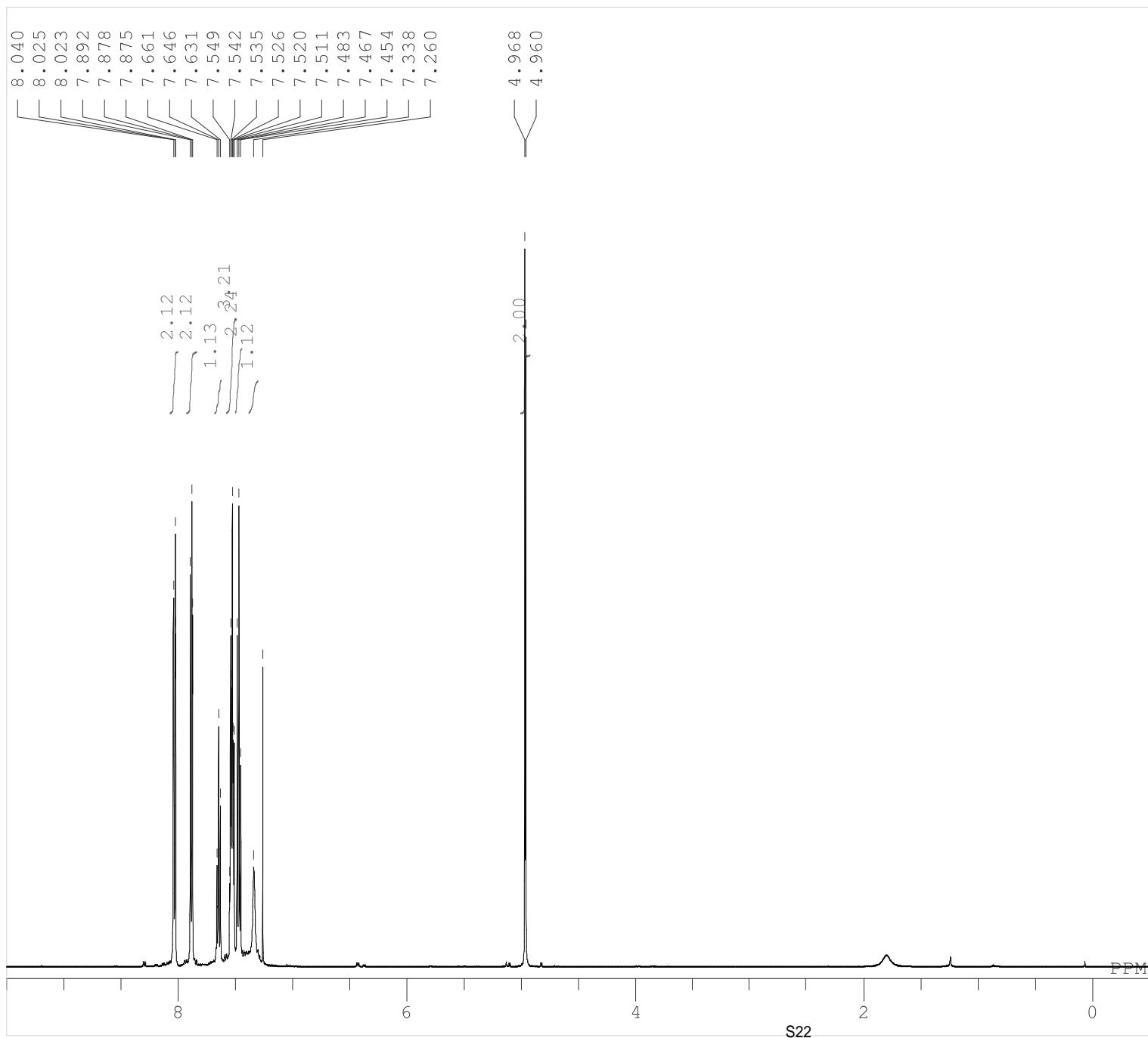
DFILE TY\_09\_007\_01-1-1.als  
COMNT dazo  
DATIM 2017-07-06 12:54:10  
OBNUC 1H  
EXMOD proton.jxp  
OBFRQ 500.16 MHz  
OBSET 2.41 kHz  
OBFIN 6.01 Hz  
POINT 13107  
FREQU 7507.51 Hz  
SCANS 8  
ACQTM 1.7459 sec  
PD 5.0000 sec  
PW1 6.85 usec  
IRNUC 1H  
CTEMP 16.4 c  
SLVNT CDCL<sub>3</sub>  
EXREF 7.26 ppm  
BF 0.10 Hz  
RGAIN 48



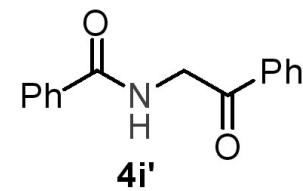


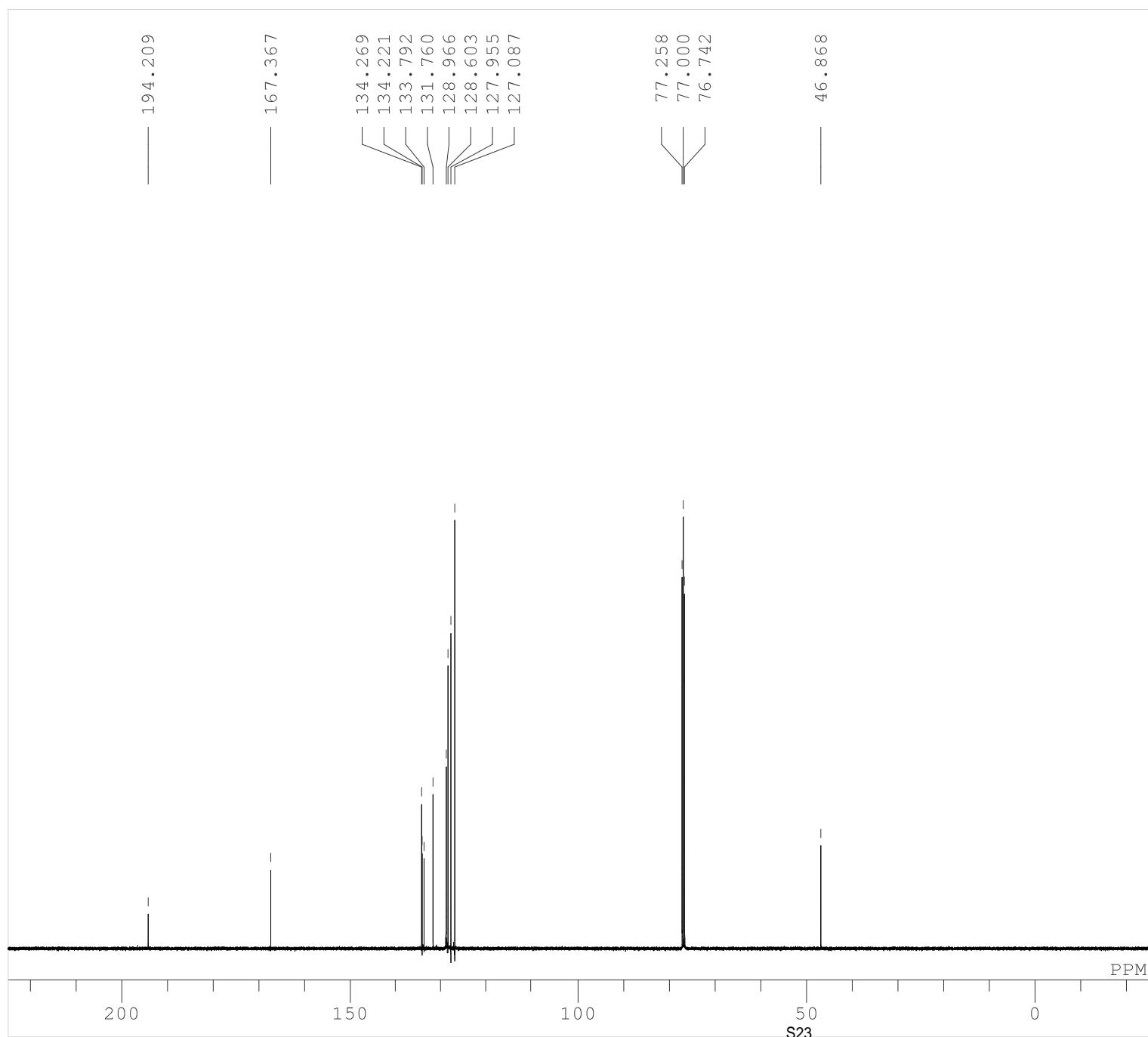
DFILE TY\_08\_132\_03\_carbon-1-1.als  
COMNT single pulse decoupled gated  
DATIM 2018-02-21 23:12:53  
OBNUC <sup>13</sup>C  
EXMOD carbon.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 kHz  
OBFIN 4.21 Hz  
POINT 26214  
FREQU 31446.54 Hz  
SCANS 9200  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 16.9 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 60



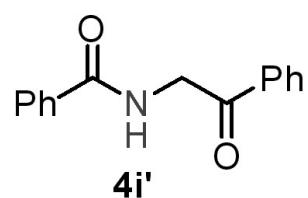


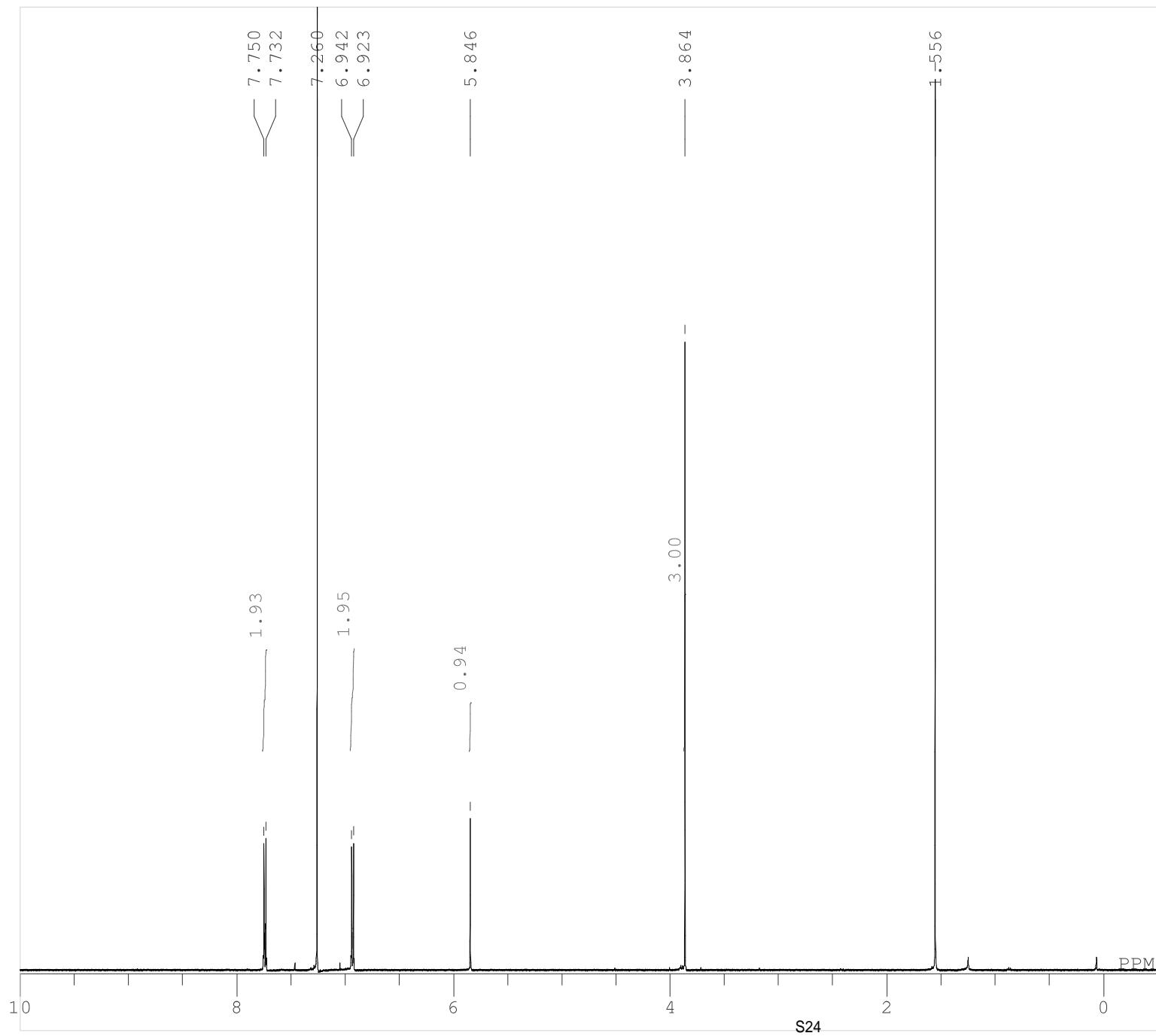
DFILE TY\_10\_062\_01\_proton-1-1.als  
 COMNT single\_pulse  
 DATIM 2018-04-12 13:14:34  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 15.4 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 36



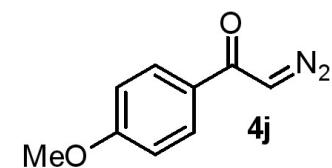


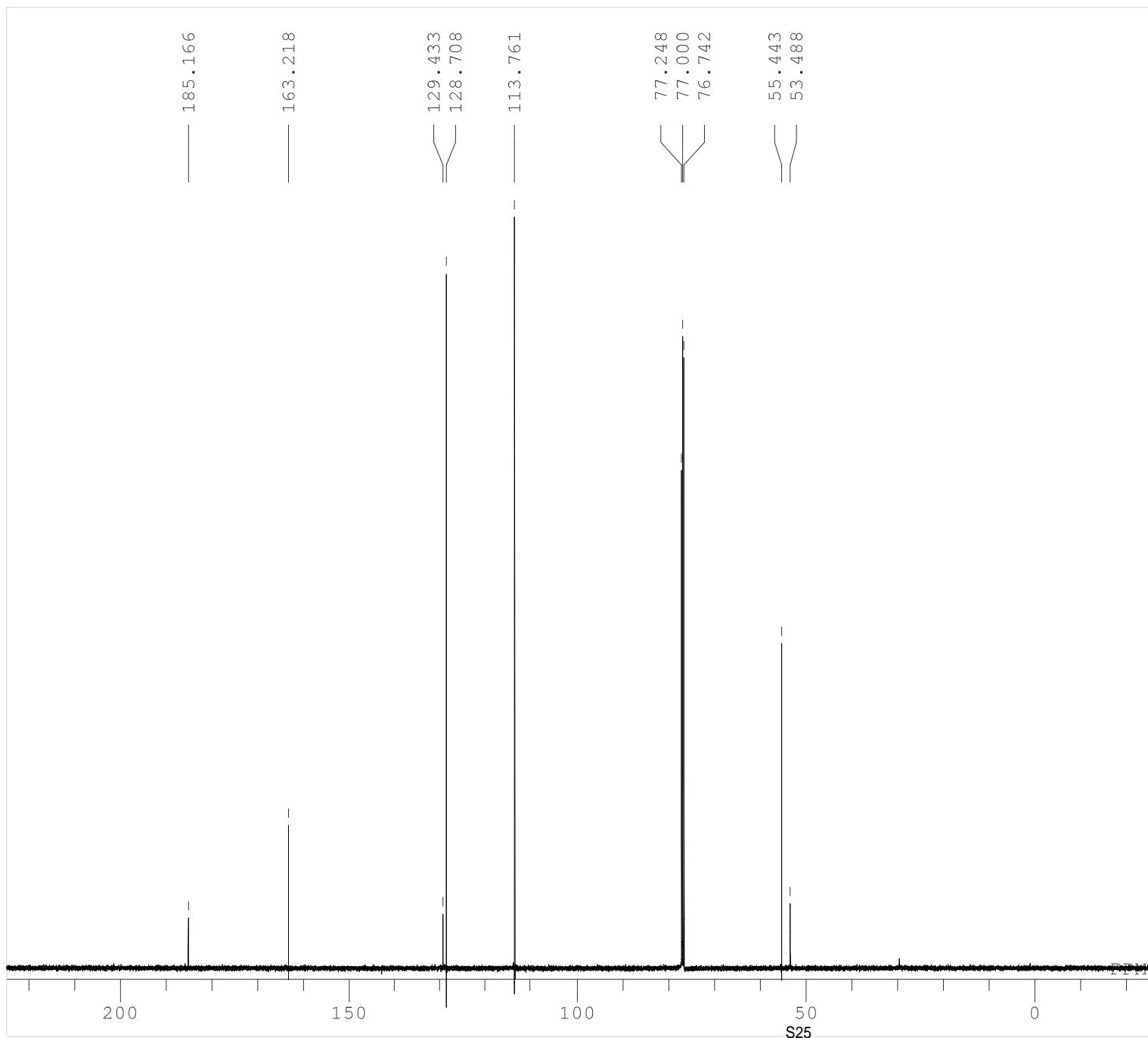
DFILE TY\_10\_062\_01\_carbon-1-1.als  
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 DATIM 2018-04-12 13:18:15  
 OBNUC <sup>13</sup>C  
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 1680  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 15.3 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60



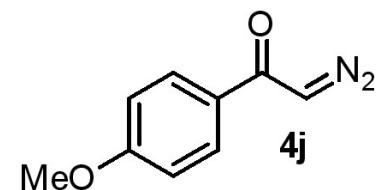


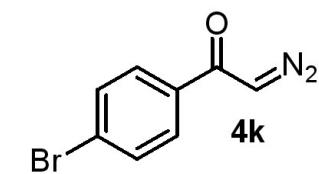
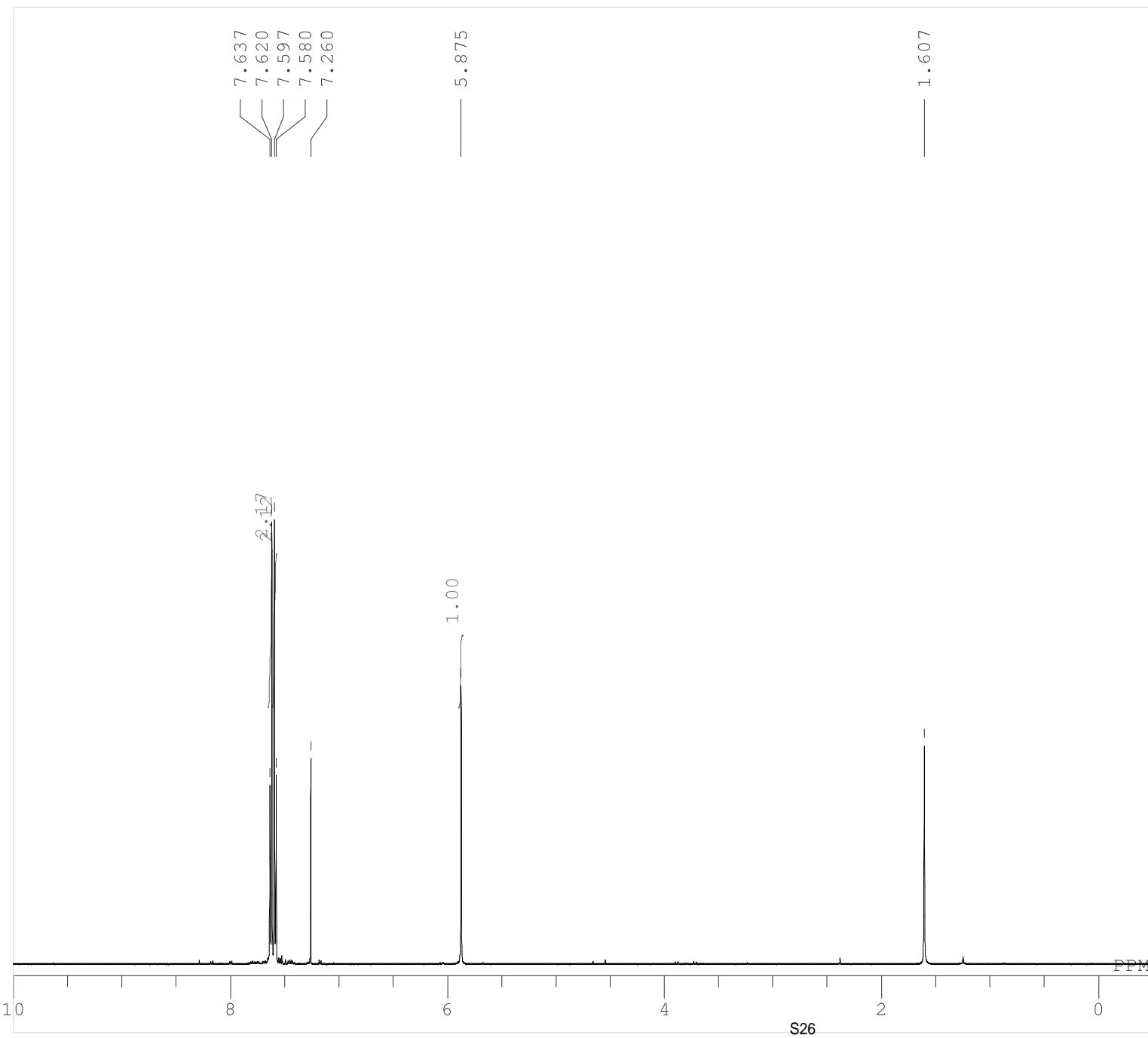
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COMNT dazo  
DATIM 2017-07-19 17:00:58  
OBNUC 1H  
EXMOD proton.jxp  
OBFRQ 500.16 MHz  
OBSET 2.41 kHz  
OBFIN 6.01 Hz  
POINT 13107  
FREQU 7507.51 Hz  
SCANS 8  
ACQTM 1.7459 sec  
PD 5.0000 sec  
PW1 6.85 usec  
IRNUC 1H  
CTEMP 19.0 c  
SLVNT CDCL<sub>3</sub>  
EXREF 7.26 ppm  
BF 0.10 Hz  
RGAIN 50

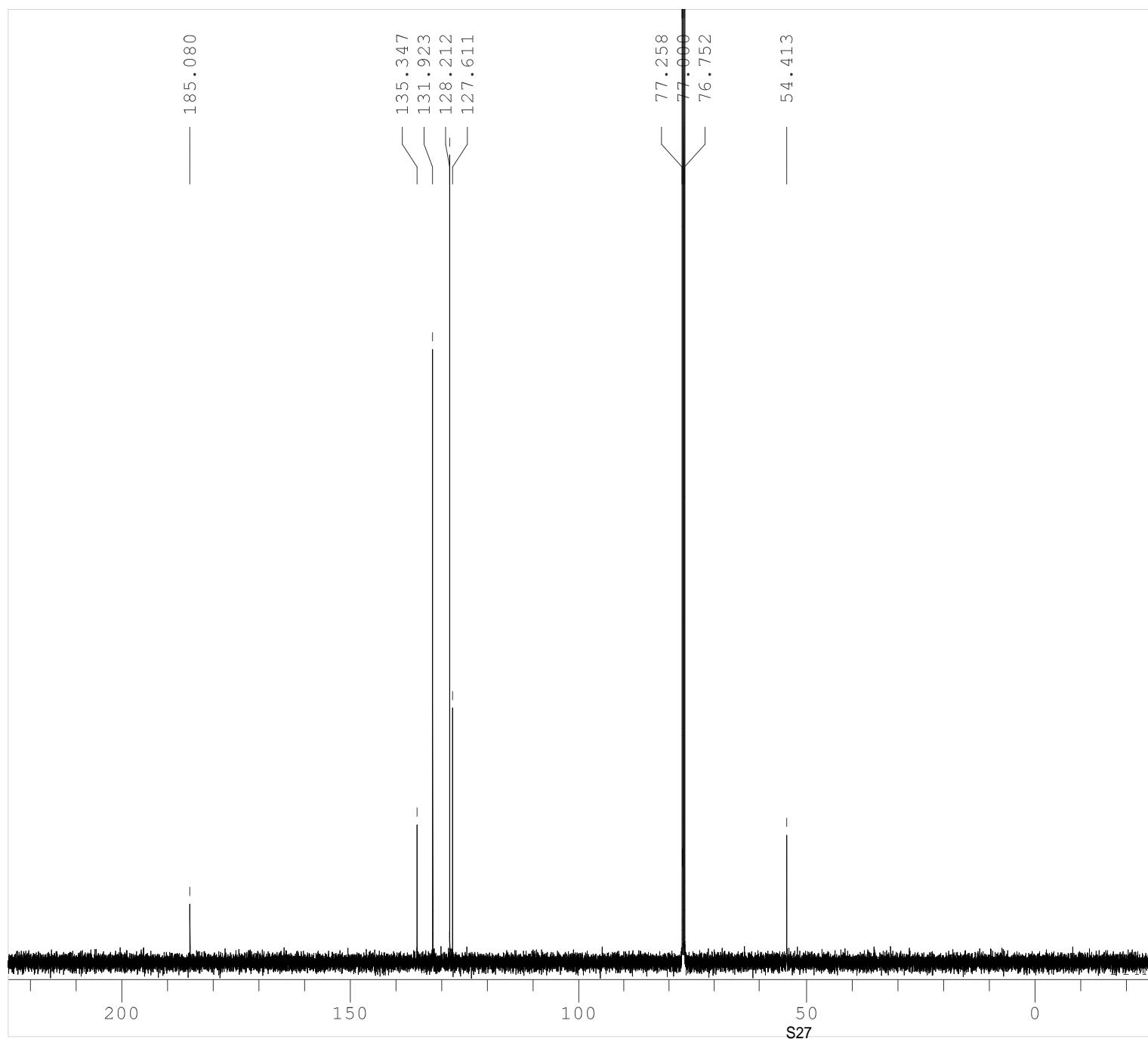




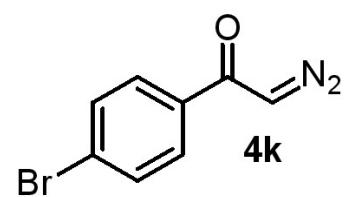
DFILE TY\_09\_031\_01\_carbon-1-1.als  
COMNT single pulse decoupled gated  
DATIM 2017-07-20 09:56:39  
OBNUC <sup>13</sup>C  
EXMOD carbon.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 kHz  
OBFIN 4.21 Hz  
POINT 26214  
FREQU 31446.54 Hz  
SCANS 1680  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 18.1 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 60

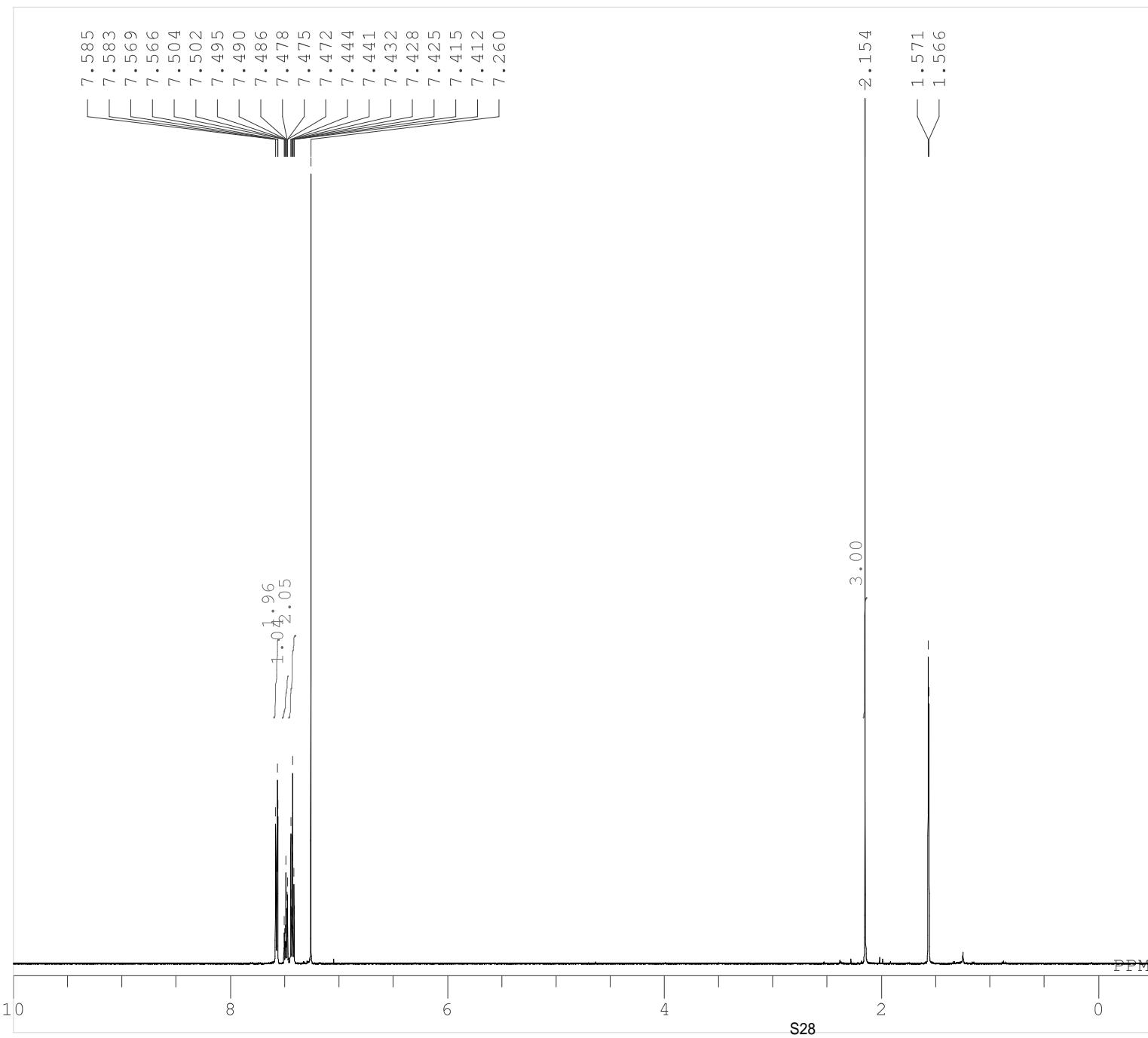




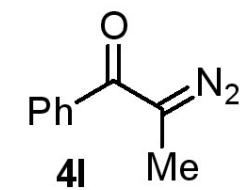


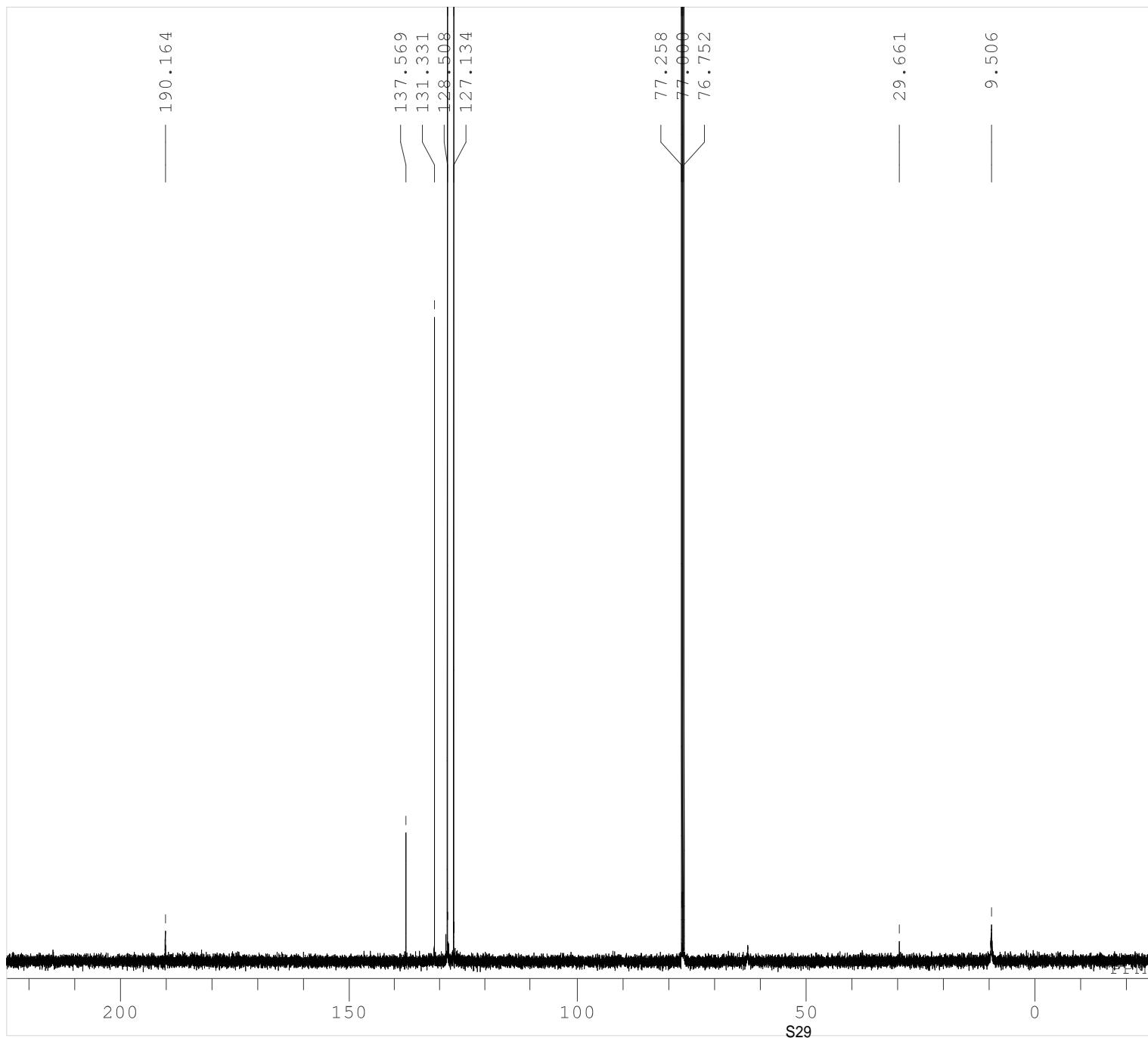
DFILE TY\_09\_054\_02\_carbon-1-1.als  
COMNT single pulse decoupled gated  
DATIM 2017-08-05 14:20:58  
OBNUC <sup>13</sup>C  
EXMOD carbon.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 kHz  
OBFIN 4.21 Hz  
POINT 26214  
FREQU 31446.54 Hz  
SCANS 1780  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 19.9 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 60



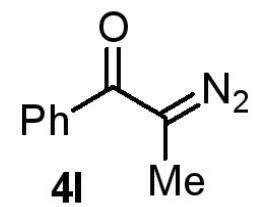


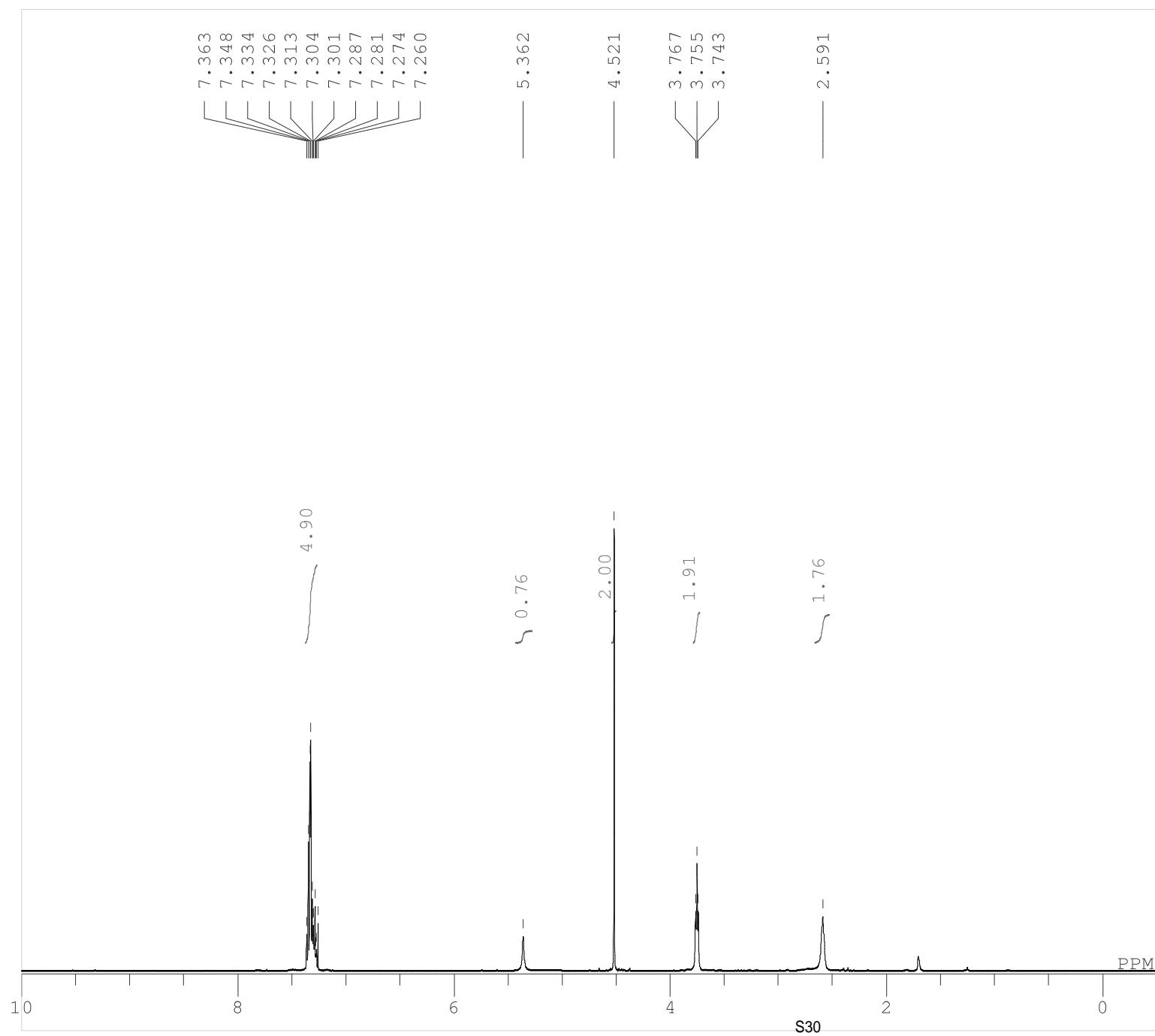
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 COMNT dazo  
 DATIM 2017-07-21 13:03:43  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 18.4 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 48





DFILE TY\_09\_038\_01\_carbon-1-1.als  
COMNT single pulse decoupled gated  
DATIM 2017-07-25 10:00:23  
OBNUC  $^{13}\text{C}$   
EXMOD carbon.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 kHz  
OBFIN 4.21 Hz  
POINT 26214  
FREQU 31446.54 Hz  
SCANS 1580  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 18.5 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 60

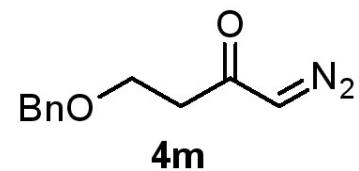


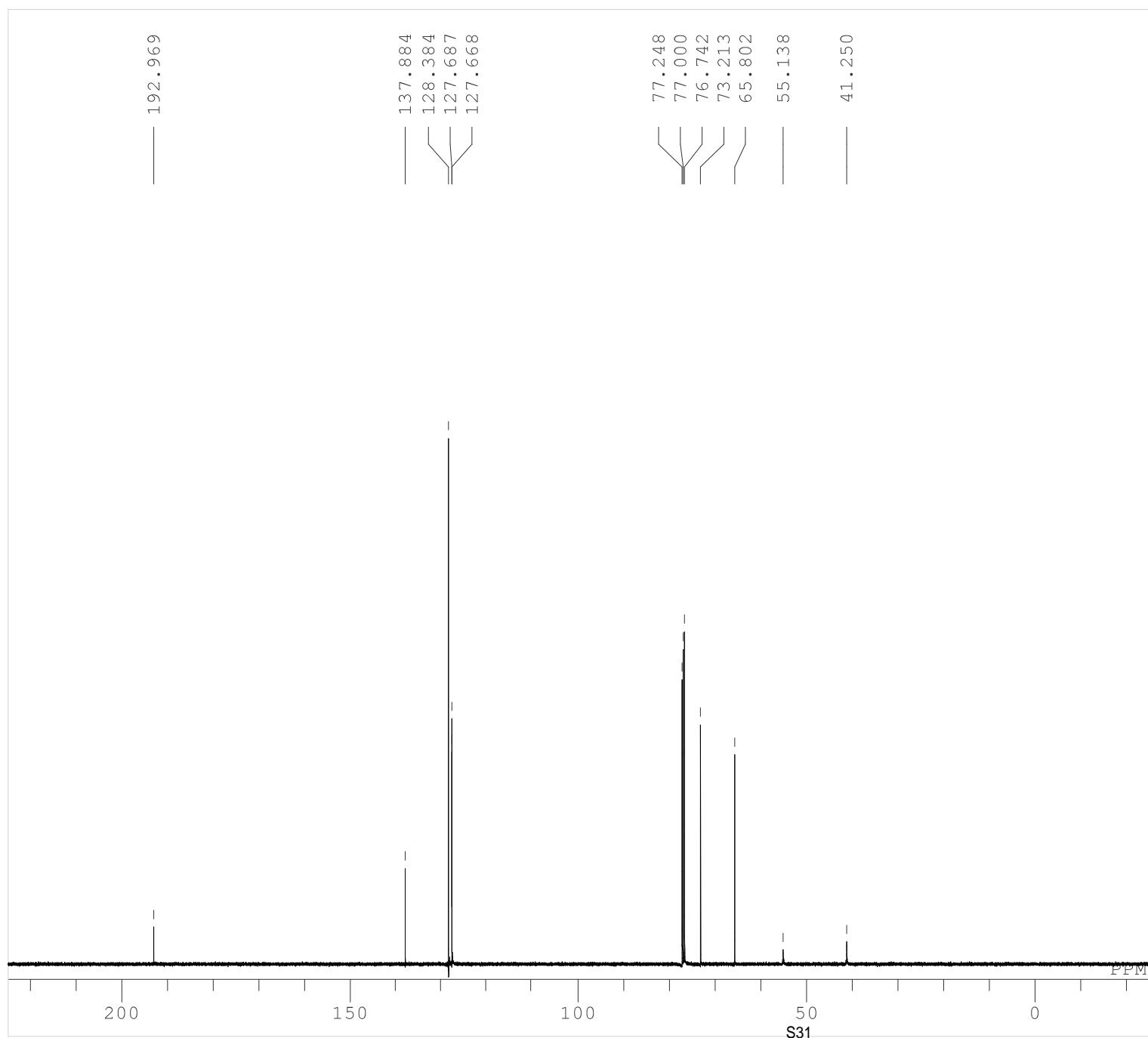


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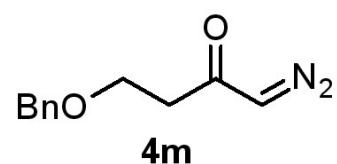
DFILE TY_09_037_02_proton-1-1.als
COMNT single_pulse
DATIM 2017-07-24 10:13:46
OBNUC 1H
EXMOD proton.jxp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 13107
FREQU 7507.51 Hz
SCANS 8
ACQTM 1.7459 sec
PD 5.0000 sec
PW1 6.85 usec
IRNUC 1H
CTEMP 18.1 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.10 Hz
RGAIN 36

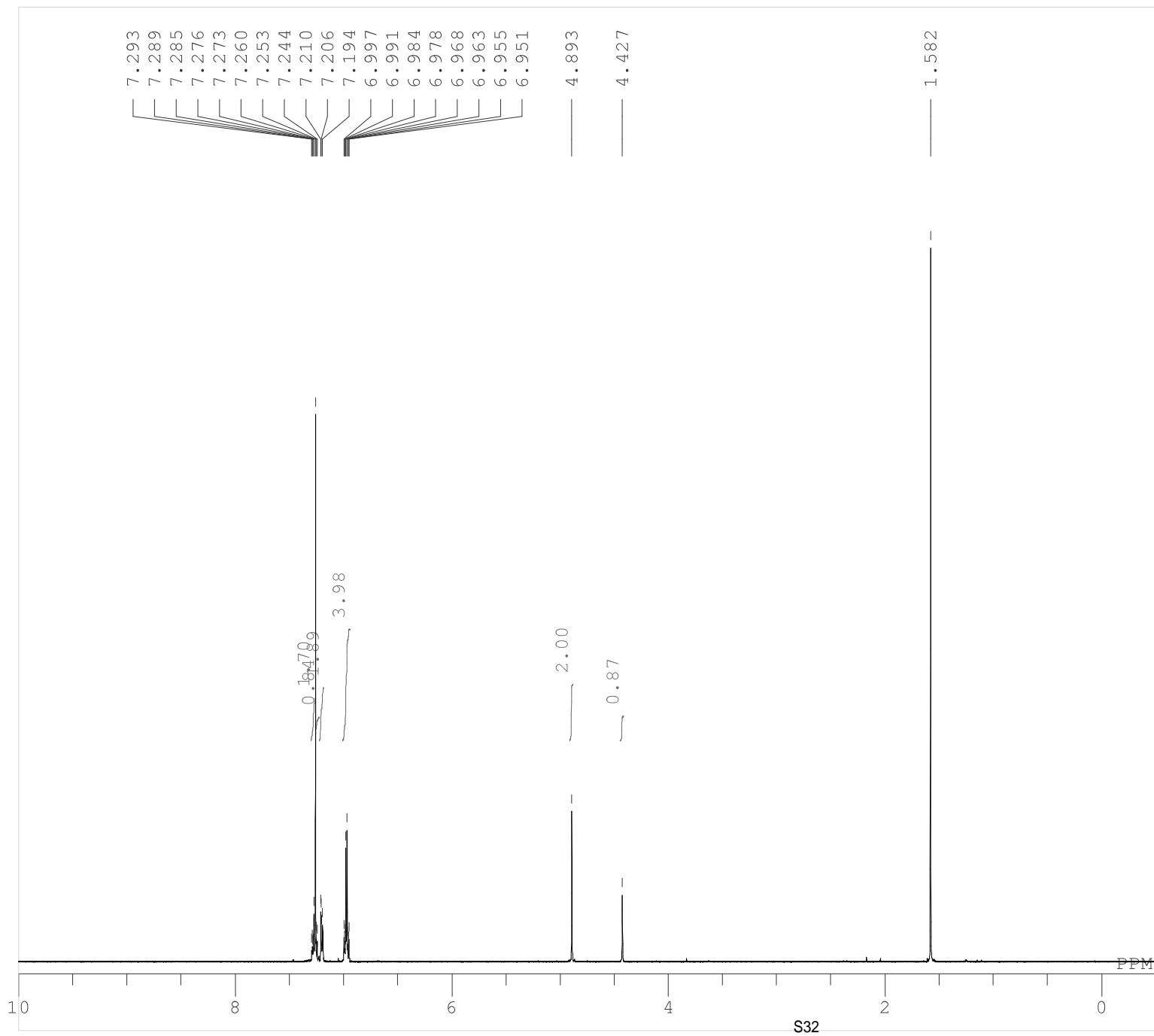
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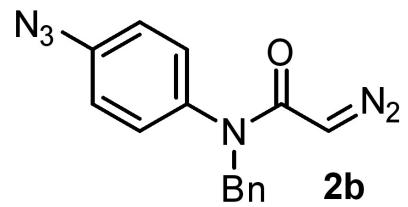


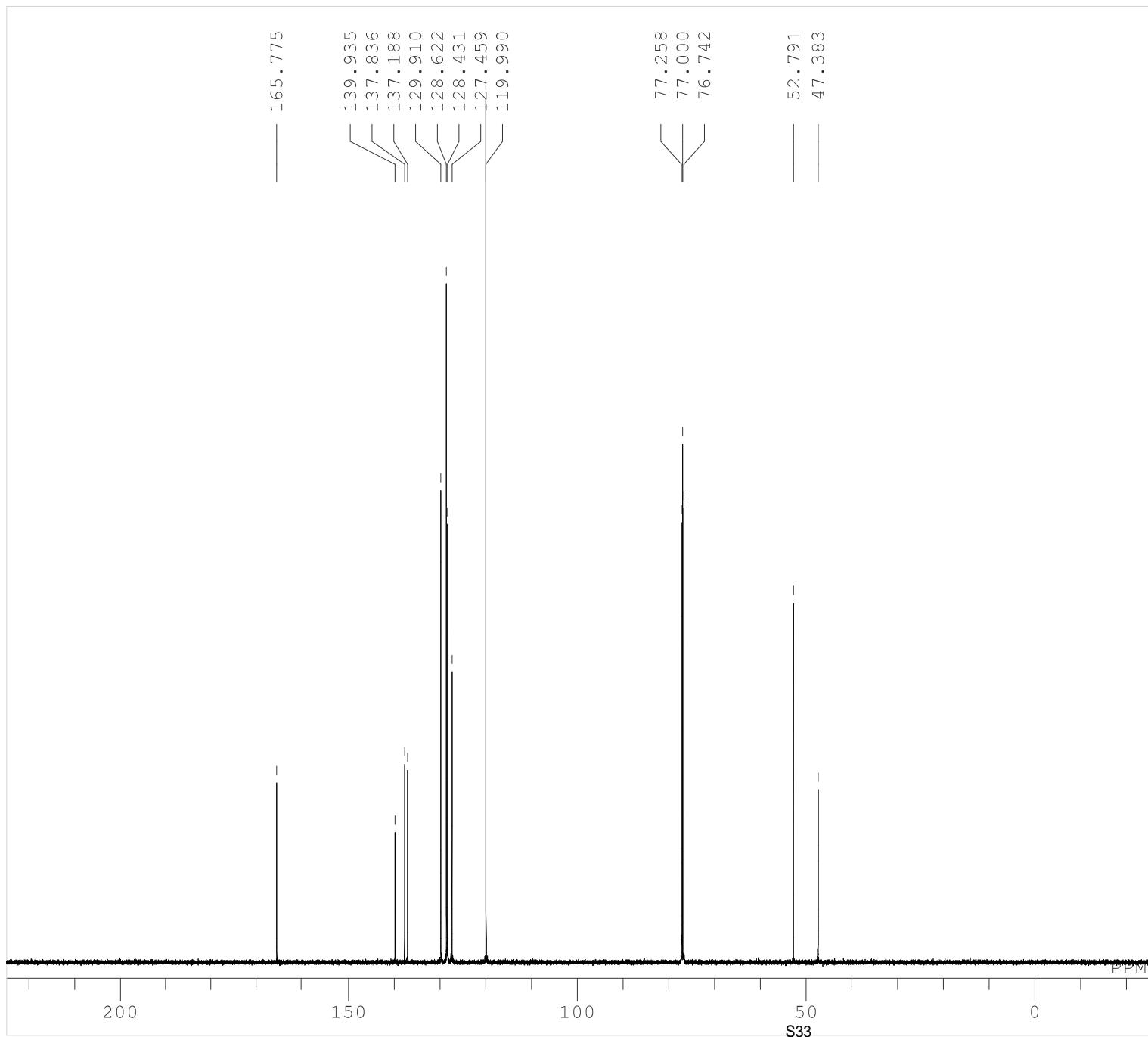
DFILE TY\_09\_037\_02\_carbon-1-1.als  
 COMNT single pulse decoupled gated  
 DATIM 2017-07-24 10:15:44  
 OBNUC <sup>13</sup>C  
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 1260  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 18.6 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60



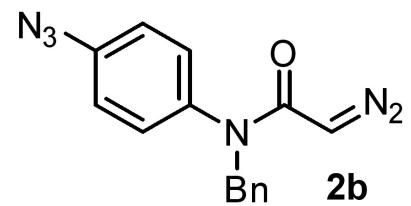


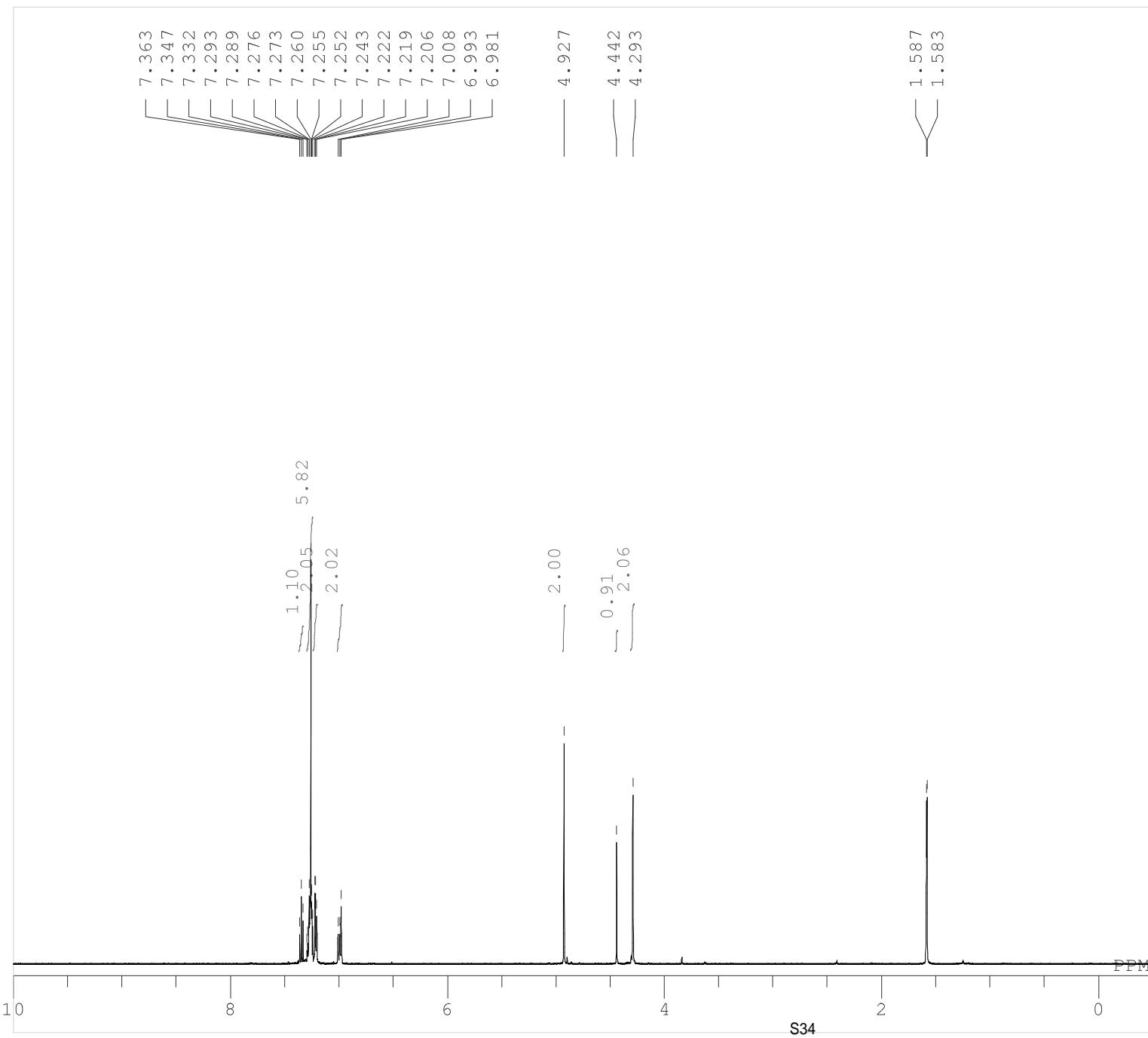
DFILE TY\_09\_056\_05-1-1.als  
 COMNT dazo-azi\_d  
 DATIM 2017-08-18 17:15:26  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 18.2 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 48



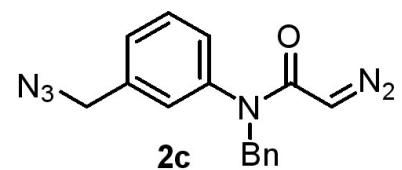


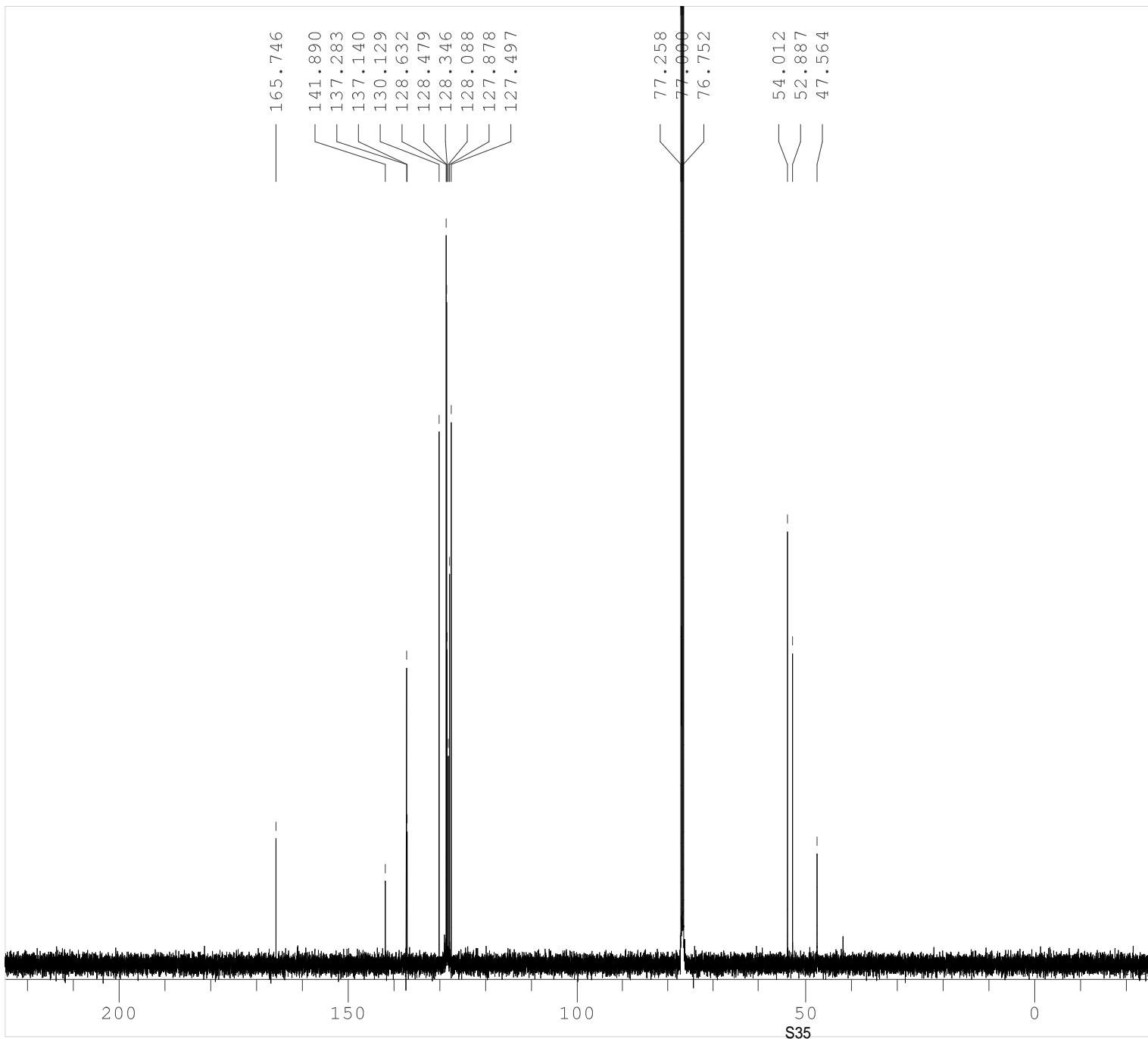
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COMNT single pulse decoupled gated  
DATIM 2017-08-19 10:46:46  
OBNUC <sup>13</sup>C  
EXMOD carbon.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 kHz  
OBFIN 4.21 Hz  
POINT 26214  
FREQU 31446.54 Hz  
SCANS 1780  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 18.4 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 60



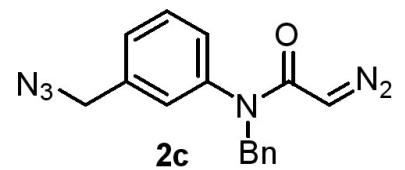


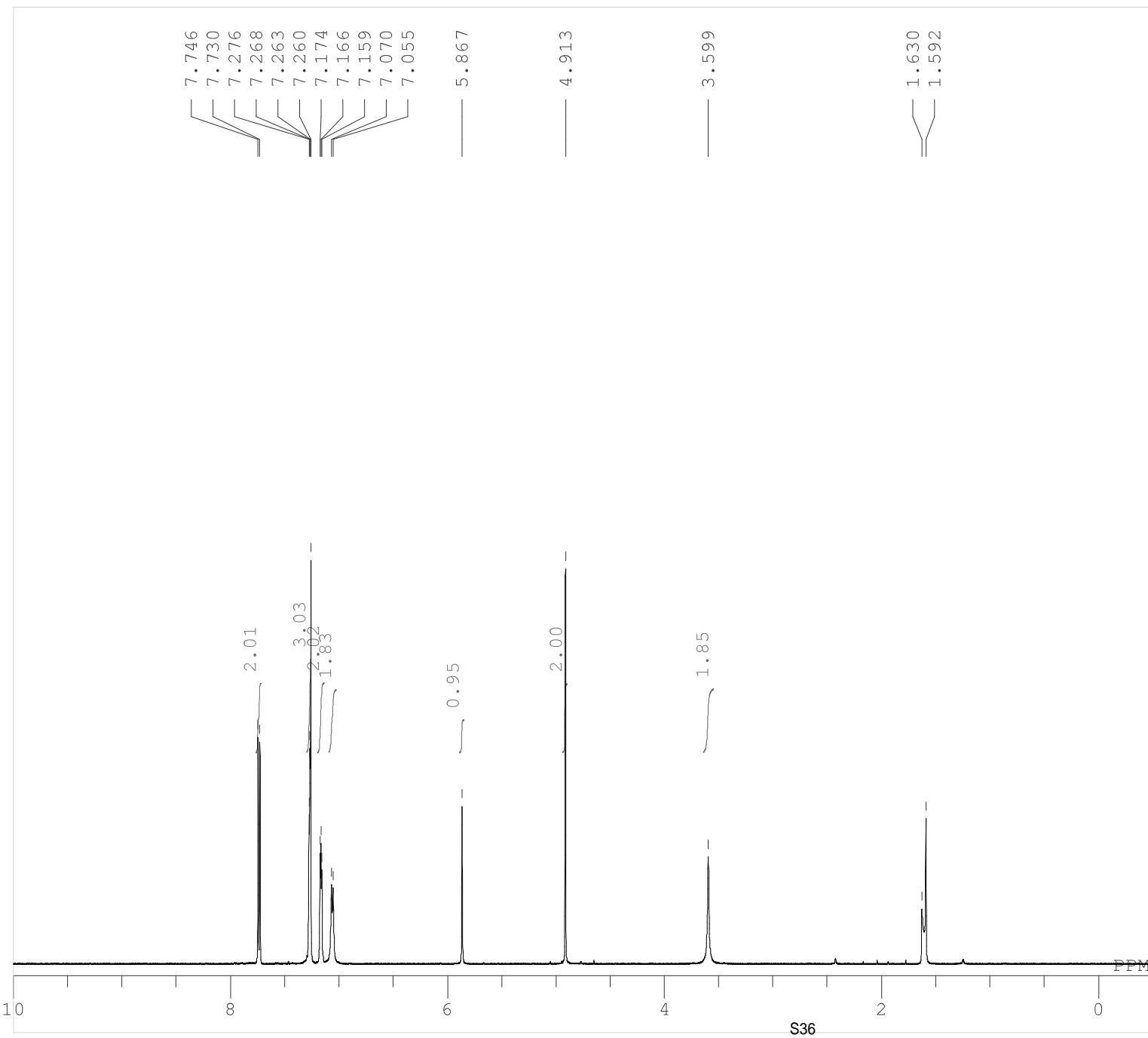
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 COMNT single\_pulse  
 DATIM 2017-10-23 23:11:42  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 16.8 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 46



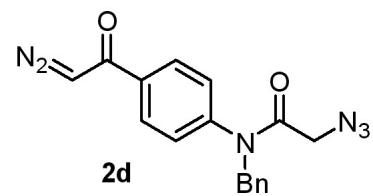


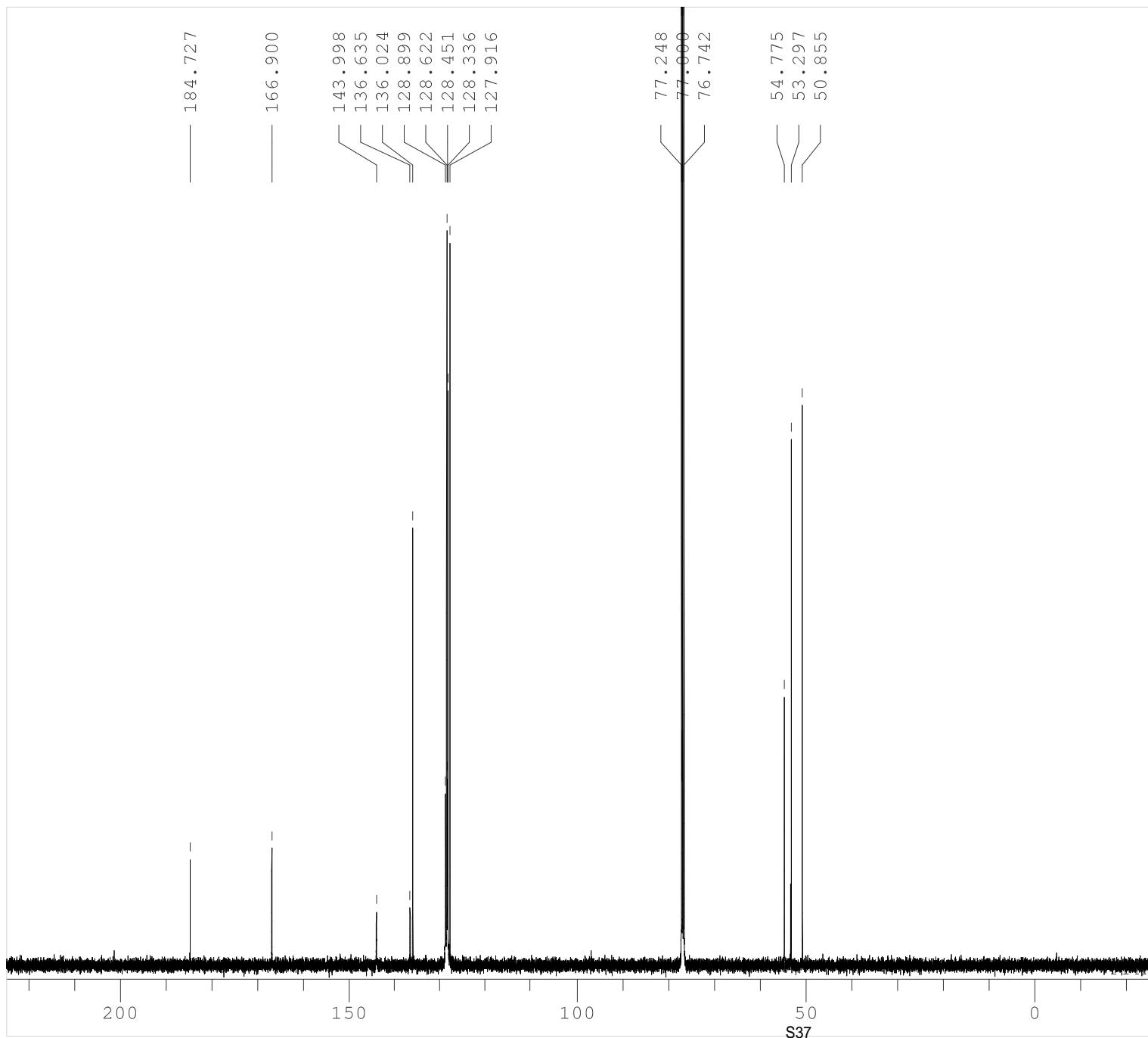
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 COMNT single pulse decoupled gated  
 DATIM 2017-10-23 23:13:21  
 OBNUC  $^{13}\text{C}$   
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 8460  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 17.8 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60



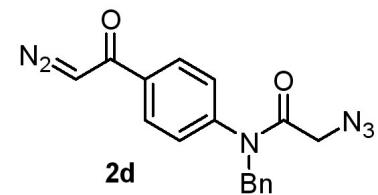


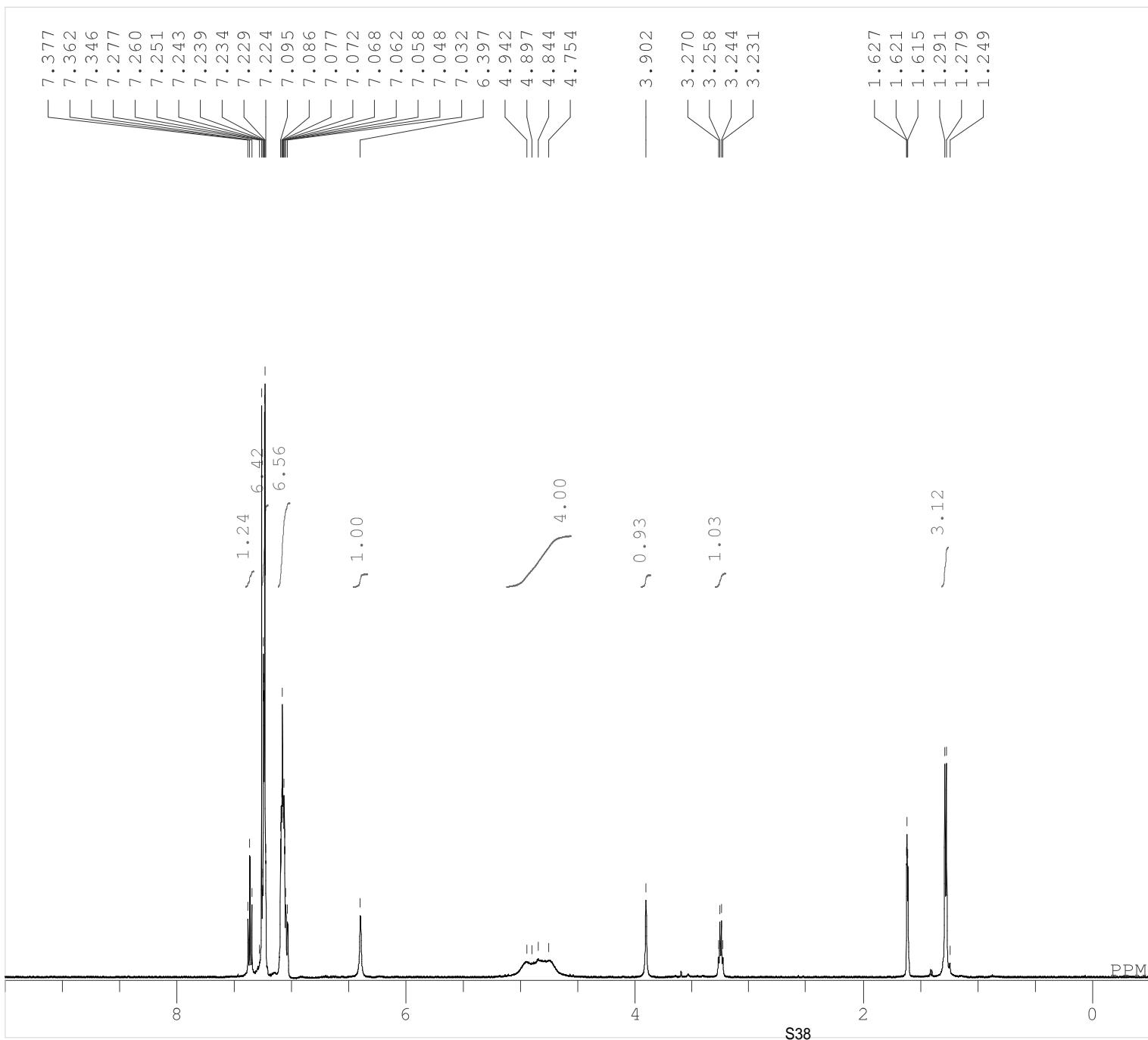
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 COMNT single\_pulse  
 DATIM 2017-08-06 14:51:11  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 19.6 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 44



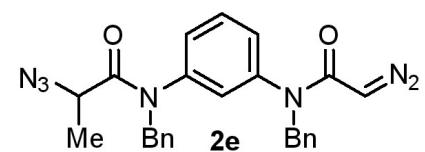


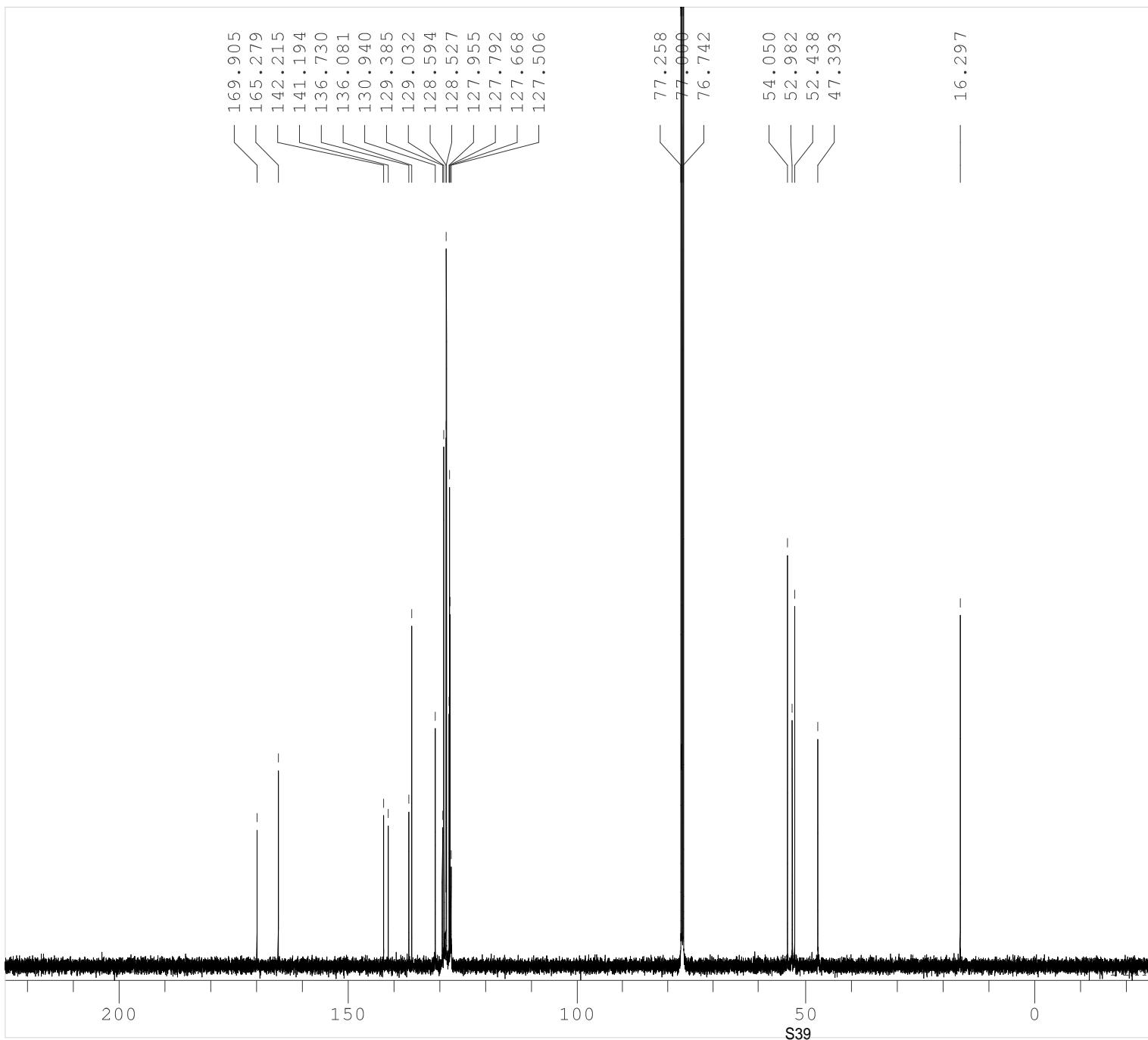
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 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 3438  
 ACQTM 0.8336 sec  
 PD 10.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 17.9 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60





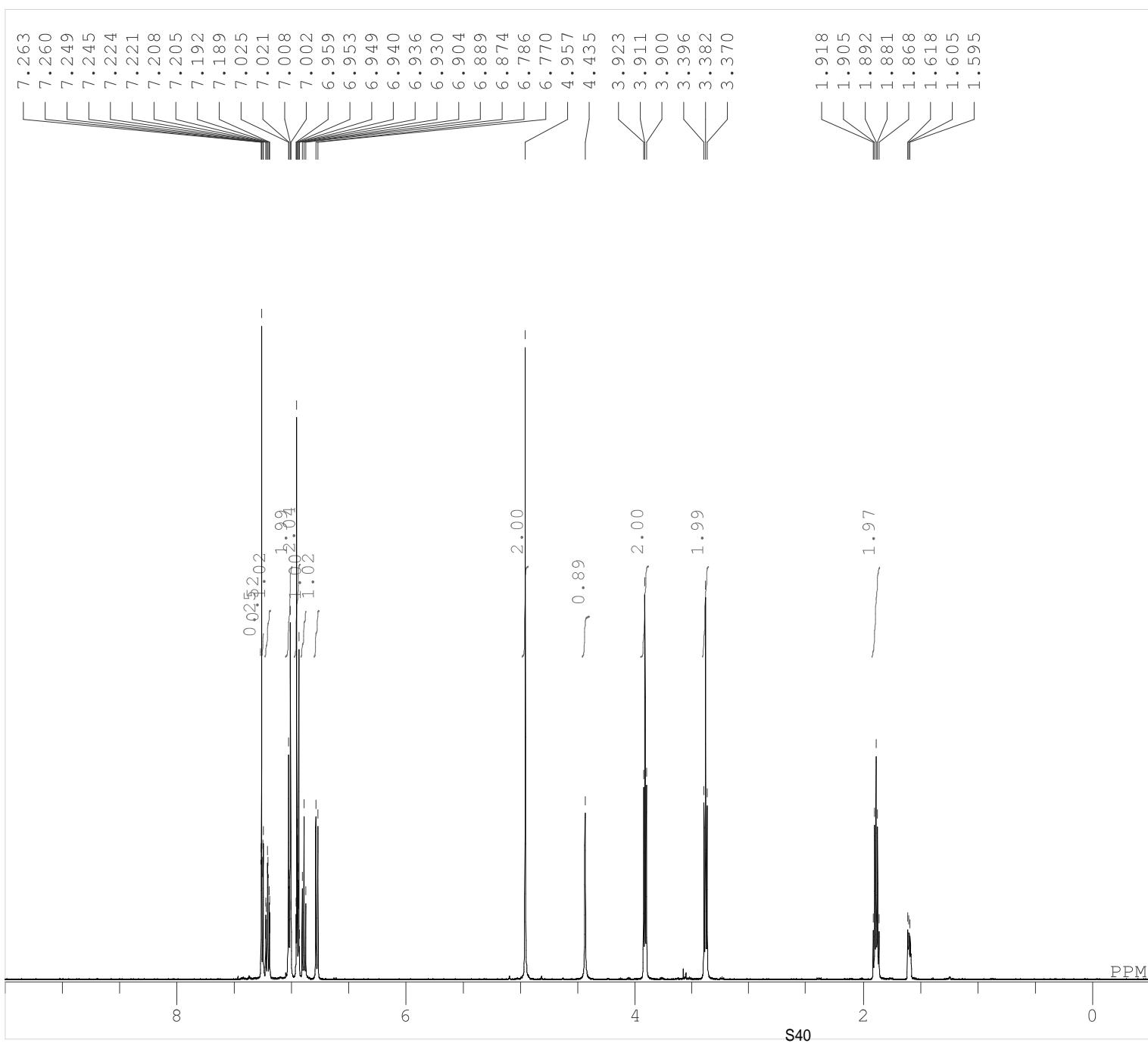
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 COMNT single\_pulse  
 DATIM 2017-10-24 23:12:57  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 17.9 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 40



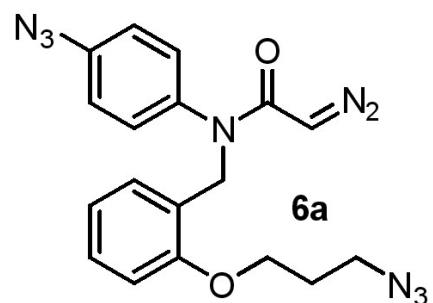


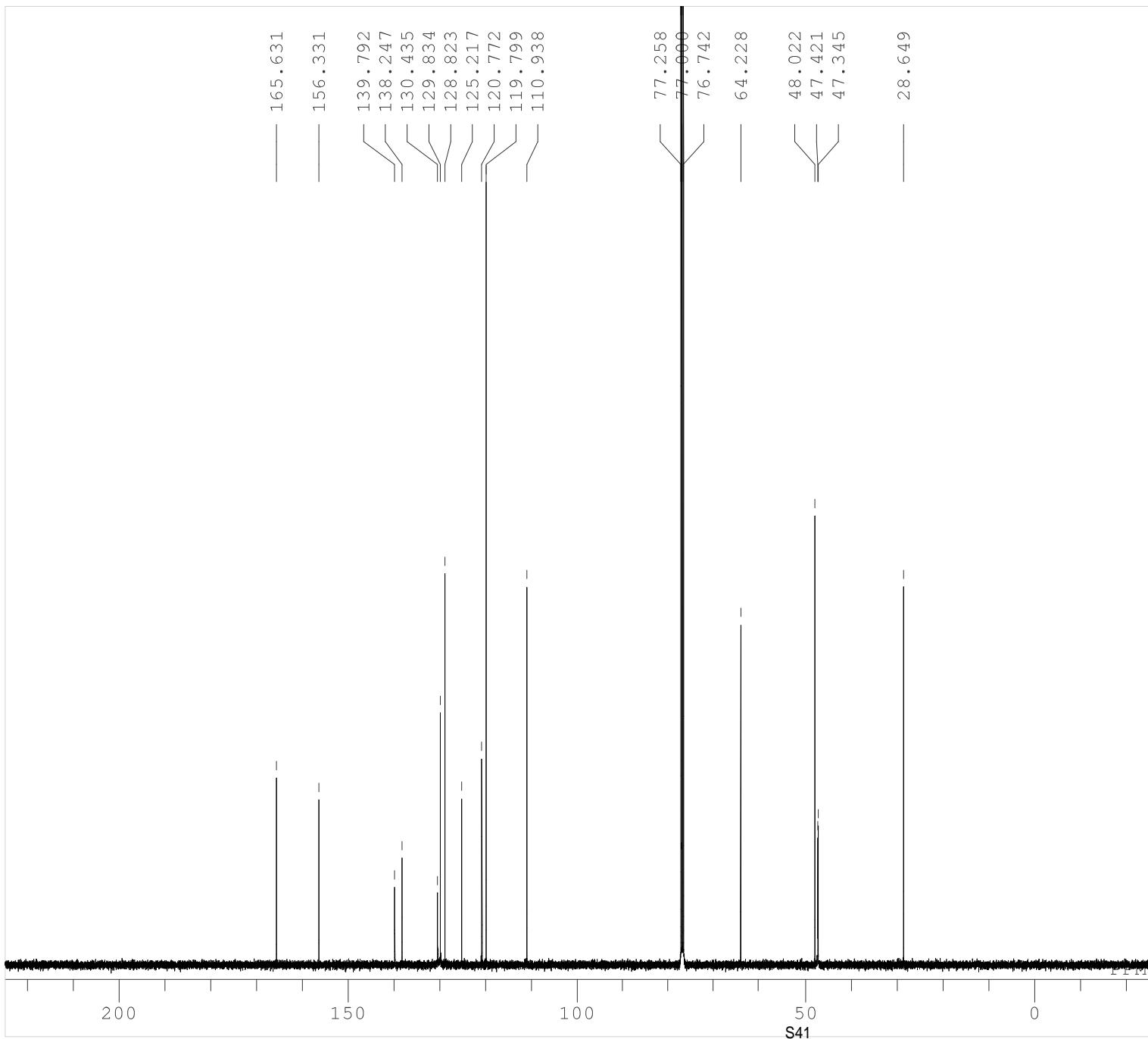
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 COMNT single pulse decoupled gated  
 DATIM 2017-10-24 23:14:28  
 OBNUC <sup>13</sup>C  
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 8860  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 19.2 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60



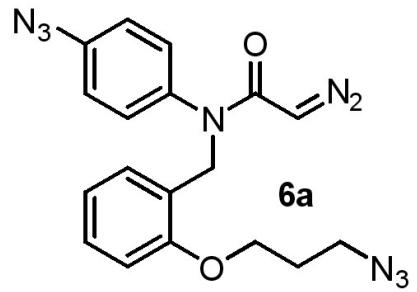


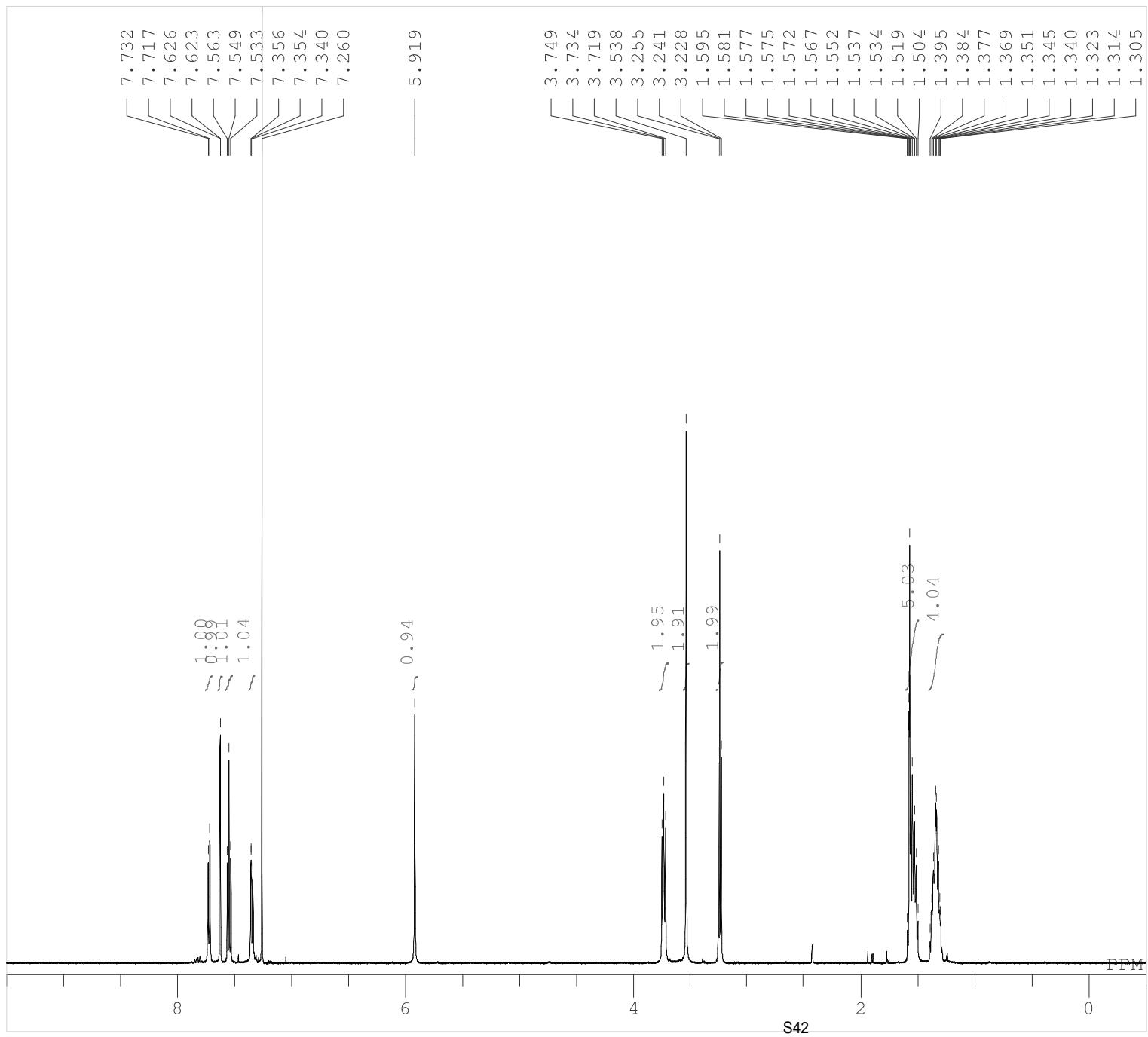
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 COMNT single\_pulse  
 DATIM 2018-01-10 23:09:05  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 17.2 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 44



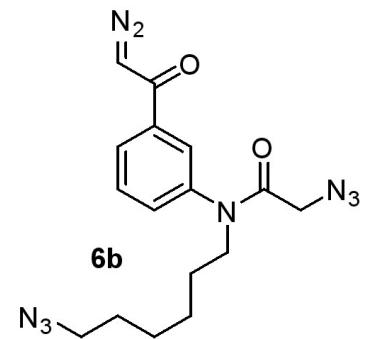


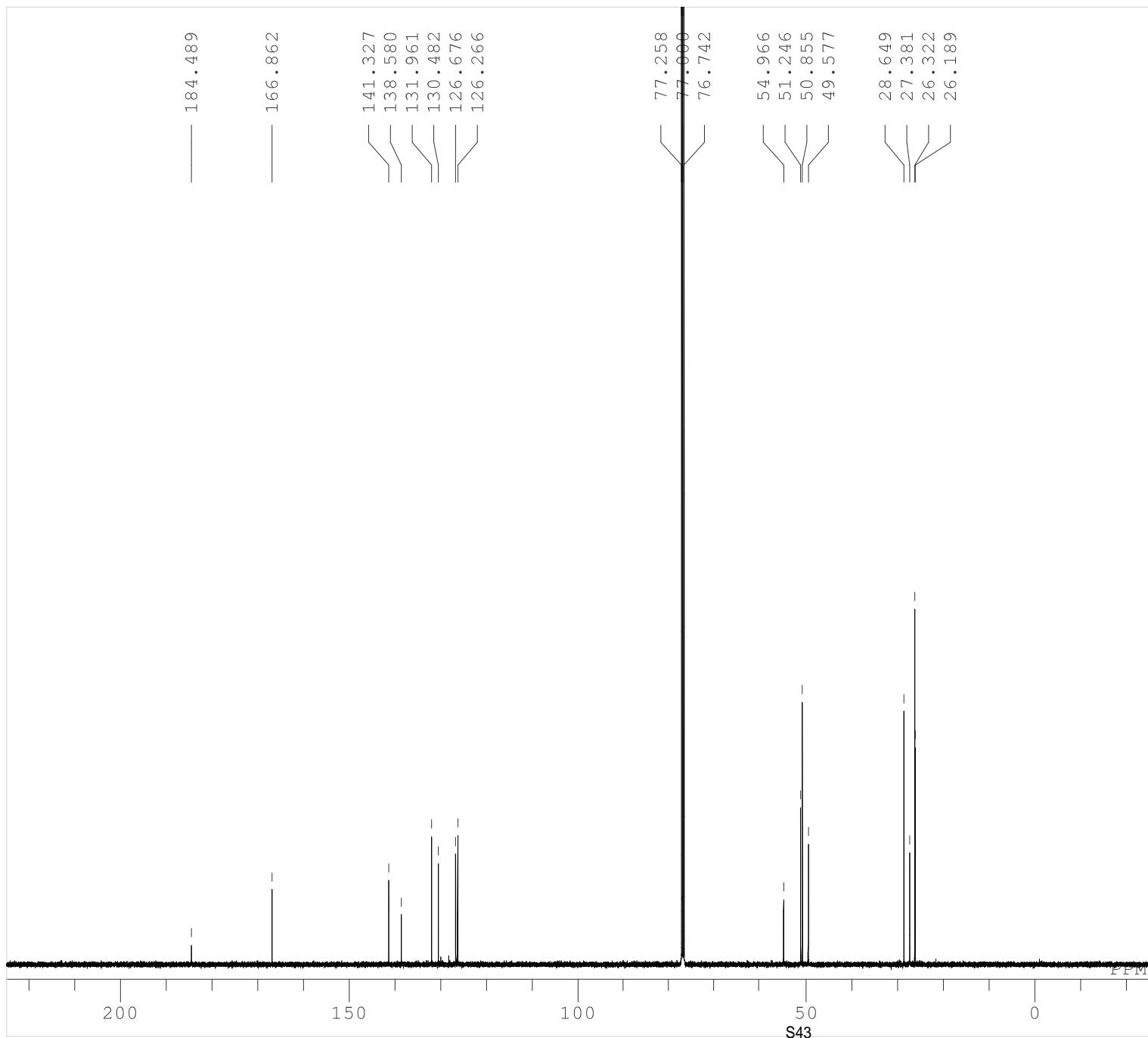
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EXMOD carbon.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 kHz  
OBFIN 4.21 Hz  
POINT 26214  
FREQU 31446.54 Hz  
SCANS 9000  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H 18.2 c  
CTEMP CDCL<sub>3</sub>  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 60



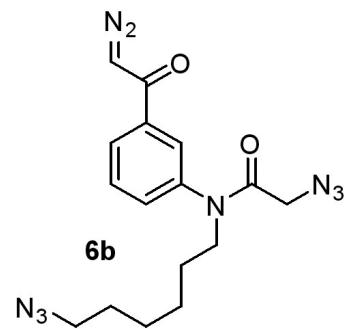


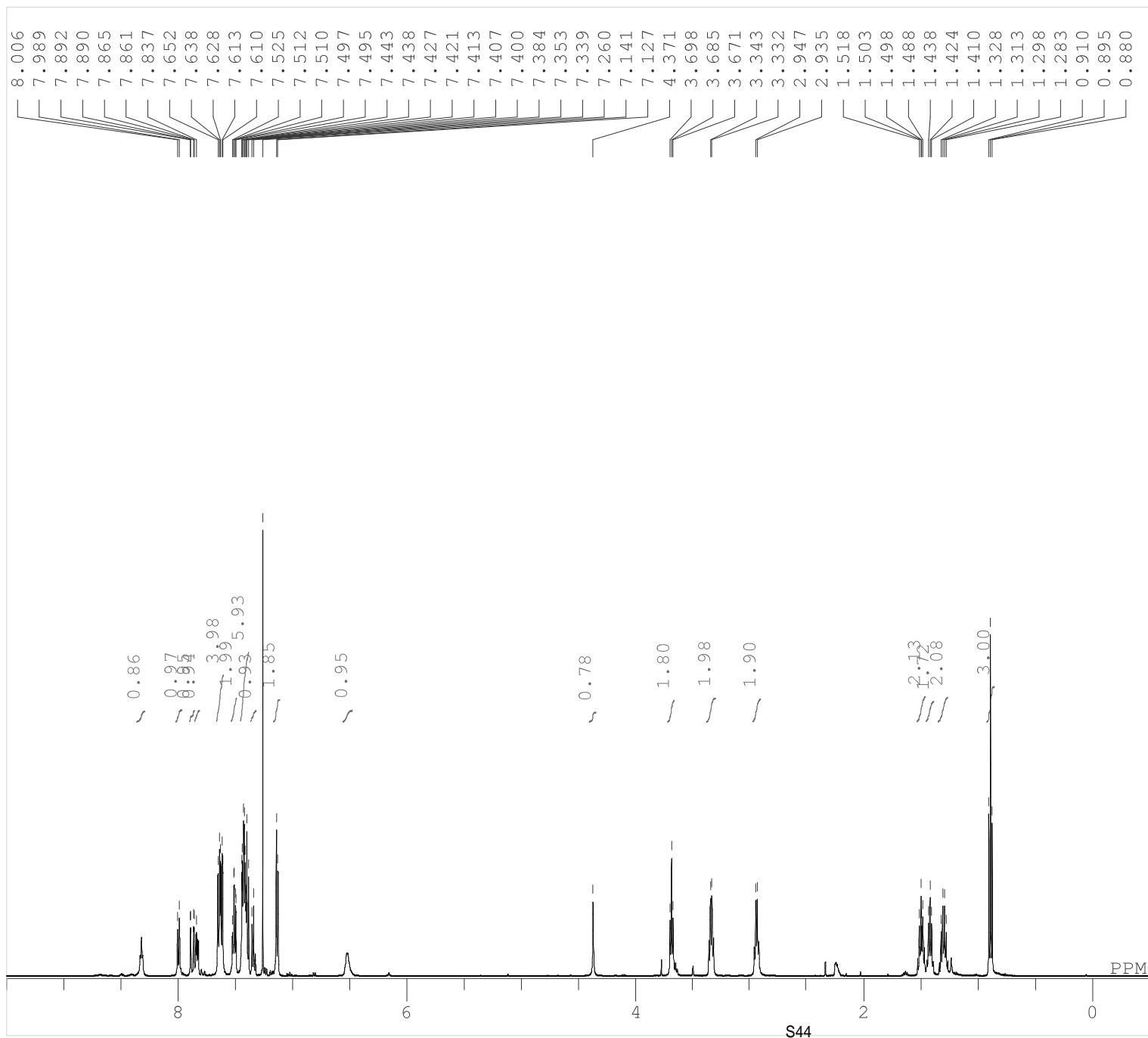
DFILE TY\_09\_136\_03-1-1.als  
 COMNT dazo-dazied  
 DATIM 2017-11-06 14:24:51  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 17.4 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 44



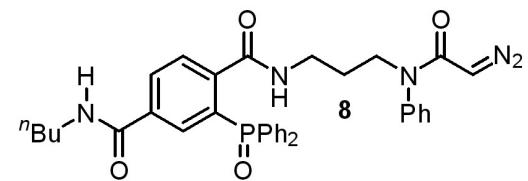


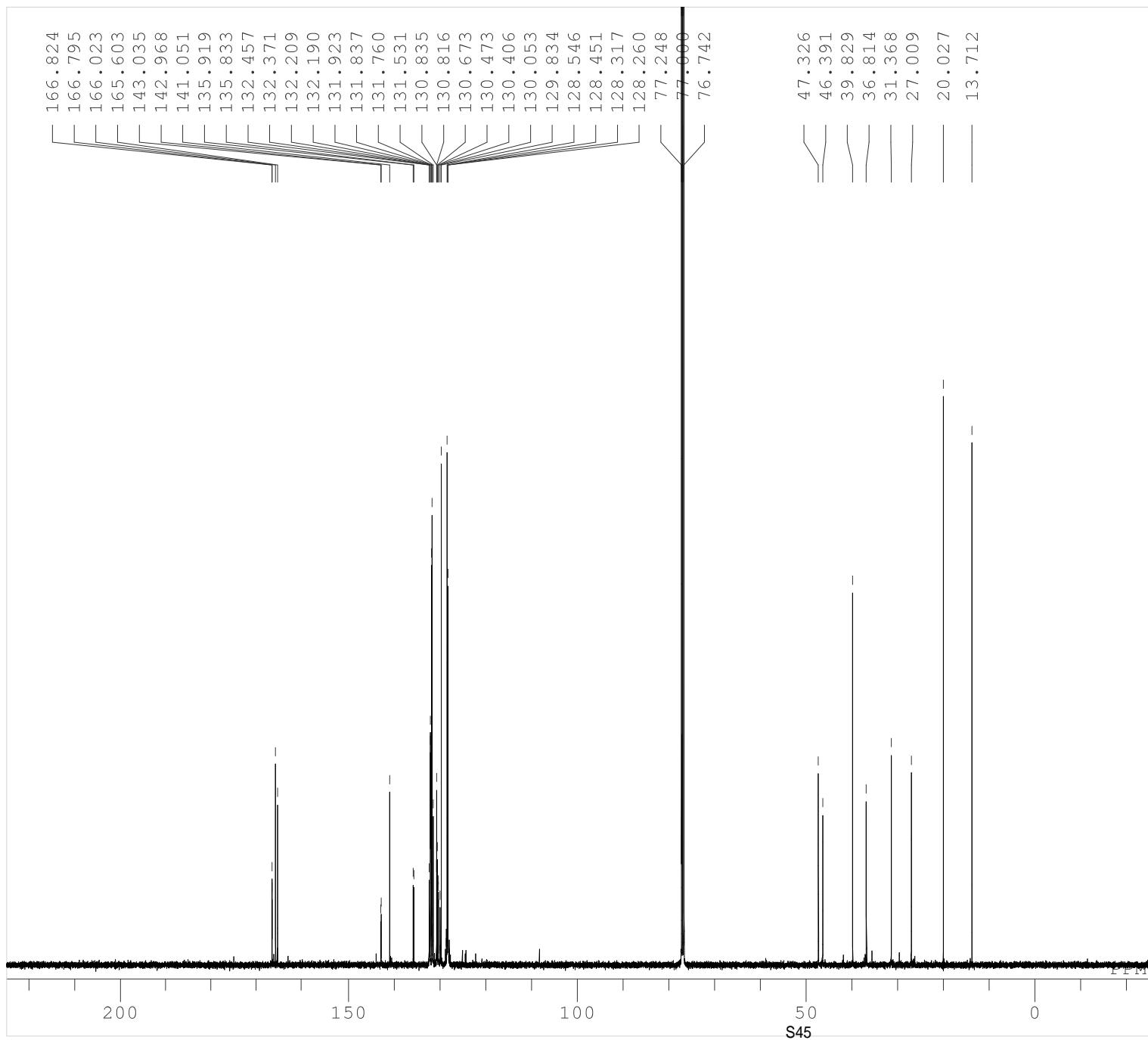
DFILE TY\_09\_136\_01\_carbon-1-1.als  
 COMNT single pulse decoupled gated  
 DATIM 2017-10-30 23:16:35  
 OBNUC <sup>13</sup>C  
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 8920  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 19.6 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60



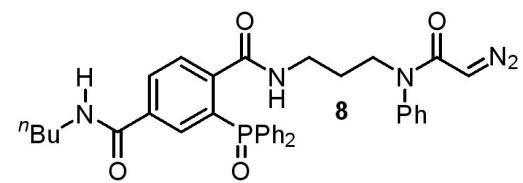


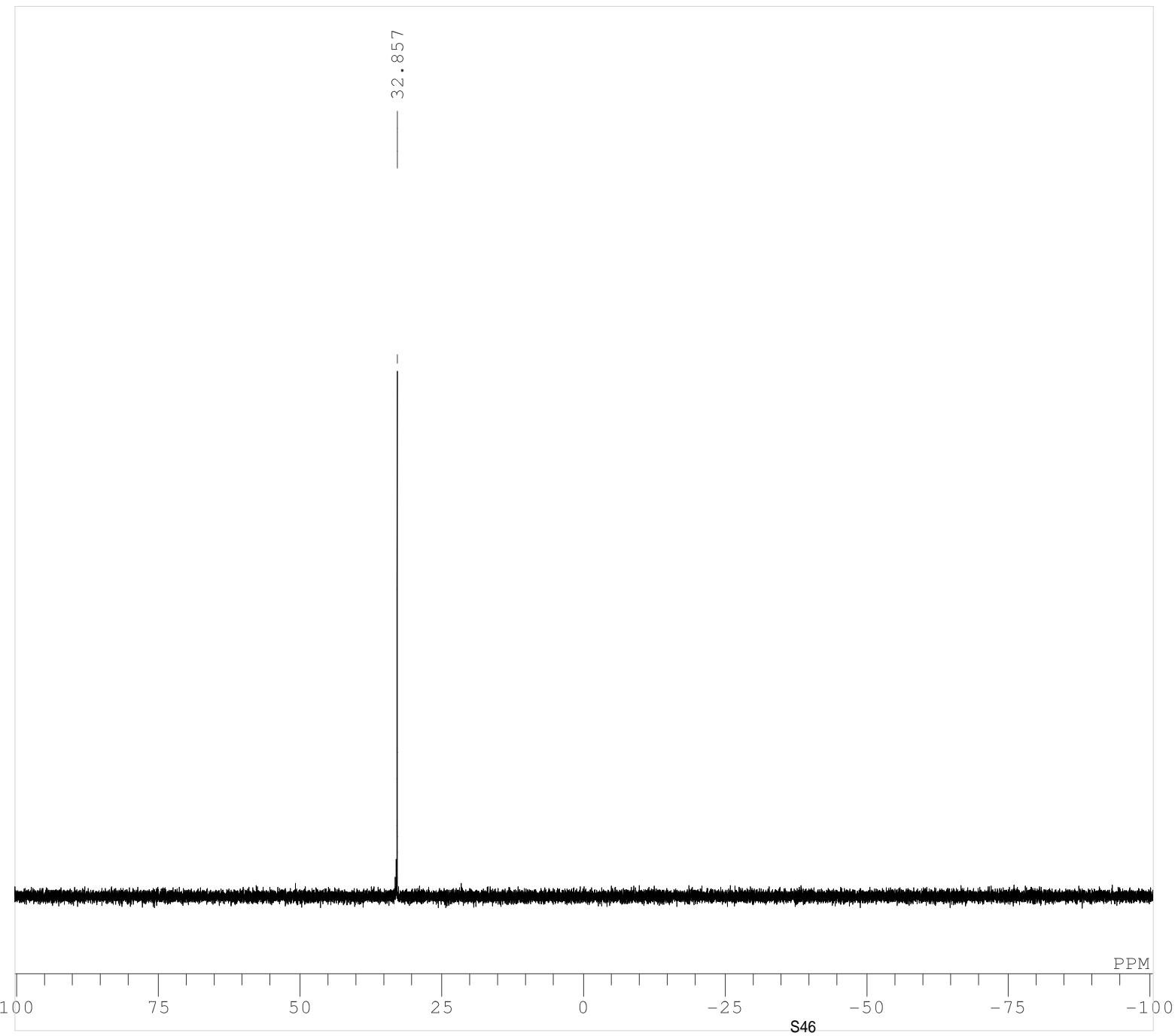
DFILE TY\_09\_095\_04\_proton-1-1.als  
 COMNT single\_pulse  
 DATIM 2018-02-14 23:16:20  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 14.8 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 34





DFILE TY\_09\_095\_04\_carbon-1-1.als  
 COMNT single pulse decoupled gated  
 DATIM 2018-02-14 23:18:56  
 OBNUC <sup>13</sup>C  
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 8900  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 16.0 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 58

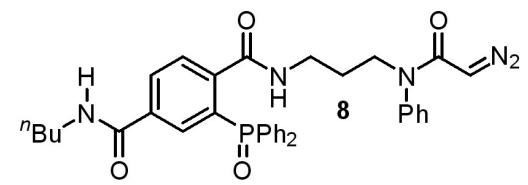


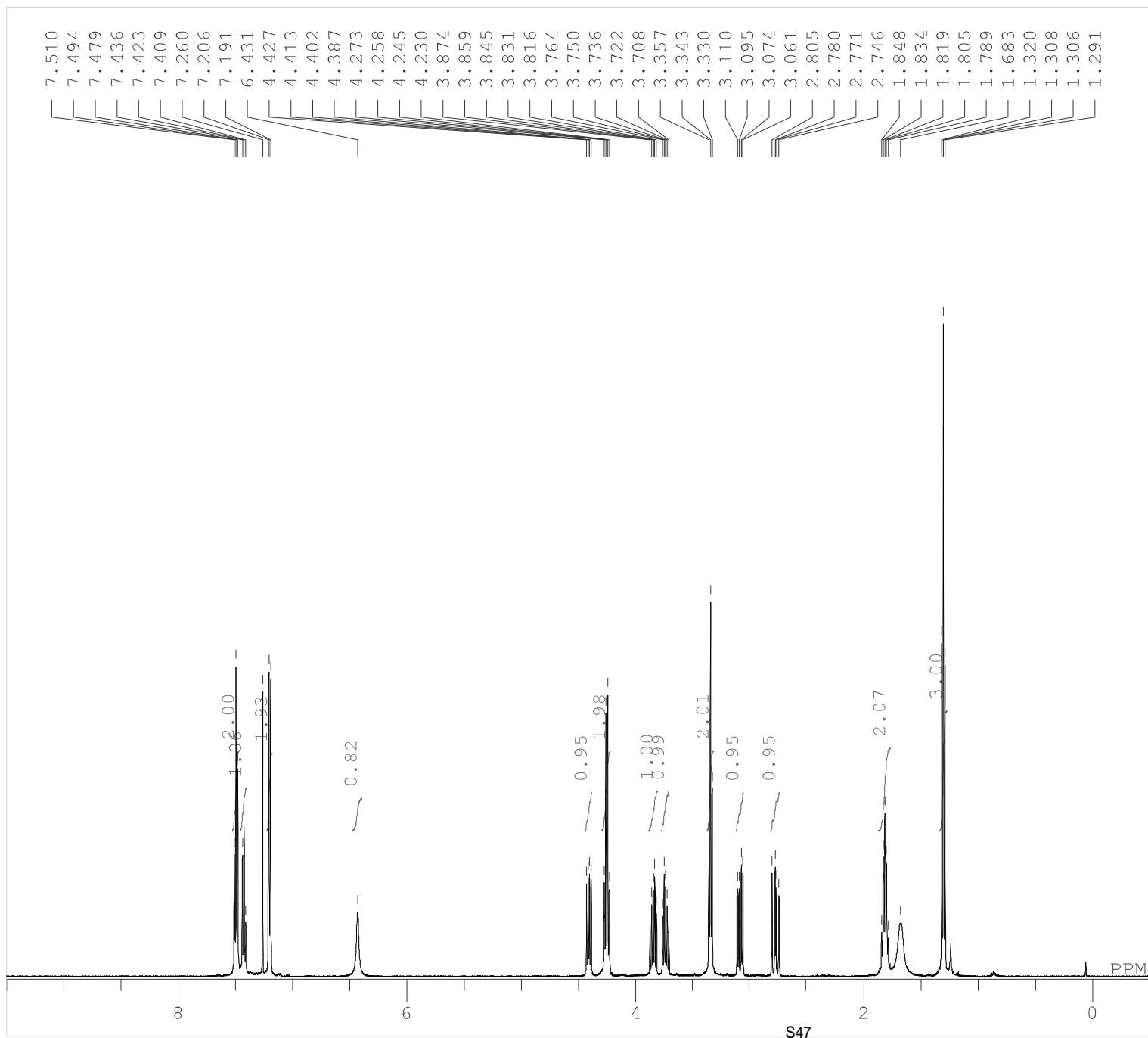


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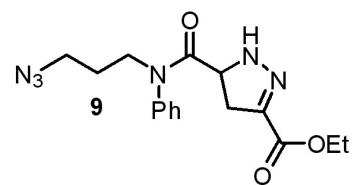
DFILE TY_09_095_04_phosphorus-1-1.a
COMNT single pulse decoupled gated
DATIM 2018-02-22 15:57:34
OBNUC 31P
EXMOD carbon.jxp
OBFRQ 202.46 MHz
OBSET 8.31 KHz
OBFIN 0.75 Hz
POINT 26214
FREQU 40650.41 Hz
SCANS 10
ACQTM 0.6449 sec
PD 2.0000 sec
PW1 3.88 usec
IRNUC 1H
CTEMP 15.1 c
SLVNT C6D6
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 58

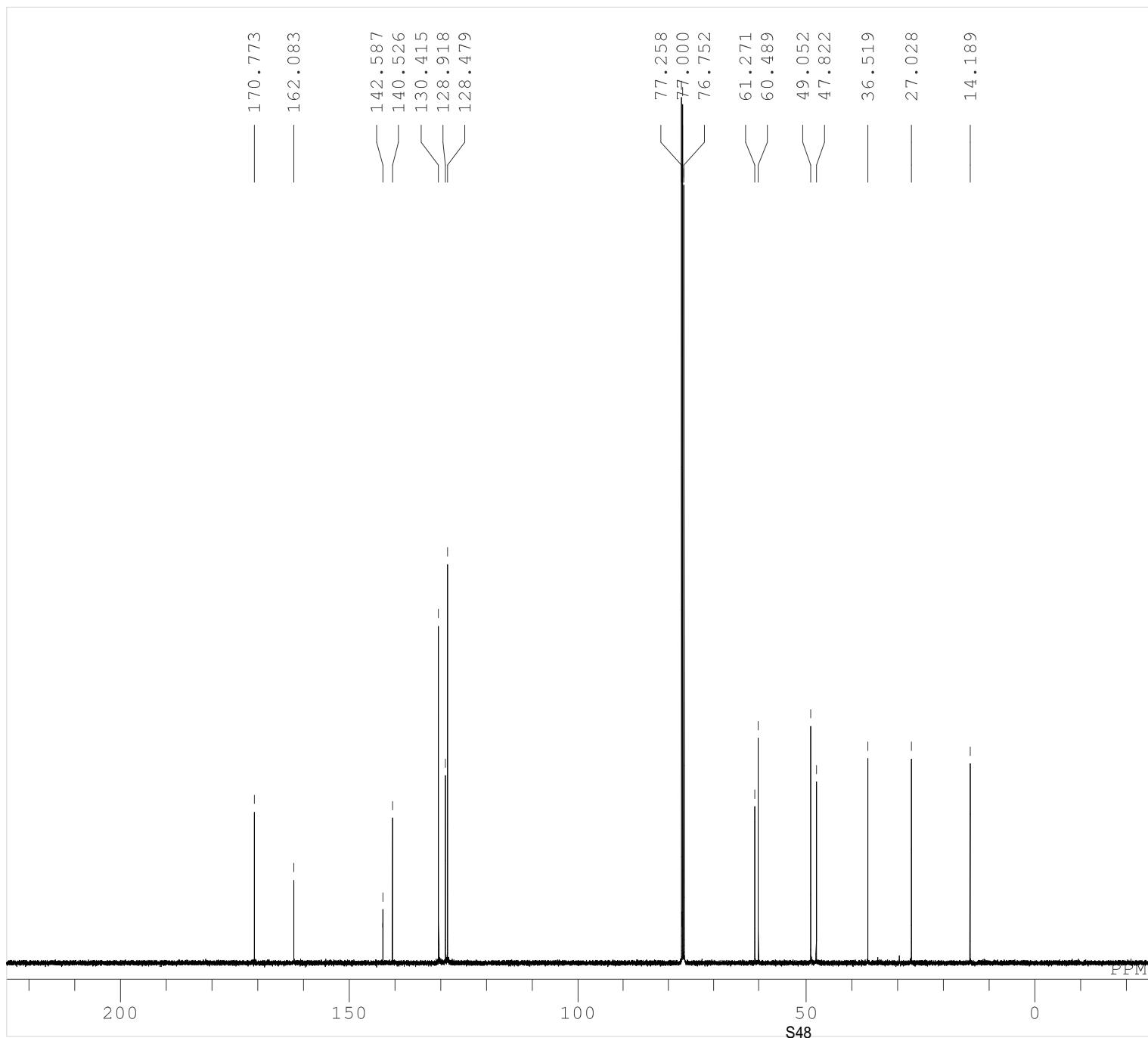
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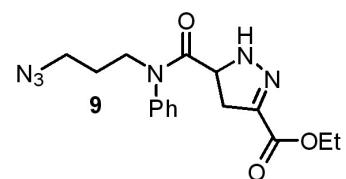


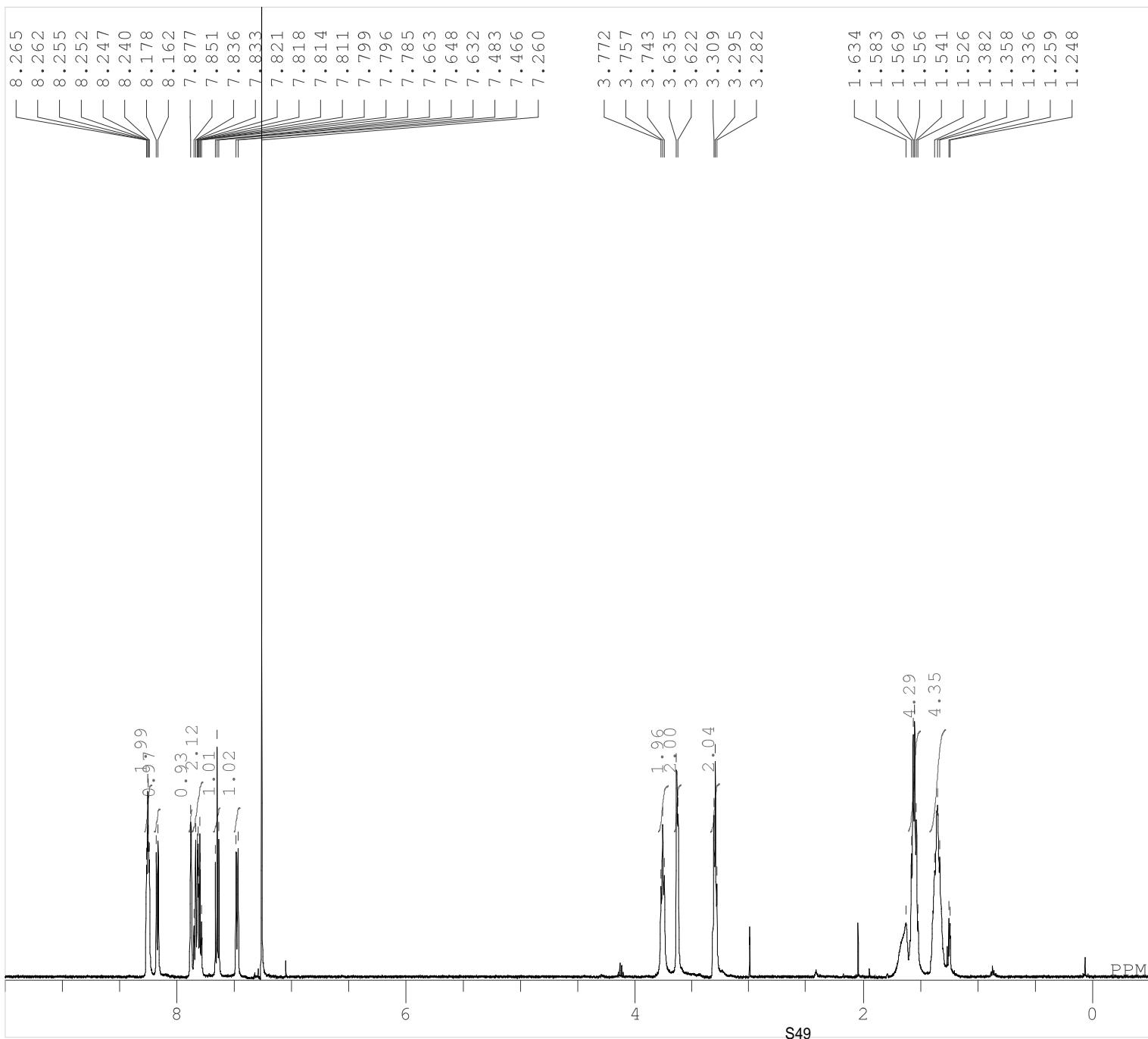
DFILE TY\_09\_064\_01\_proton-1-1.als  
 COMNT single\_pulse  
 DATIM 2017-08-23 23:08:18  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 18.4 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 38





DFILE TY\_09\_064\_01\_carbon-1-1.als  
 COMNT single pulse decoupled gated  
 DATIM 2017-08-23 23:10:02  
 OBNUC <sup>13</sup>C  
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 8880  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 18.4 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60

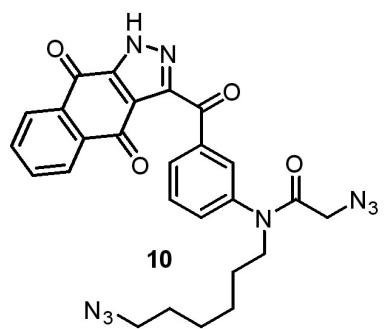


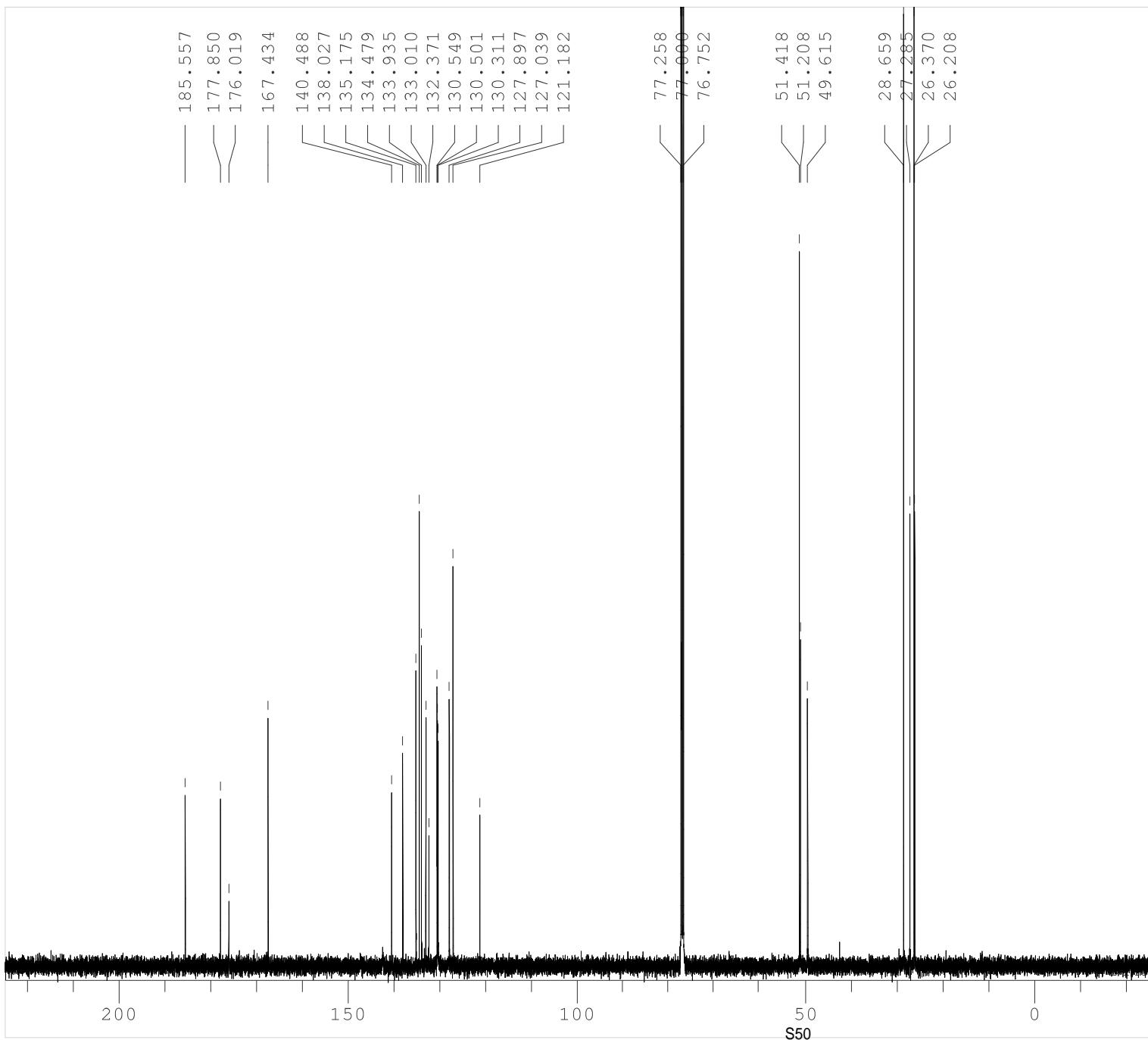


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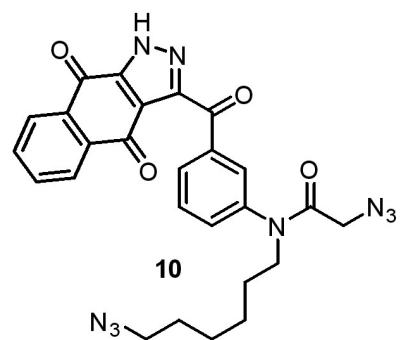
DFILE      TY_10_033_01-1-1.als
COMNT      desired
DATIM      2017-12-14 15:44:38
OBNUC      1H
EXMOD     proton.jxp
OBFRQ      500.16 MHz
OBSET      2.41 kHz
OBFIN      6.01 Hz
POINT      13107
FREQU     7507.51 Hz
SCANS       8
ACQTM      1.7459 sec
PD         5.0000 sec
PW1        6.85 usec
IRNUC      1H
CTEMP       18.6 c
SLVNT      CDCL3
EXREF      7.26 ppm
BF          0.10 Hz
RGAIN       46

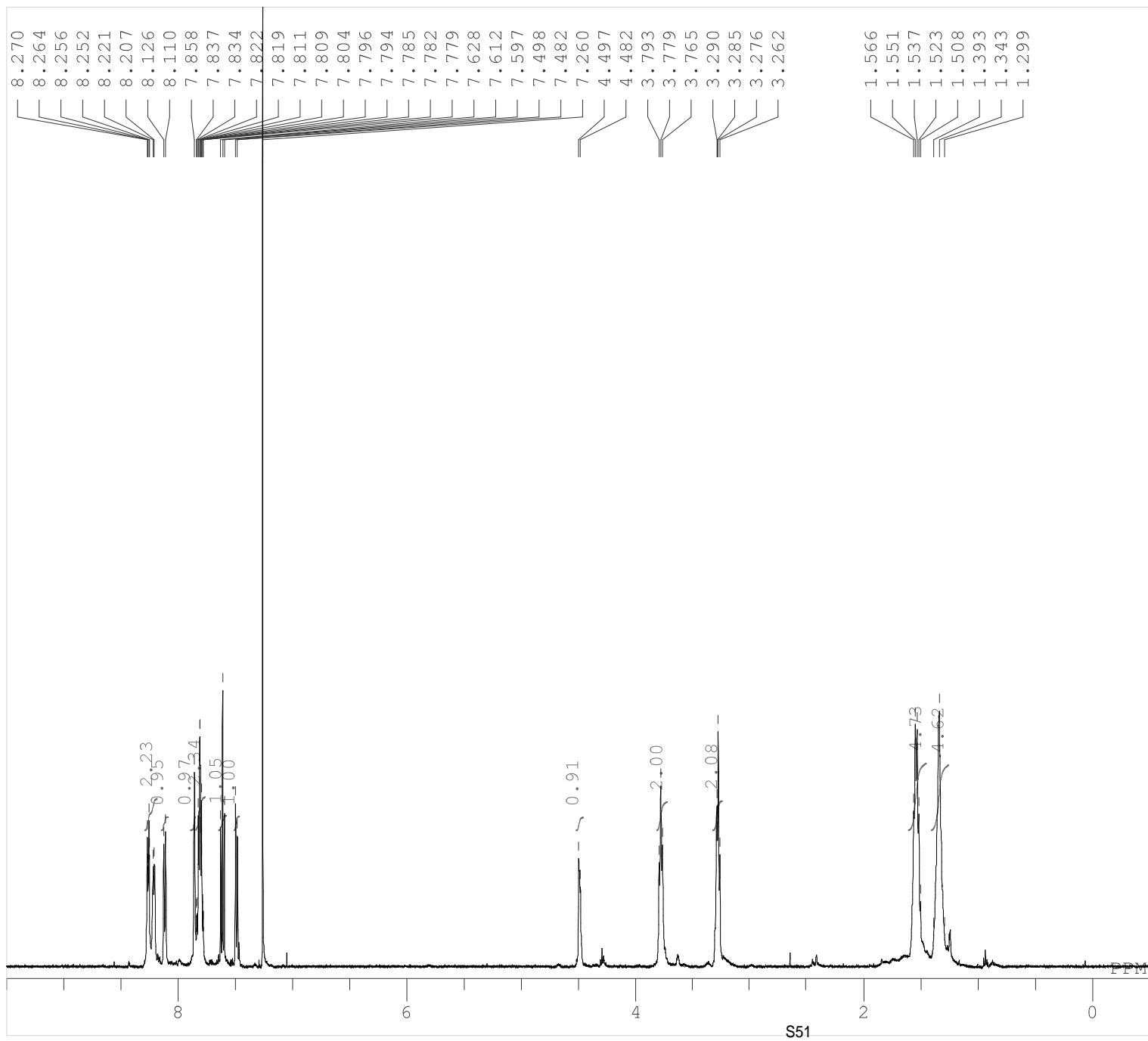
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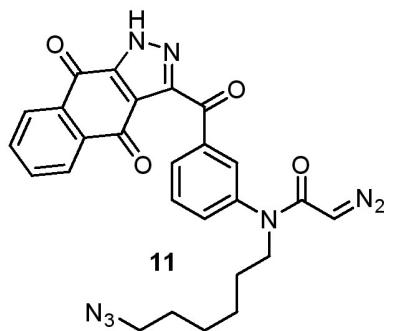


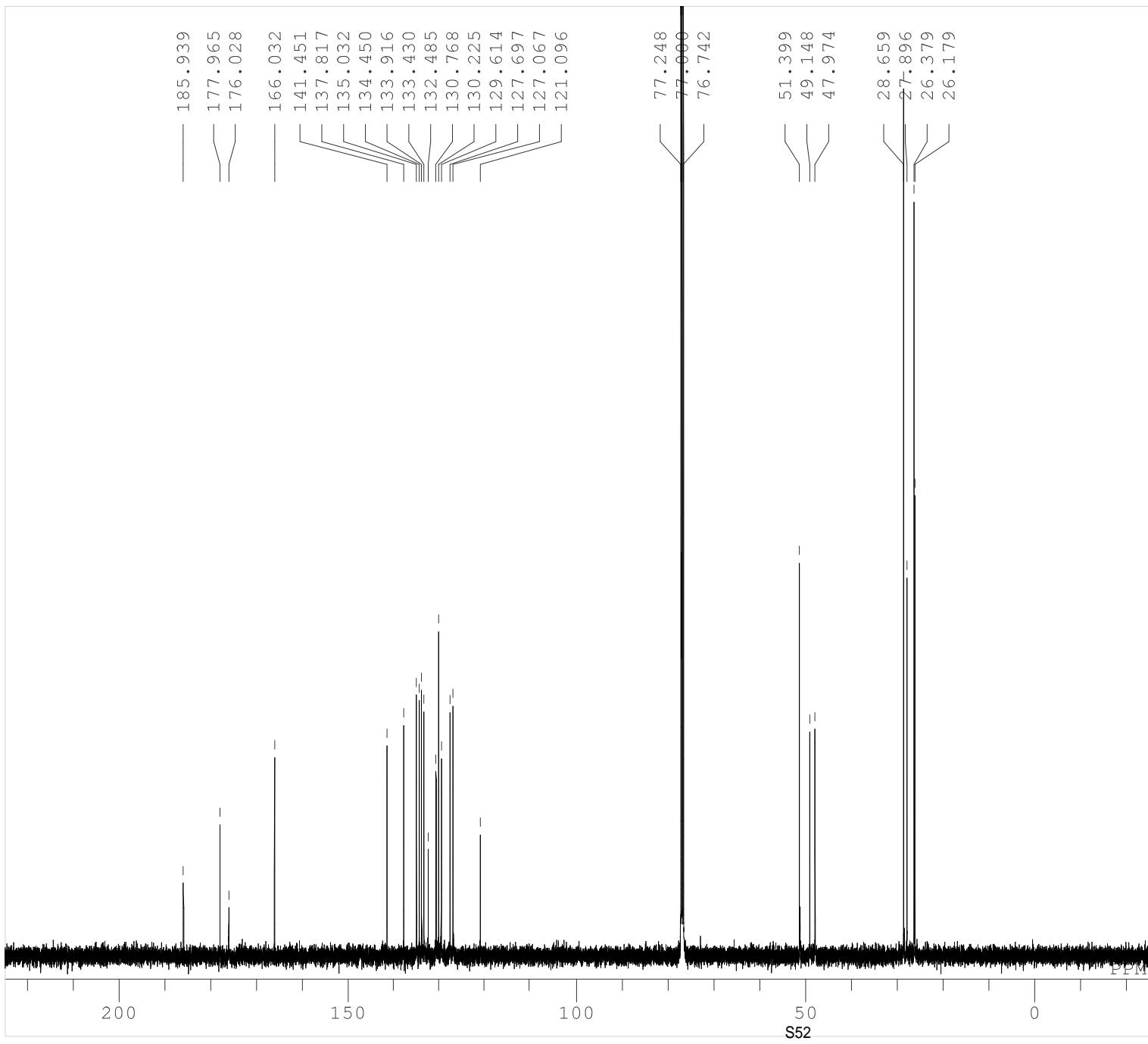
DFILE TY\_10\_033\_01\_carbon-1-1.als  
 COMNT single pulse decoupled gated  
 DATIM 2017-12-18 23:19:47  
 OBNUC <sup>13</sup>C  
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 8680  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 19.9 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60



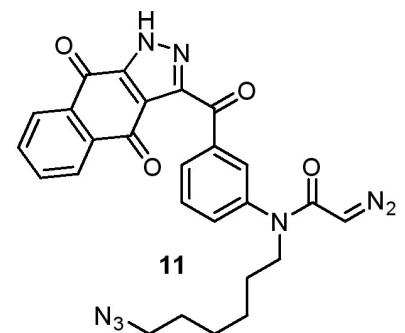


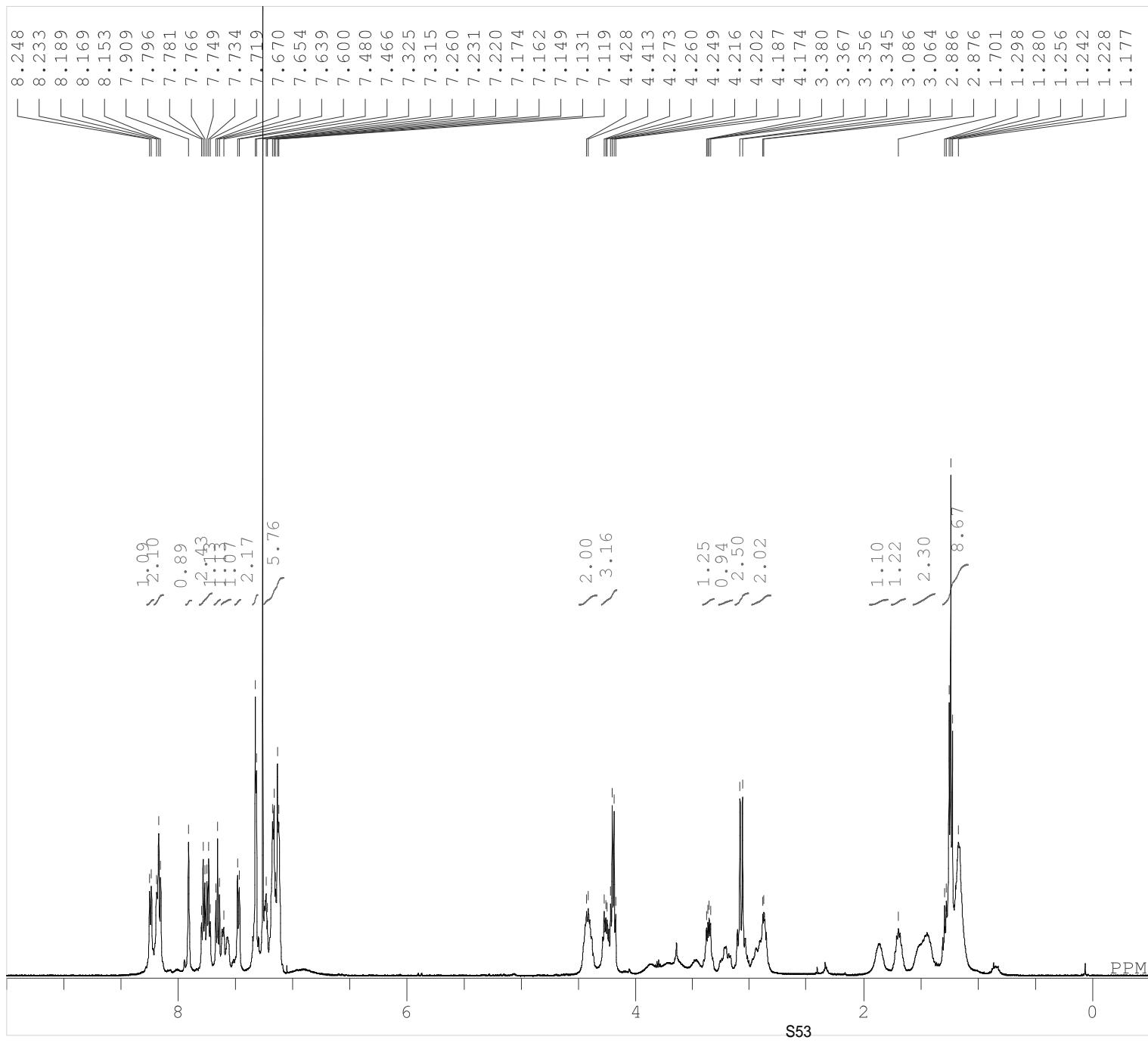
DFILE TY\_10\_051\_01-1-1.als  
 COMNT dazo  
 DATIM 2018-02-01 21:17:19  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 17.6 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 46





DFILE TY\_10\_051\_01\_carbon-1-1.als  
 COMNT single pulse decoupled gated  
 DATIM 2018-02-05 23:15:43  
 OBNUC  $^{13}\text{C}$   
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 8860  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 18.9 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 58

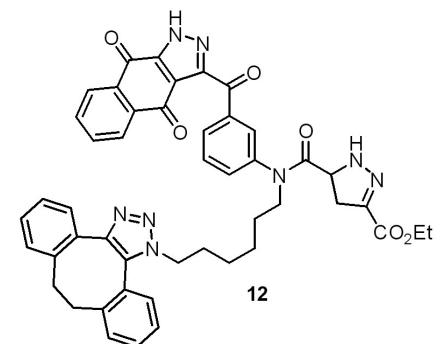


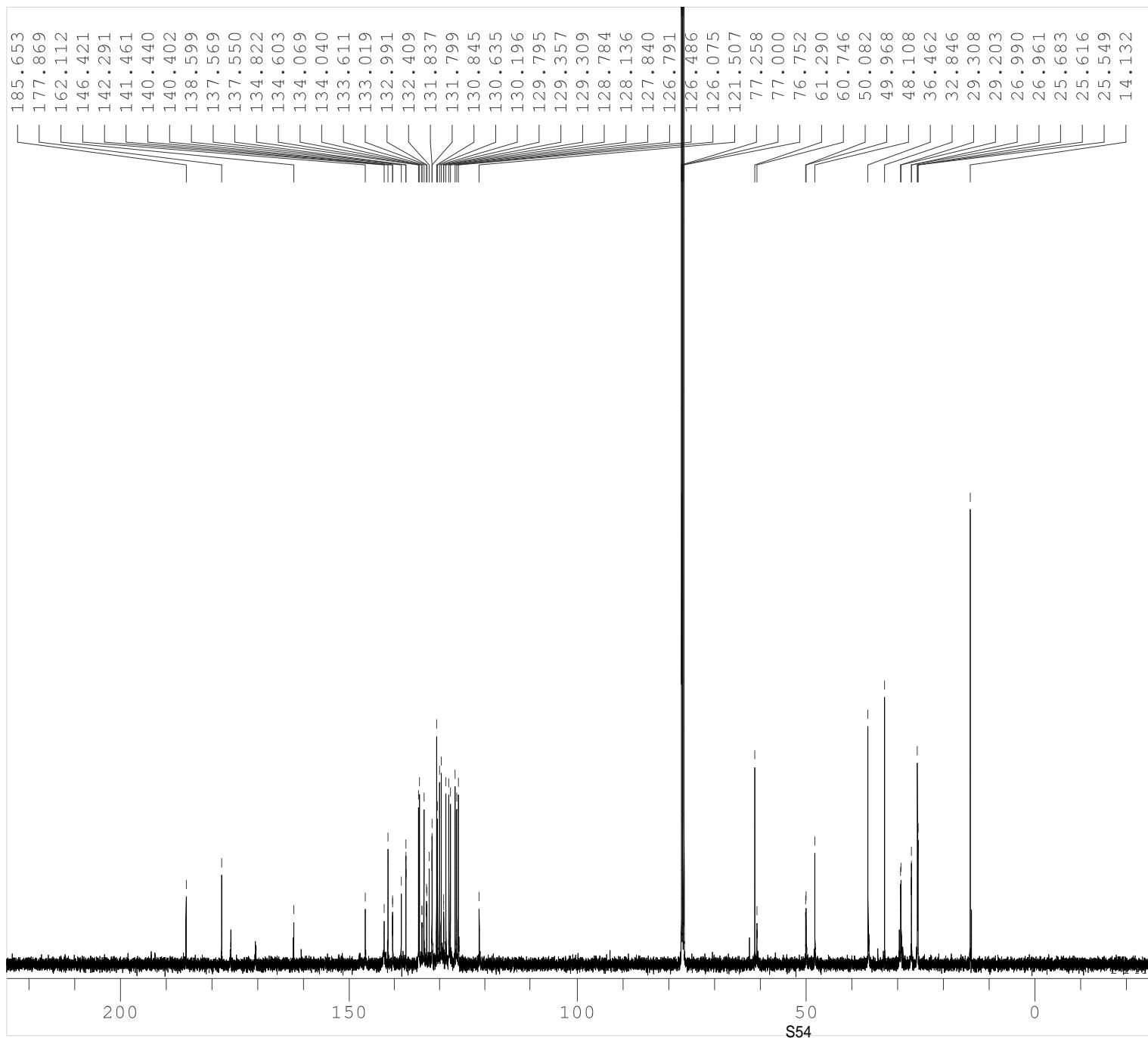


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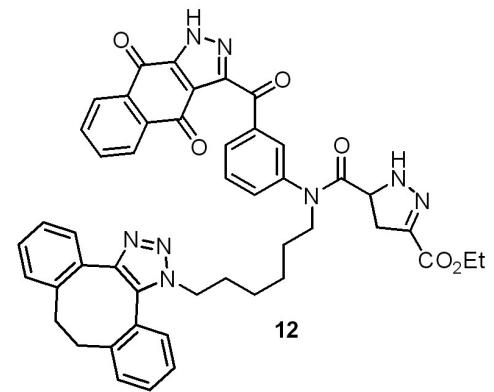
DFILE      TY_10_061_02_proton-1-1.als
COMNT      single_pulse
DATIM      2018-04-06 23:22:52
OBNUC      1H
EXMOD     proton.jxp
OBFRQ      500.16 MHz
OBSET      2.41 kHz
OBFIN      6.01 Hz
POINT      13107
FREQU     7507.51 Hz
SCANS       8
ACQTM      1.7459 sec
PD         5.0000 sec
PW1        6.85 usec
IRNUC      1H
CTEMP       16.5 c
SLVNT      CDCL3
EXREF      7.26 ppm
BF          0.10 Hz
RGAIN       30

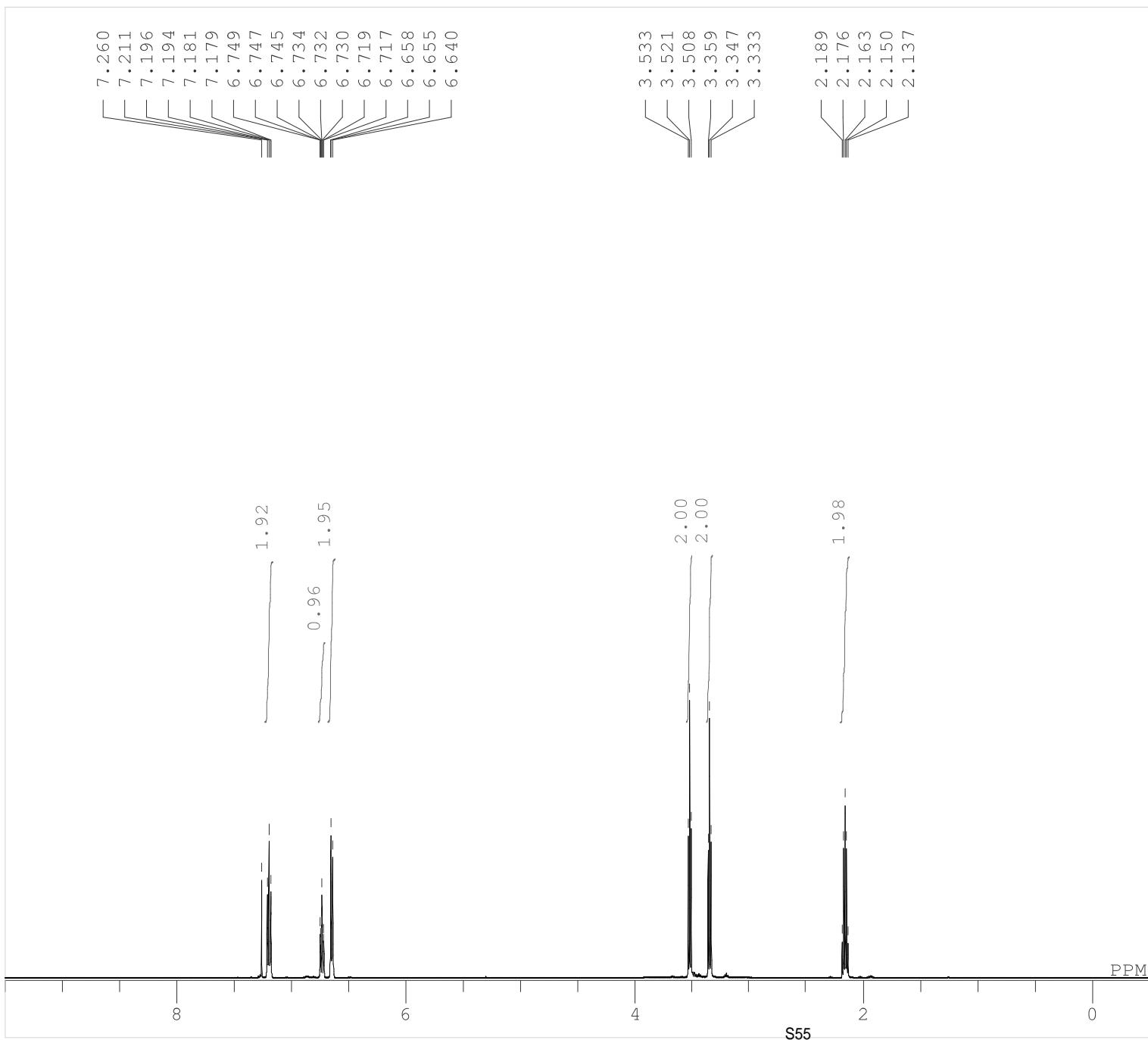
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DFILE TY\_10\_061\_02\_carbon-1-1.als  
 COMNT single pulse decoupled gated  
 DATIM 2018-04-06 23:24:27  
 OBNUC <sup>13</sup>C  
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 8900  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 18.2 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60

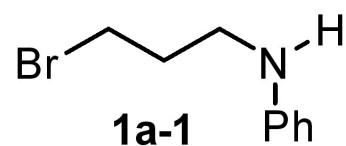


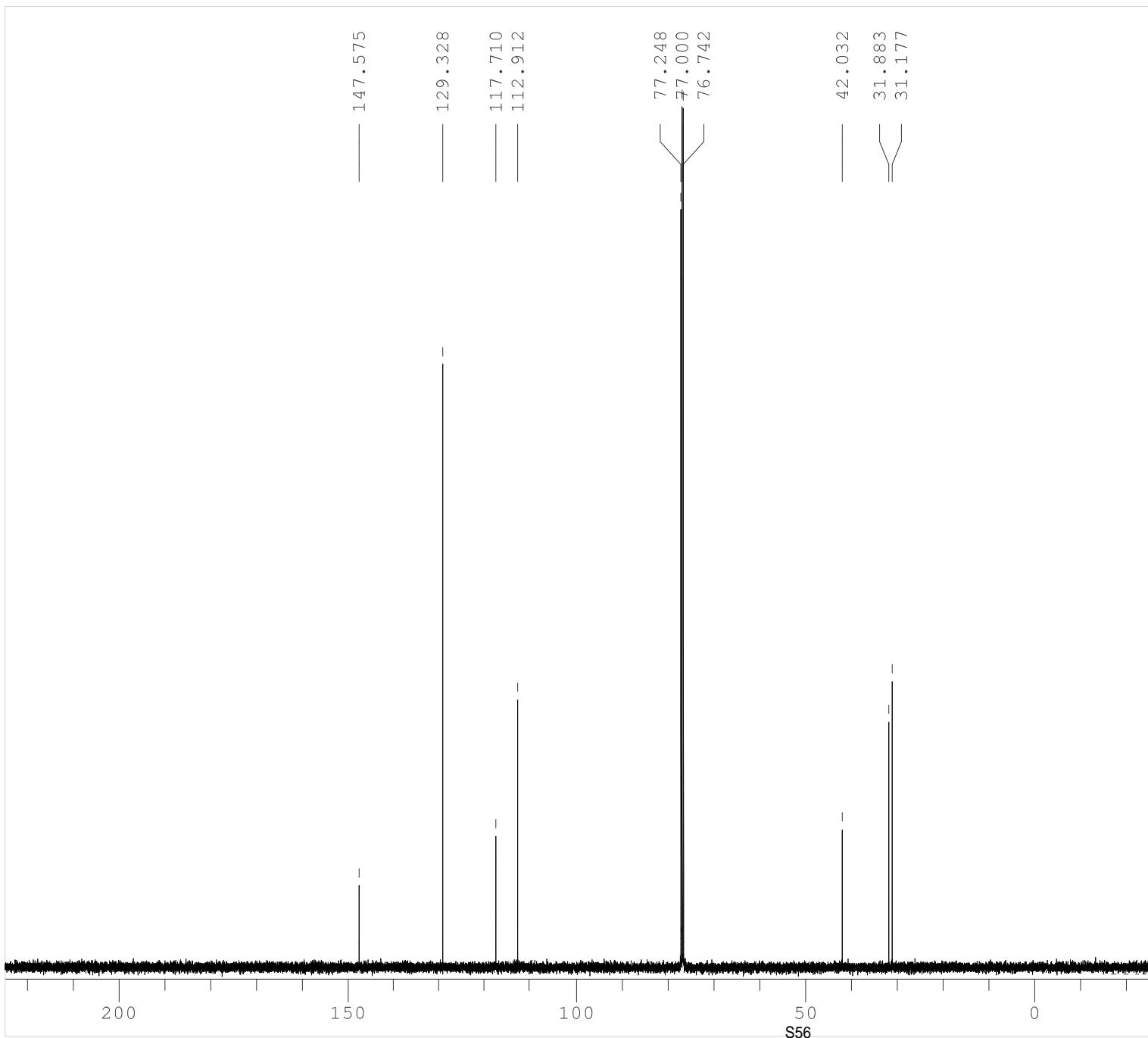


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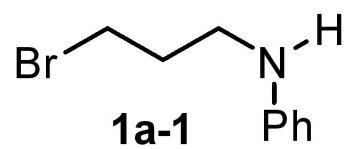
DFILE      TY_07_067_03_proton-1-1.als
COMNT      single_pulse
DATIM      2016-09-26 17:49:12
OBNUC      1H
EXMOD     proton.jxp
OBFRQ      500.16 MHz
OBSET      2.41 kHz
OBFIN      6.01 Hz
POINT      13107
FREQU     7507.51 Hz
SCANS       8
ACQTM      1.7459 sec
PD         5.0000 sec
PW1        6.85 usec
IRNUC      1H
CTEMP       18.3 c
SLVNT      CDCL3
EXREF      7.26 ppm
BF         0.10 Hz
RGAIN       40

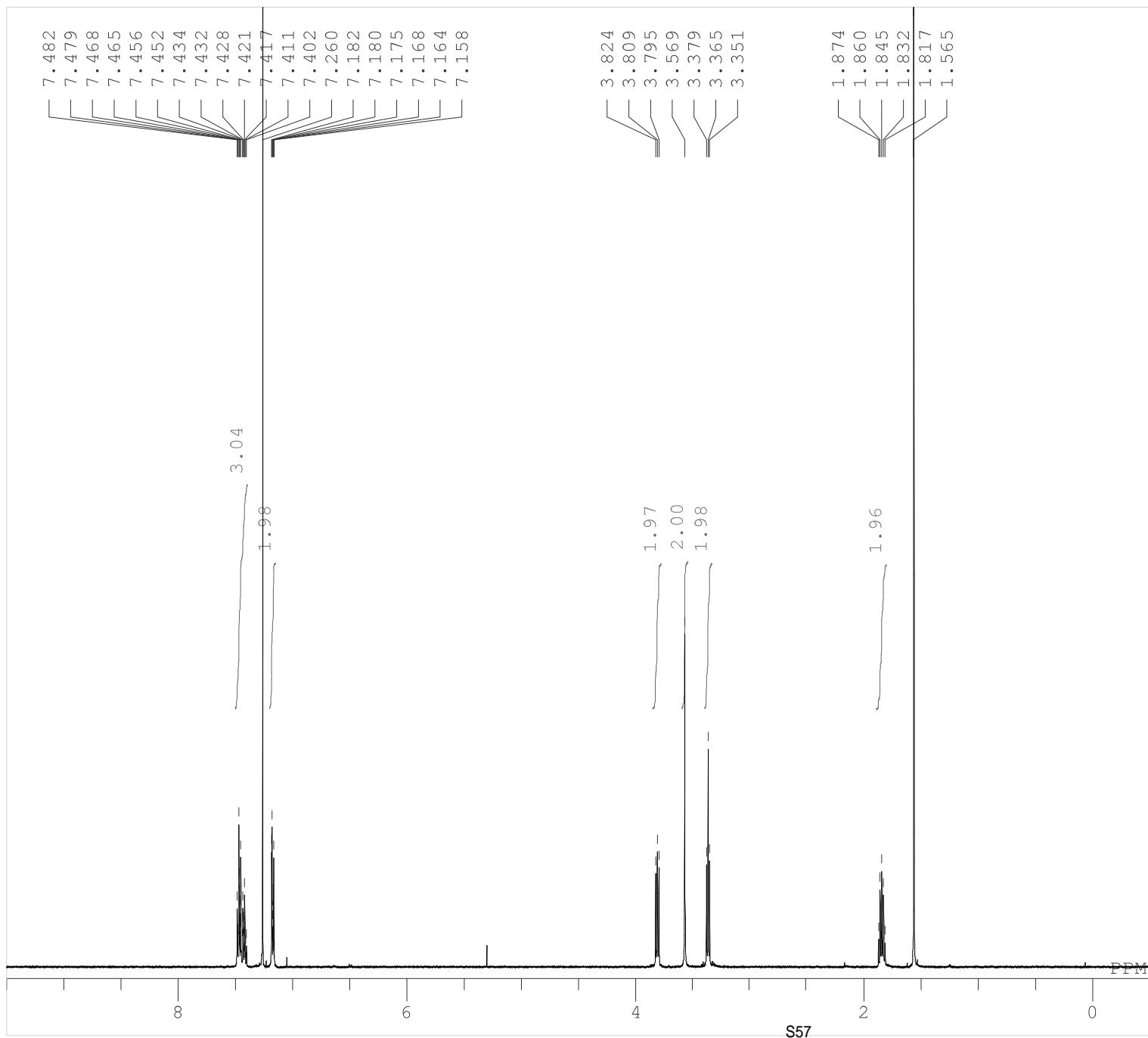
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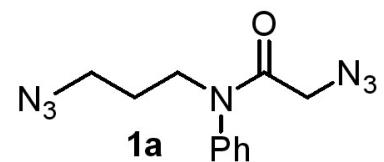


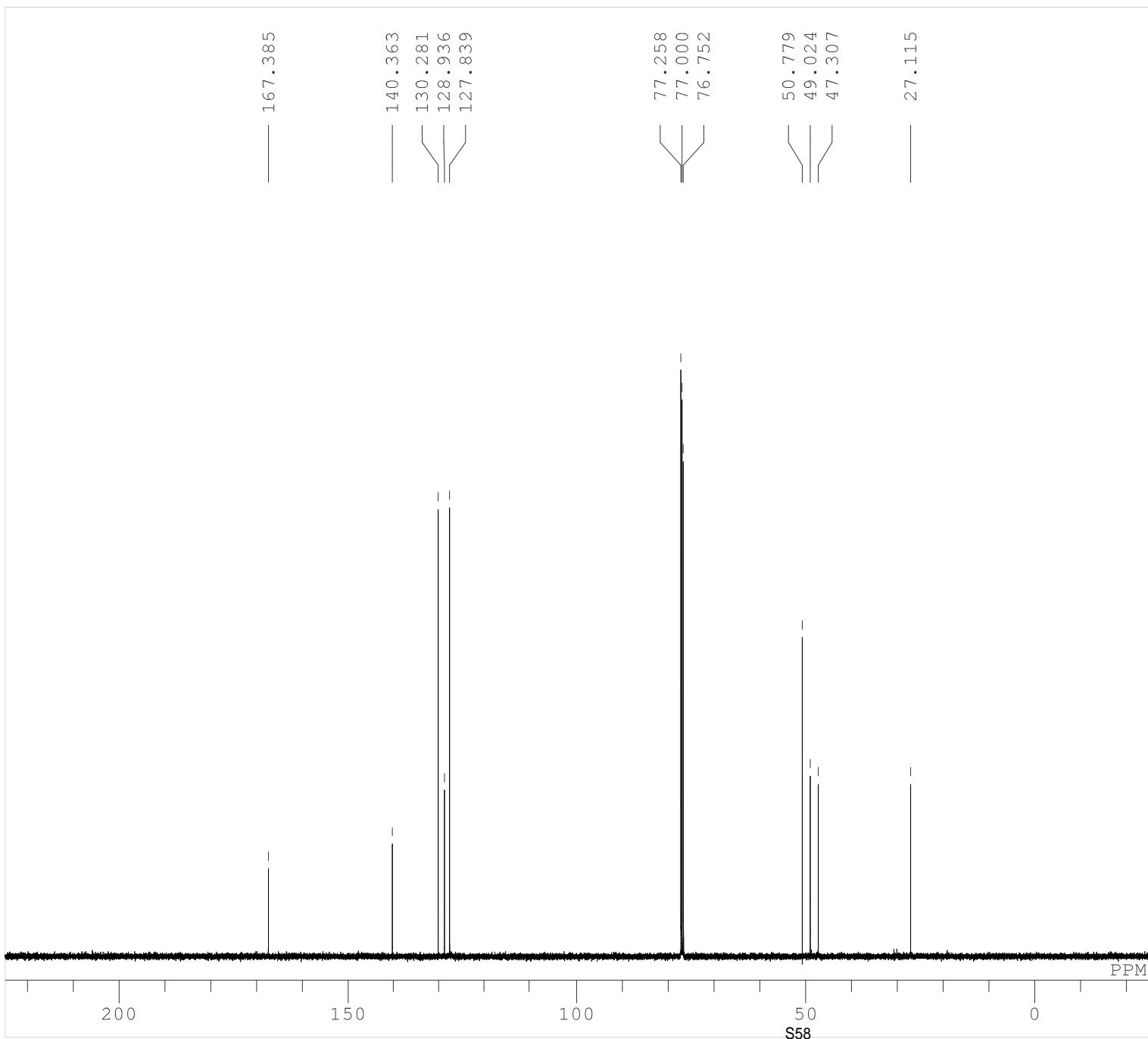
DFILE TY\_07\_067\_03\_carbon-1-1.als  
COMNT single pulse decoupled gated  
DATIM 2016-09-26 17:51:11  
OBNUC <sup>13</sup>C  
EXMOD carbon.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 kHz  
OBFIN 4.21 Hz  
POINT 26214  
FREQU 31446.54 Hz  
SCANS 620  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 18.8 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 58



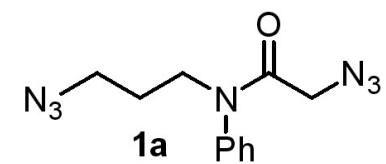


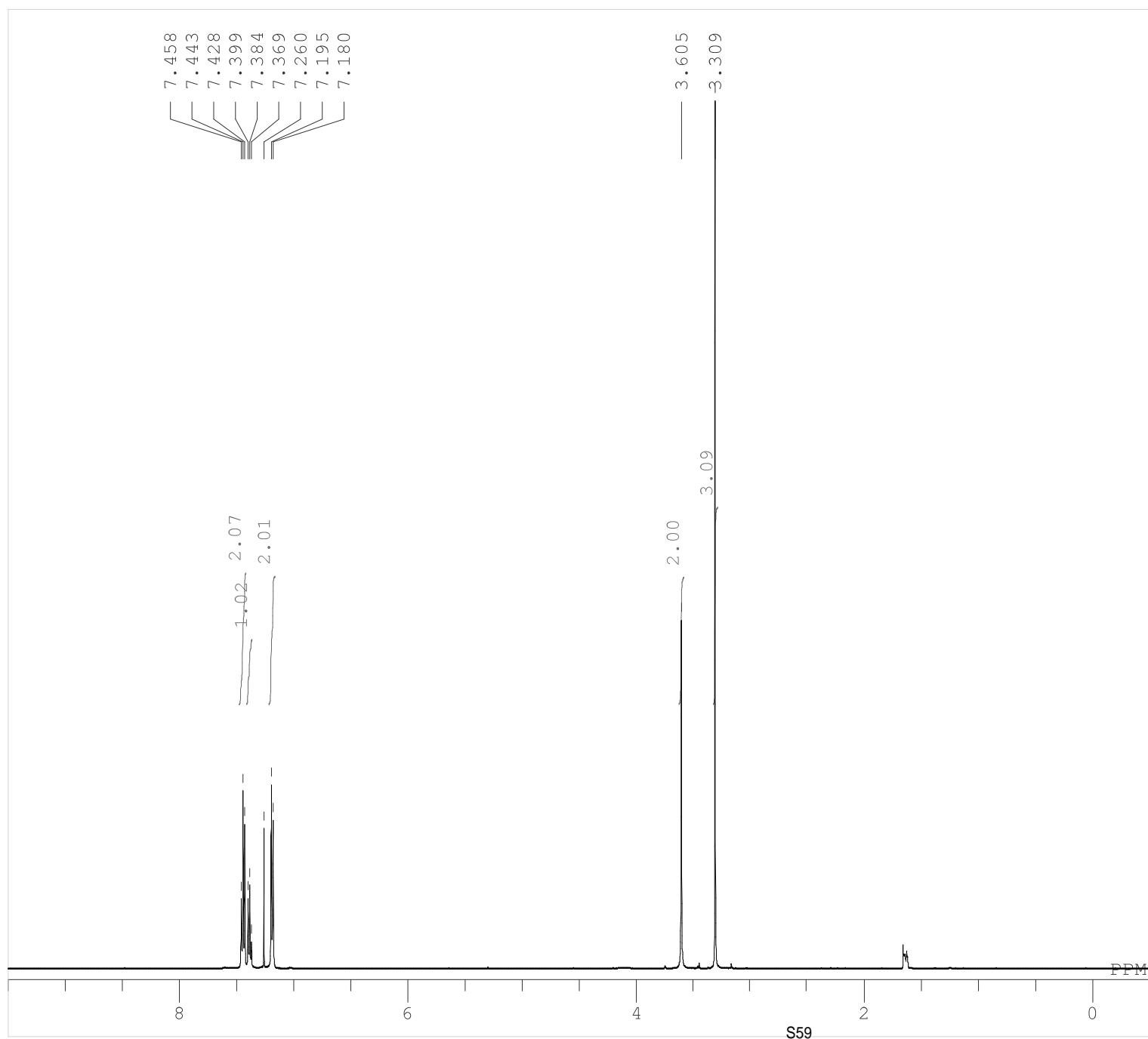
DFILE TY\_07\_069\_02-1-1.als  
 COMNT dazid  
 DATIM 2016-09-27 15:59:16  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 18.8 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 48



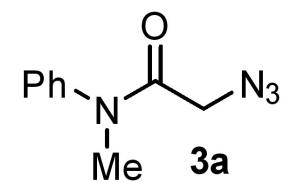


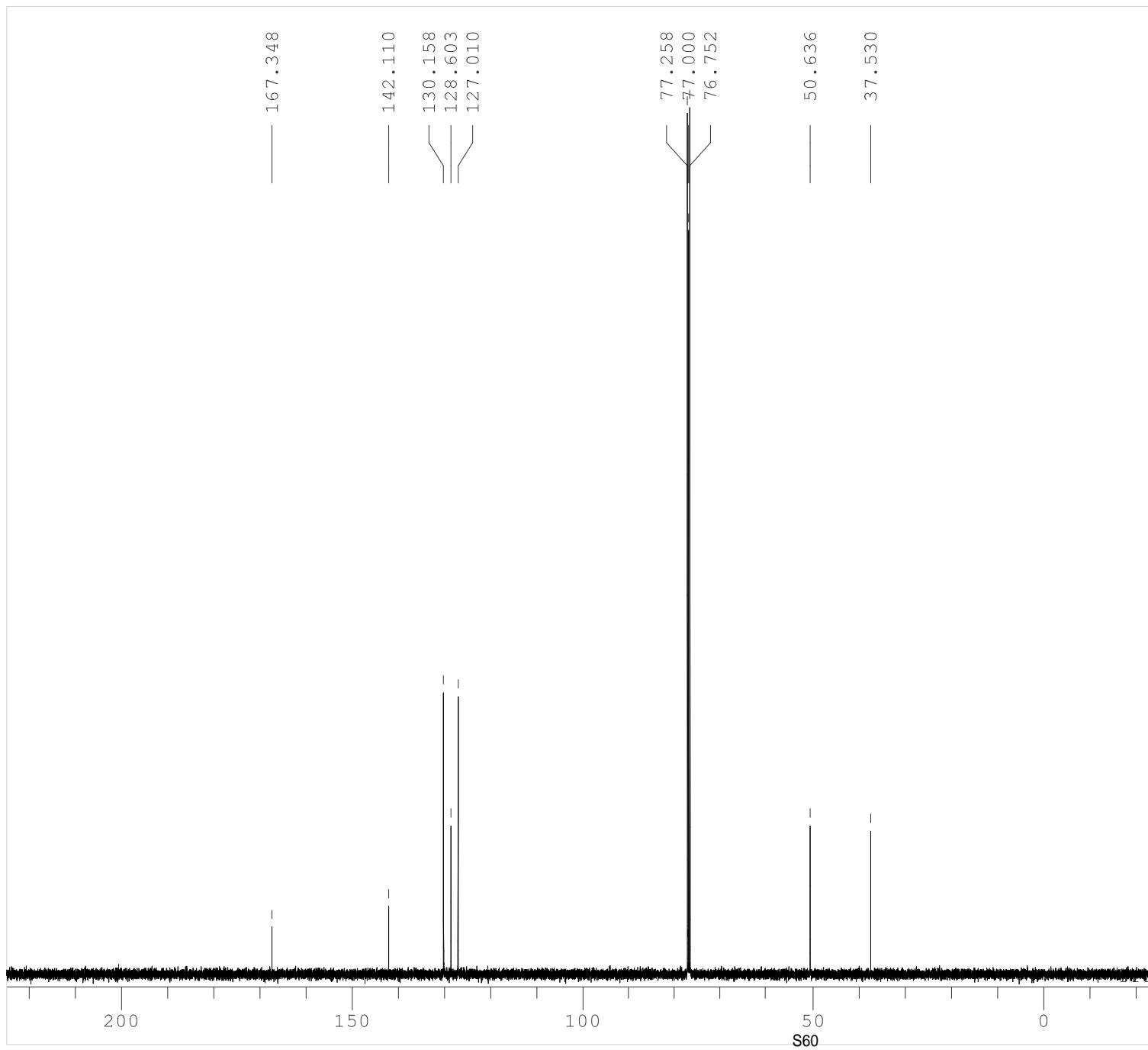
DFILE TY\_07\_015\_04\_carbon-1-1.jdf  
COMNT single pulse decoupled gated  
DATIM 2016-09-21 18:22:35  
OBNUC <sup>13</sup>C  
EXMOD carbon.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 kHz  
OBFIN 4.21 Hz  
POINT 32767  
FREQU 39308.18 Hz  
SCANS 620  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 18.9 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 60



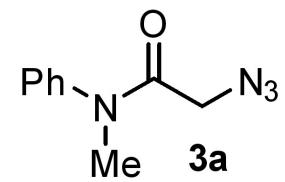


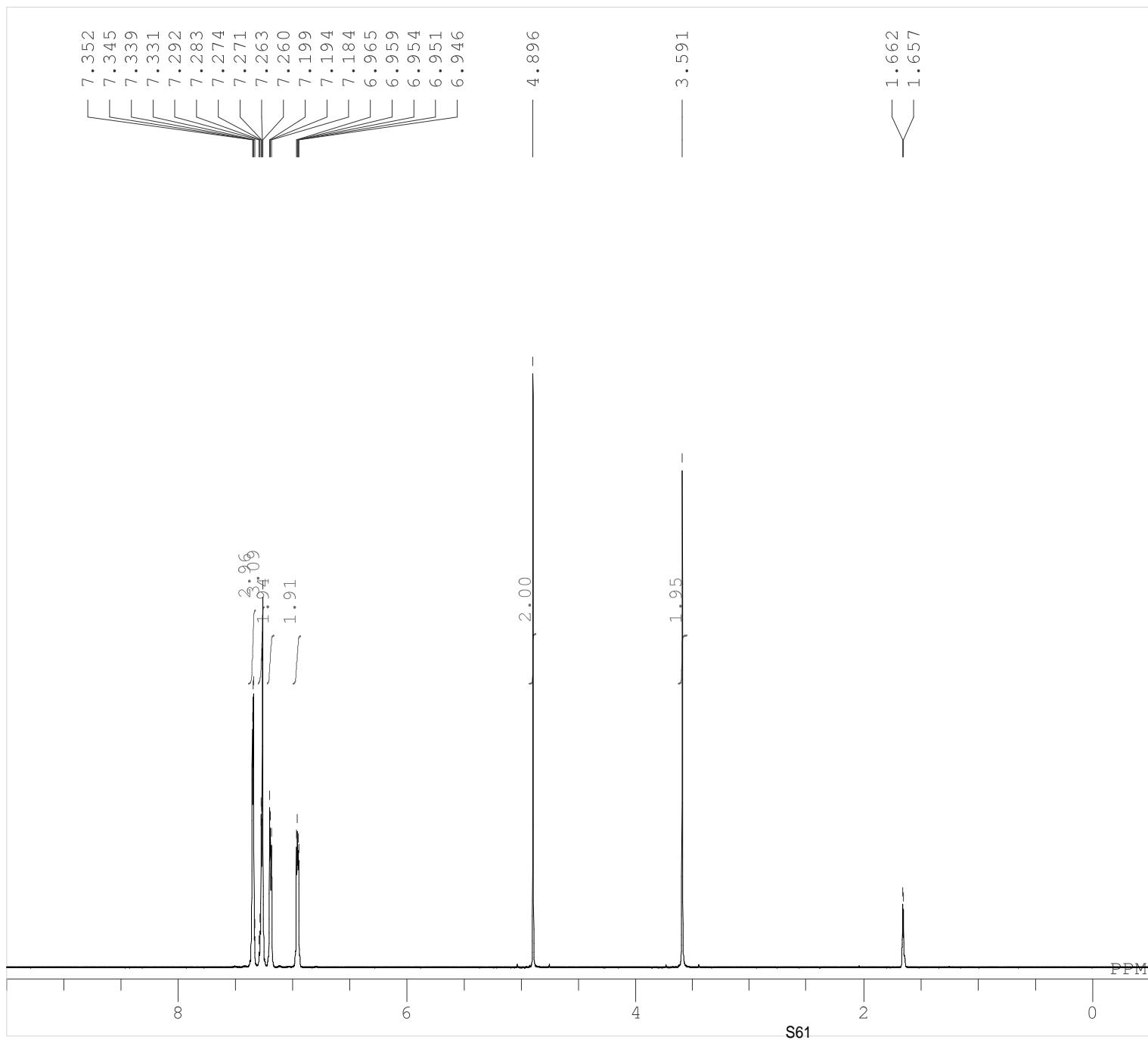
DFILE TY\_07\_048\_02\_proton-1-1.als  
COMNT single\_pulse  
DATIM 2016-09-24 15:10:01  
OBNUC 1H  
EXMOD proton.jxp  
OBFRQ 500.16 MHz  
OBSET 2.41 kHz  
OBFIN 6.01 Hz  
POINT 13107  
FREQU 7507.51 Hz  
SCANS 8  
ACQTM 1.7459 sec  
PD 5.0000 sec  
PW1 6.85 usec  
IRNUC 1H  
CTEMP 18.7 c  
SLVNT CDCL<sub>3</sub>  
EXREF 7.26 ppm  
BF 0.10 Hz  
RGAIN 40



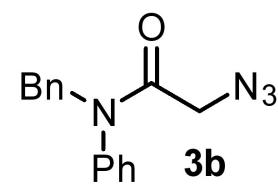


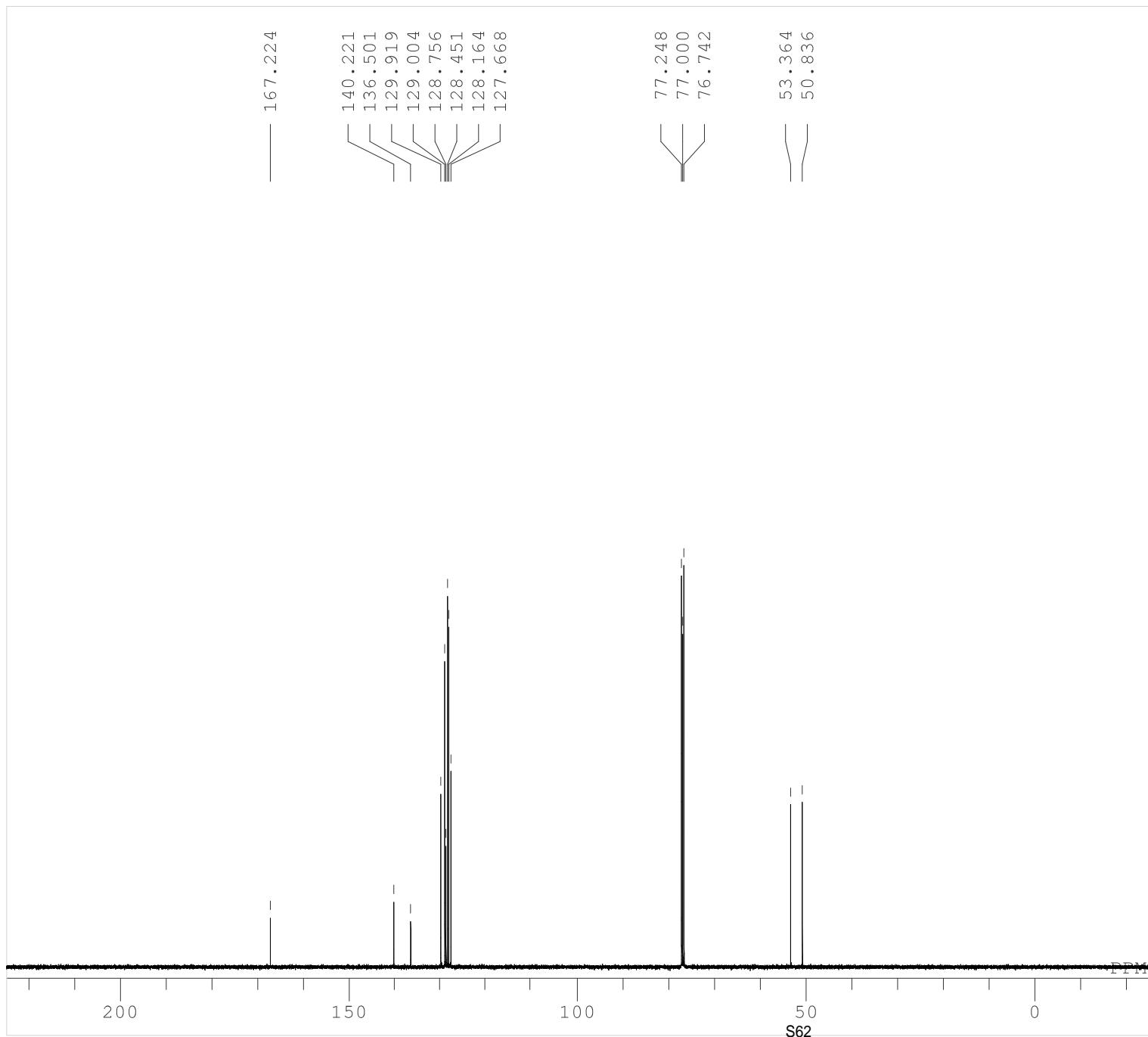
DFILE TY\_07\_048\_02\_carbon-1-1.als  
COMNT single pulse decoupled gated  
DATIM 2016-09-24 15:11:50  
OBNUC  $^{13}\text{C}$   
EXMOD carbon.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 kHz  
OBFIN 4.21 Hz  
POINT 26214  
FREQU 31446.54 Hz  
SCANS 620  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 19.0 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 60



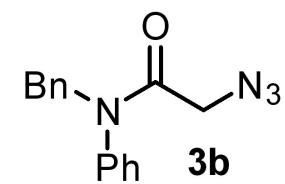


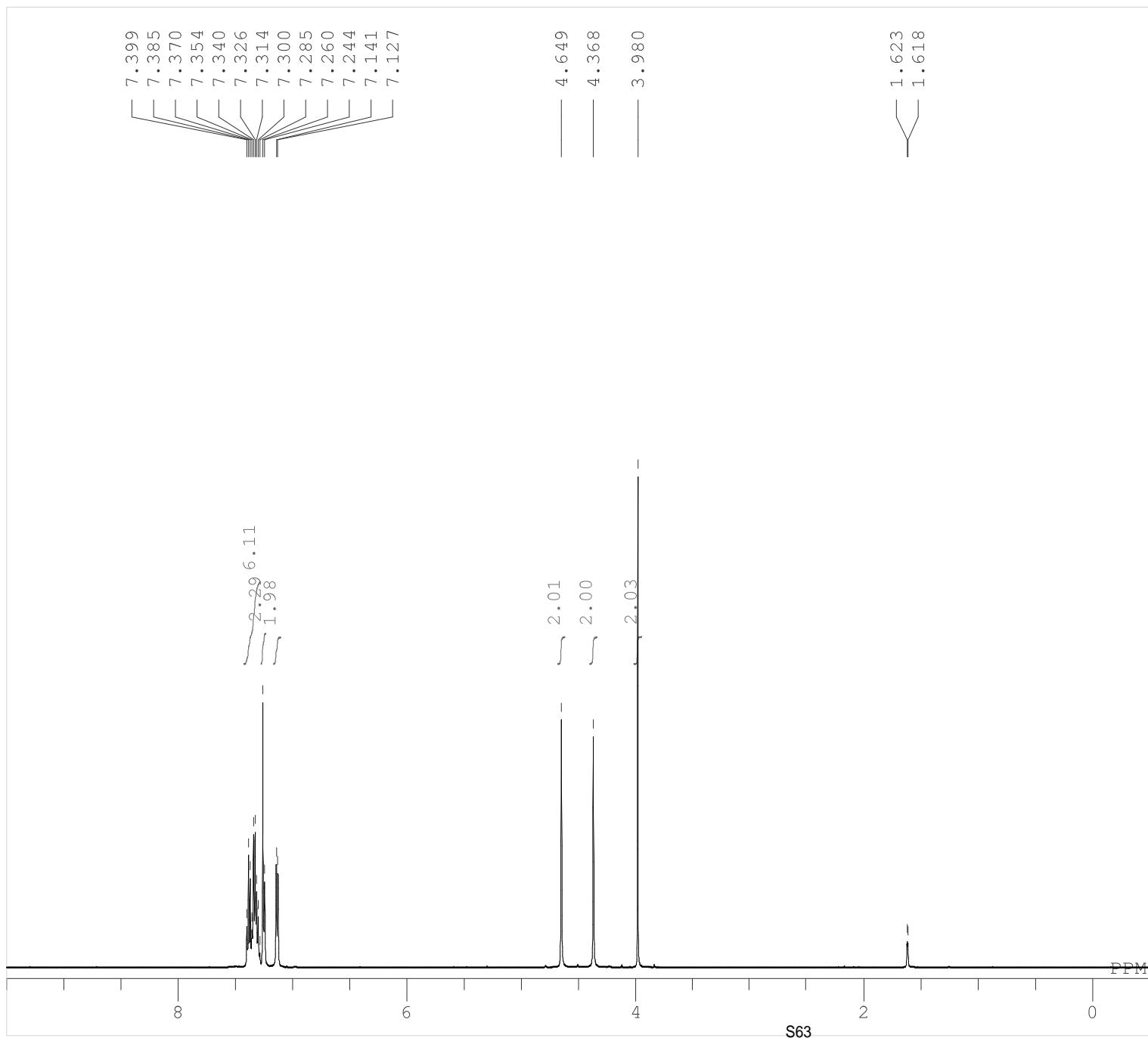
DFILE TY\_08\_137\_01\_proton-1-1.als  
 COMNT single\_pulse  
 DATIM 2017-07-01 10:05:41  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 16.8 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 36





DFILE TY\_08\_137\_01\_carbon-1-1.als  
 COMNT single pulse decoupled gated  
 DATIM 2017-07-01 10:07:16  
 OBNUC  $^{13}\text{C}$   
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 1260  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 17.4 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60

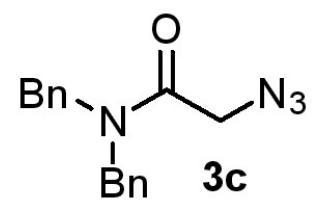


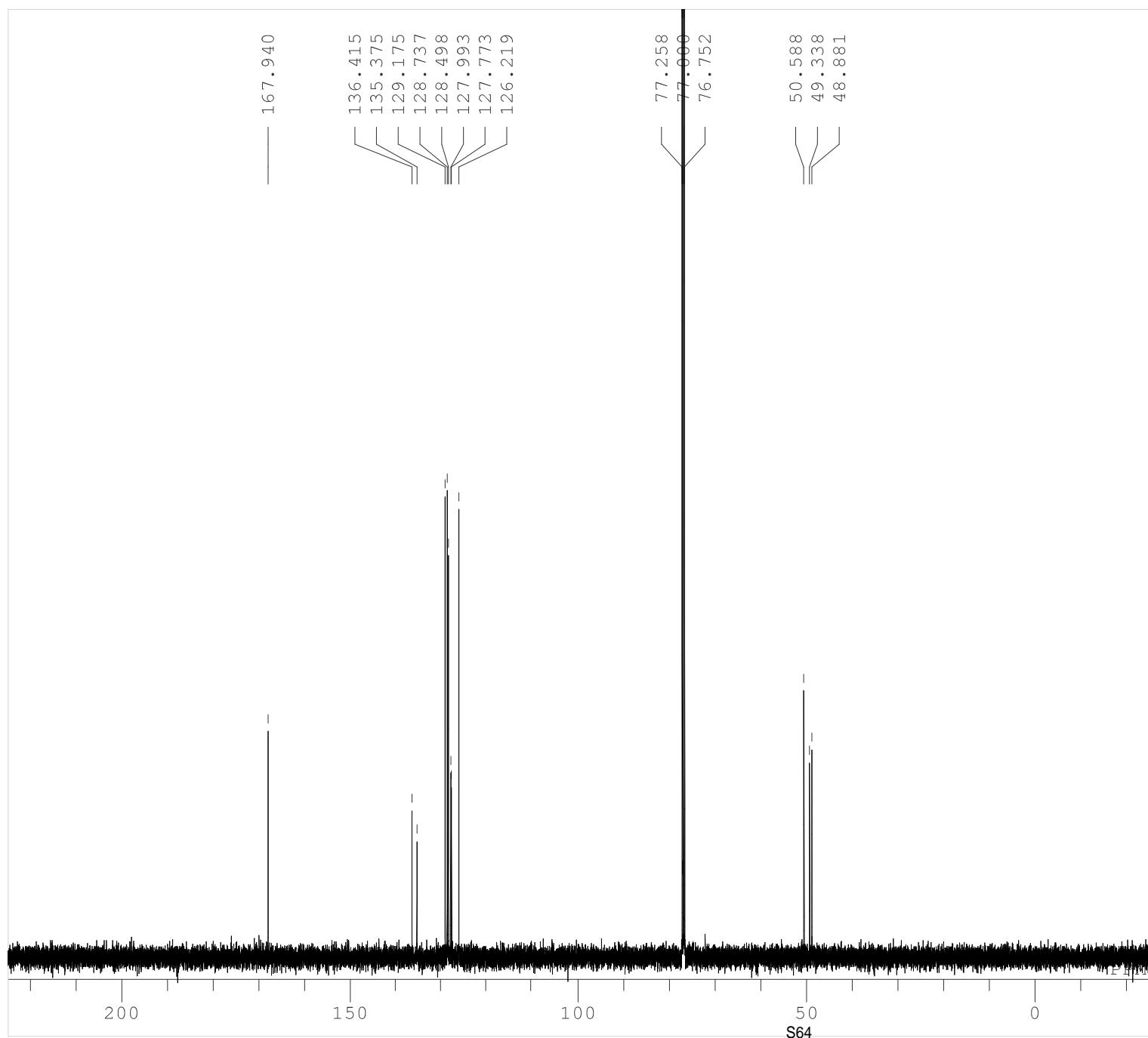


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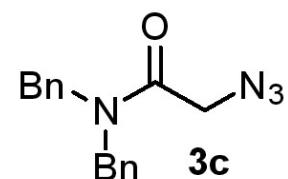
DFILE TY_07_106_02_proton-1-1.als
COMNT single_pulse
DATIM 2016-10-18 14:58:27
OBNUC 1H
EXMOD proton.jxp
OBFRQ      500.16 MHz
OBSET       2.41 kHz
OBFIN        6.01 Hz
POINT        13107
FREQU      7507.51 Hz
SCANS          8
ACQTM      1.7459 sec
PD           5.0000 sec
PW1           6.85 usec
IRNUC        1H
CTEMP         18.2 c
SLVNT      CDCL3
EXREF        7.26 ppm
BF            0.10 Hz
RGAIN          38

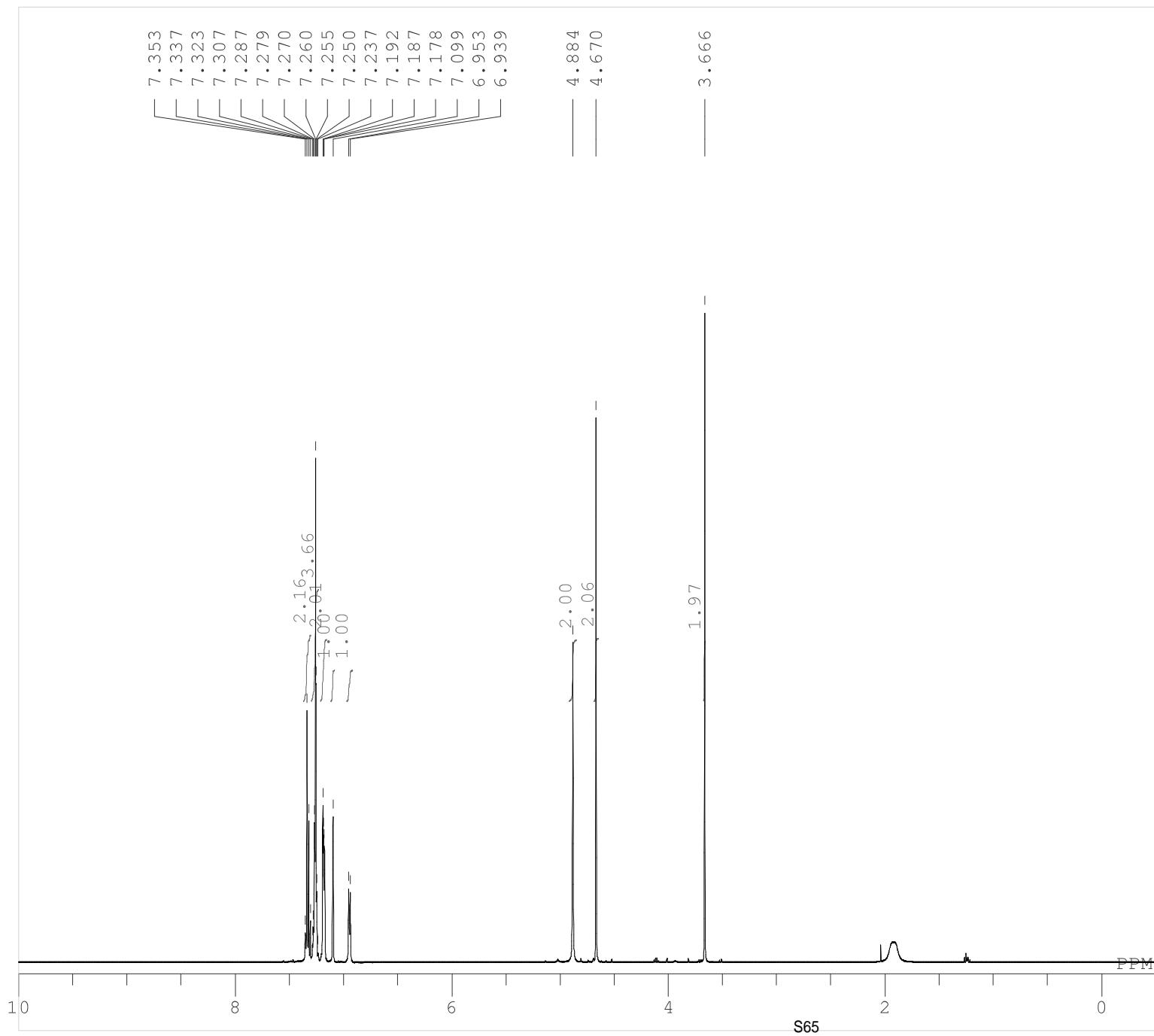
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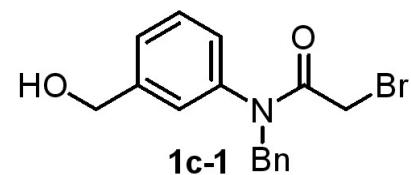


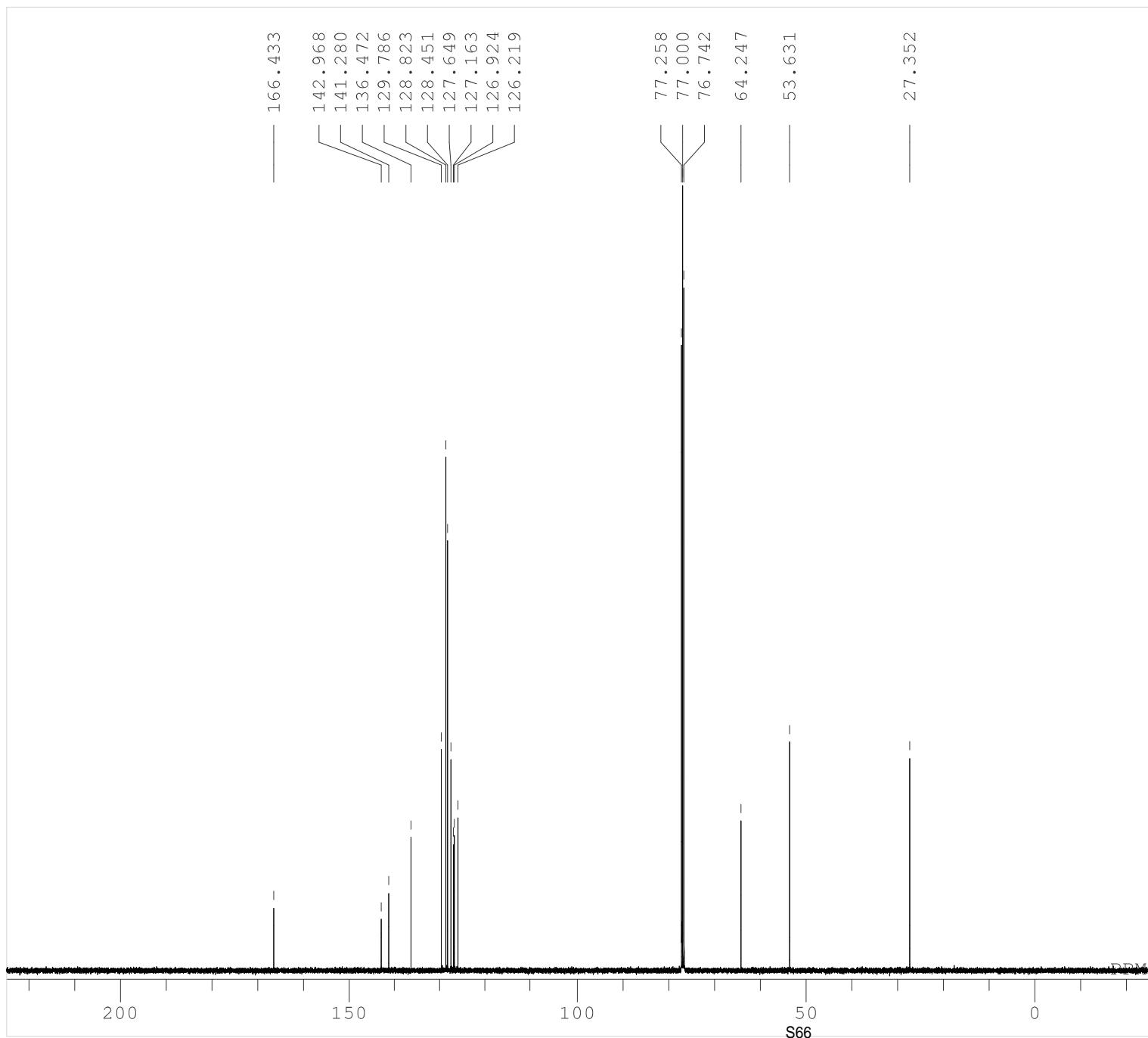
DFILE TY\_07\_106\_02\_carbon-1-1.als  
 COMNT single pulse decoupled gated  
 DATIM 2016-10-18 15:00:36  
 OBNUC <sup>13</sup>C  
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 620  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 19.1 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 56



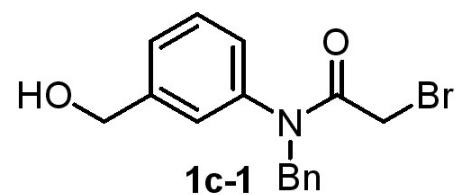


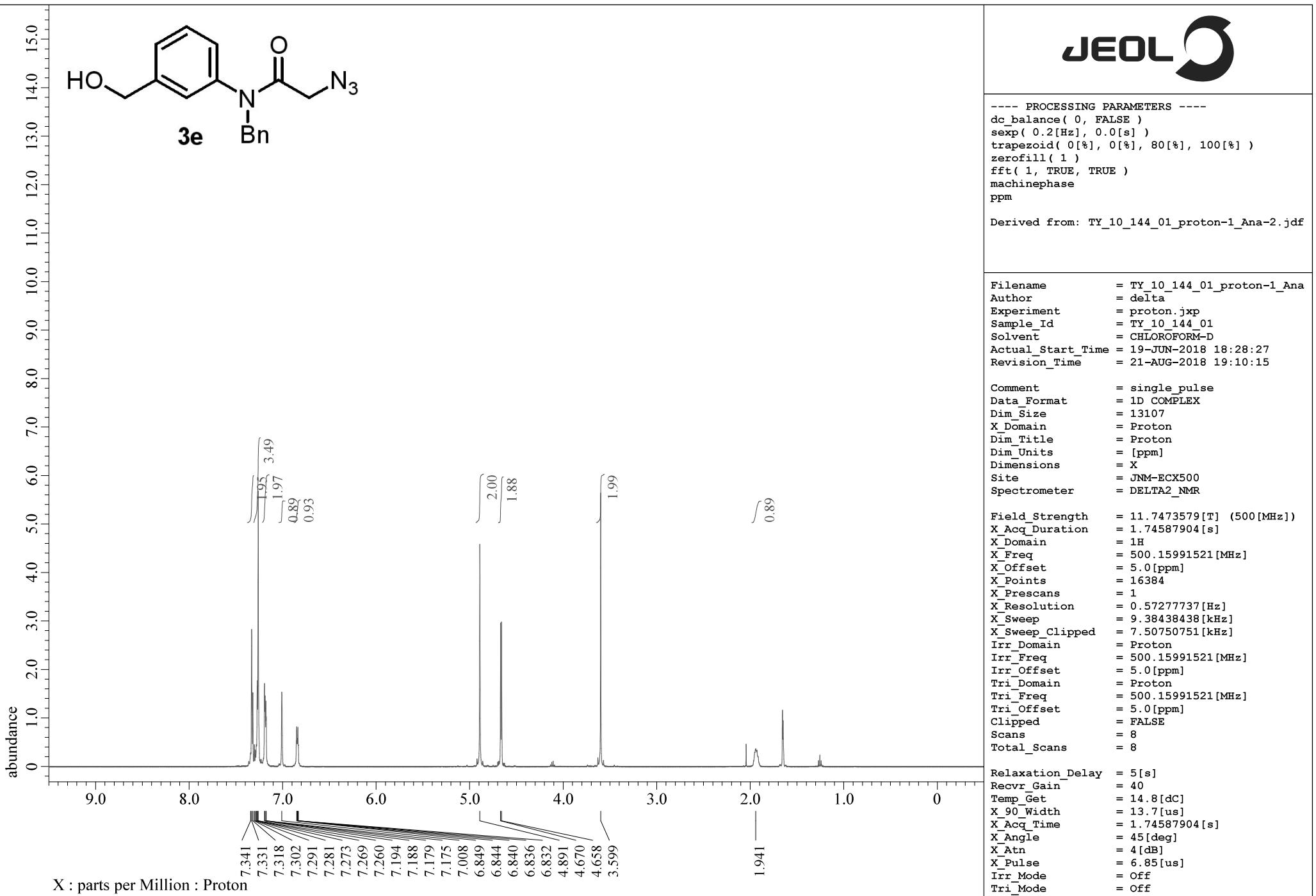
DFILE TY\_09\_099\_01\_proton-1-1.als  
 COMNT single\_pulse  
 DATIM 2017-09-30 11:55:25  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 14.2 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 38

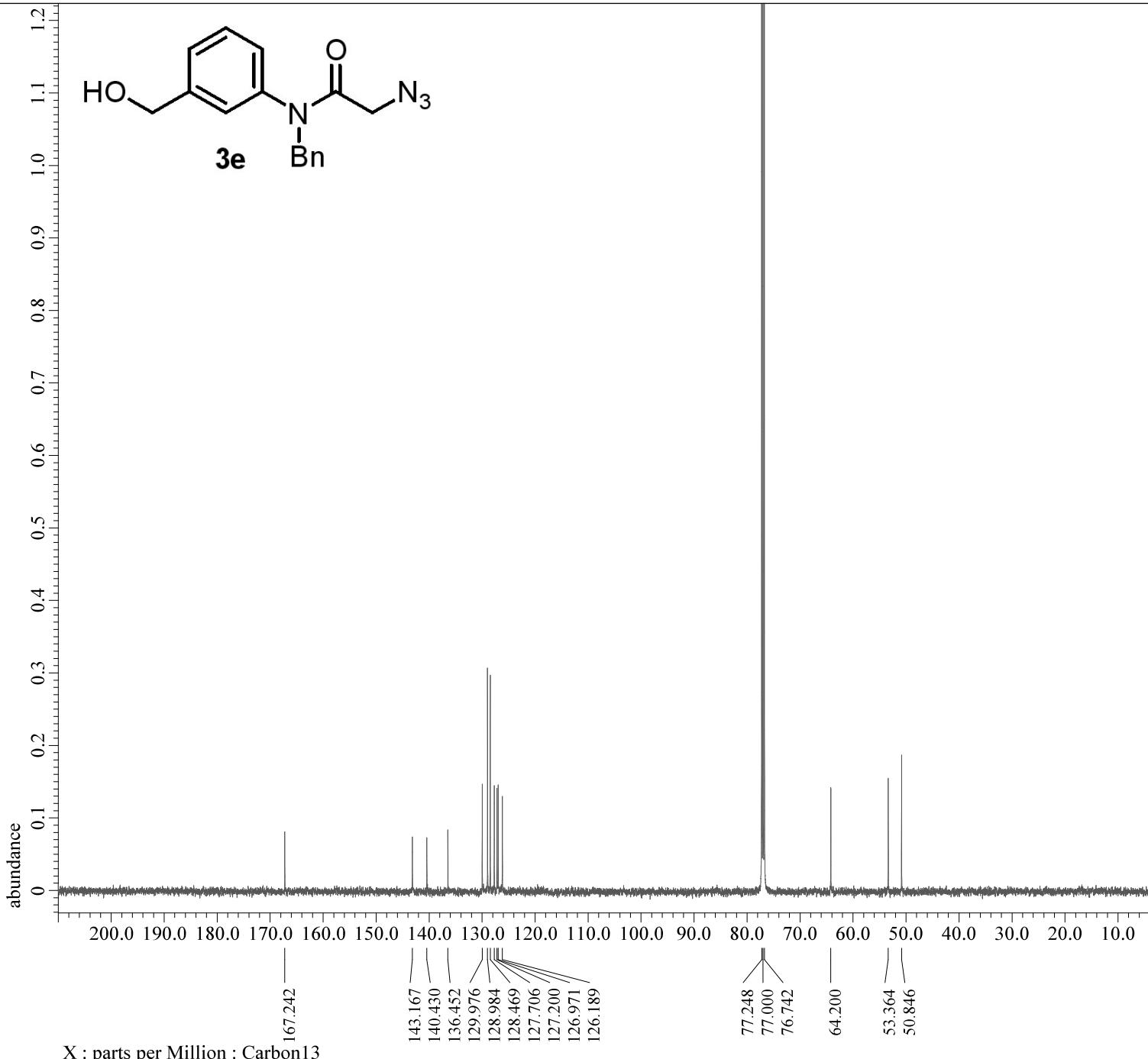
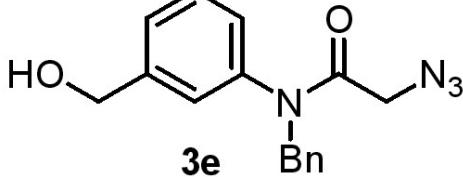




DFILE TY\_09\_099\_01\_carbon-1-1.als  
 COMNT single pulse decoupled gated  
 DATIM 2017-09-30 11:57:05  
 OBNUC <sup>13</sup>C  
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 1680  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 14.2 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 58



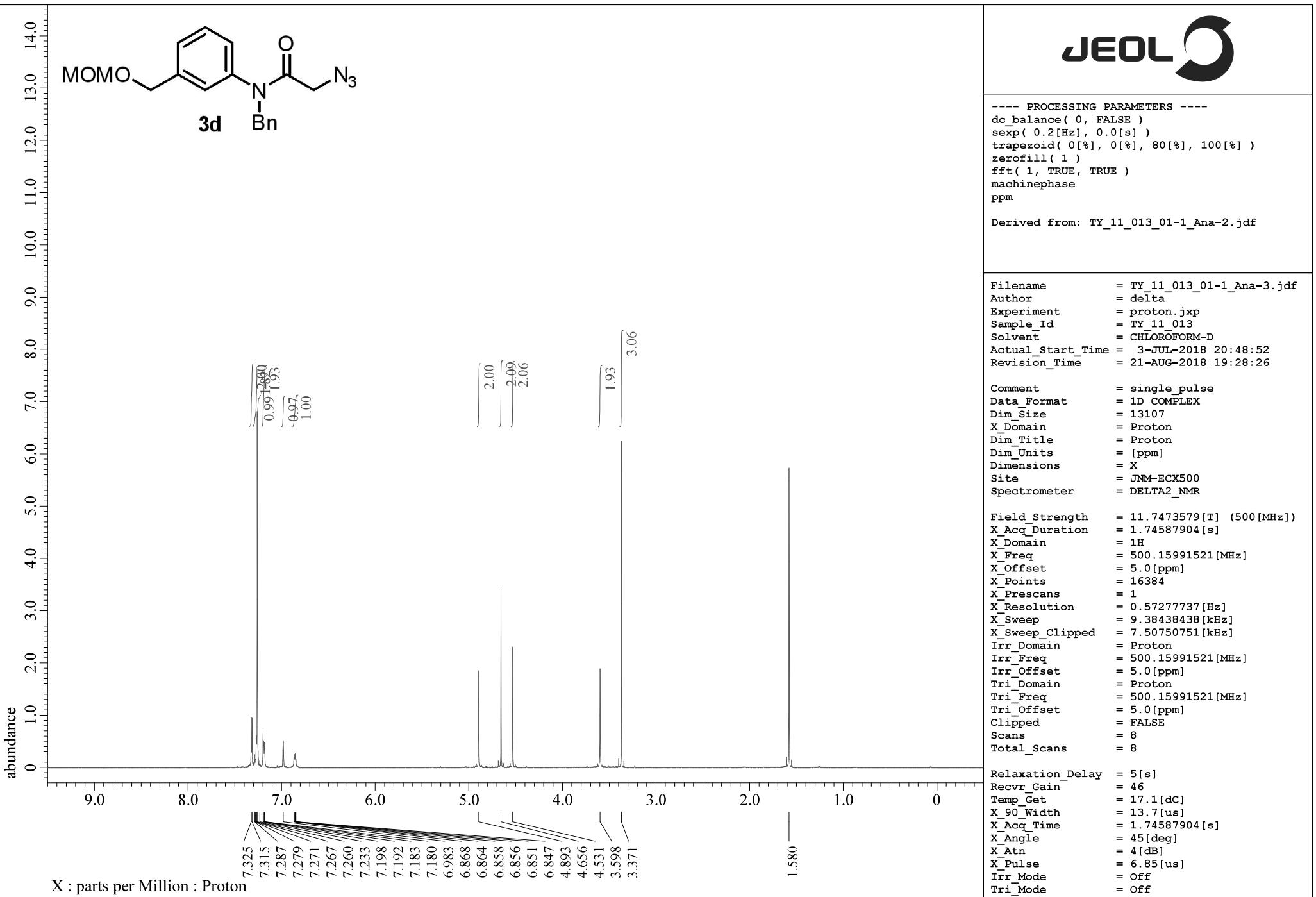


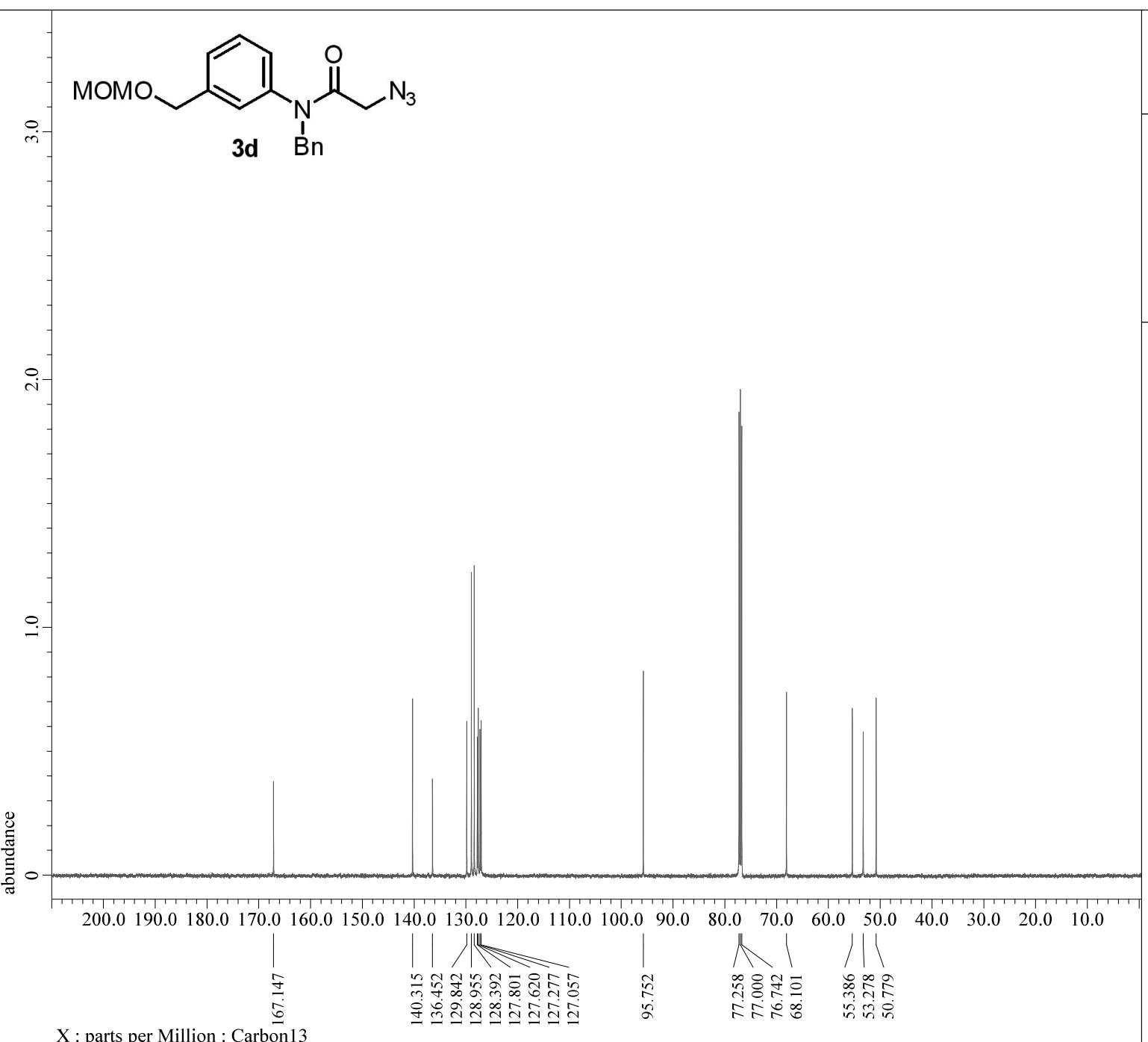
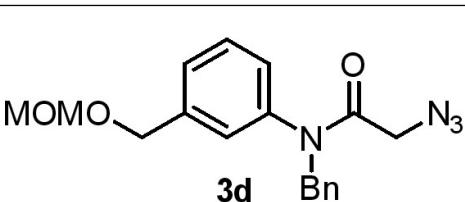


**JEOL**

---- PROCESSING PARAMETERS ----  
dc\_balance( 0, FALSE )  
sexp( 2.0[Hz], 0.0[s] )  
trapezoid( 0[%], 0[%], 80[%], 100[%] )  
zerofill( 1 )  
fft( 1, TRUE, TRUE )  
machinephase  
ppm  
Derived from: TY\_10\_144\_01\_carbon-1\_Ana-1.jdf

Filename = TY\_10\_144\_01\_carbon-1\_Ana  
Author = delta  
Experiment = carbon.jxp  
Sample\_Id = TY\_10\_144\_01  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 19-JUN-2018 18:30:17  
Revision\_Time = 21-AUG-2018 19:11:42  
Comment = single pulse decoupled ga  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
X\_Domain = Carbon  
Dim\_Title = Carbon13  
Dim\_Units = [ppm]  
Dimensions = X  
Site = JNM-ECX500  
Spectrometer = DELTA2\_NMR  
Field\_Strength = 11.7473579[T] (500[MHz])  
X\_Acq\_Duration = 0.83361792[s]  
X\_Domain = 13C  
X\_Freq = 125.76529768[MHz]  
X\_Offset = 100[ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 1.19959034[Hz]  
X\_Sweep = 39.3081761[kHz]  
X\_Sweep\_Clipped = 31.44654088[kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 500.15991521[MHz]  
Irr\_Offset = 5.0[ppm]  
Clipped = TRUE  
Scans = 1260  
Total\_Scans = 1260  
Relaxation\_Delay = 2[s]  
Recv\_Gain = 58  
Temp\_Get = 15.2[dC]  
X\_90\_Width = 9.36[us]  
X\_Acq\_Time = 0.83361792[s]  
X\_Angle = 30[deg]  
X\_Atn = 3[dB]  
X\_Pulse = 3.12[us]  
Irr\_Atn\_Dec = 20.54[dB]  
Irr\_Atn\_Noe = 20.54[dB]  
Irr\_Noise = WALTZ  
Irr\_Pwidth = 92[us]  
Decoupling = TRUE

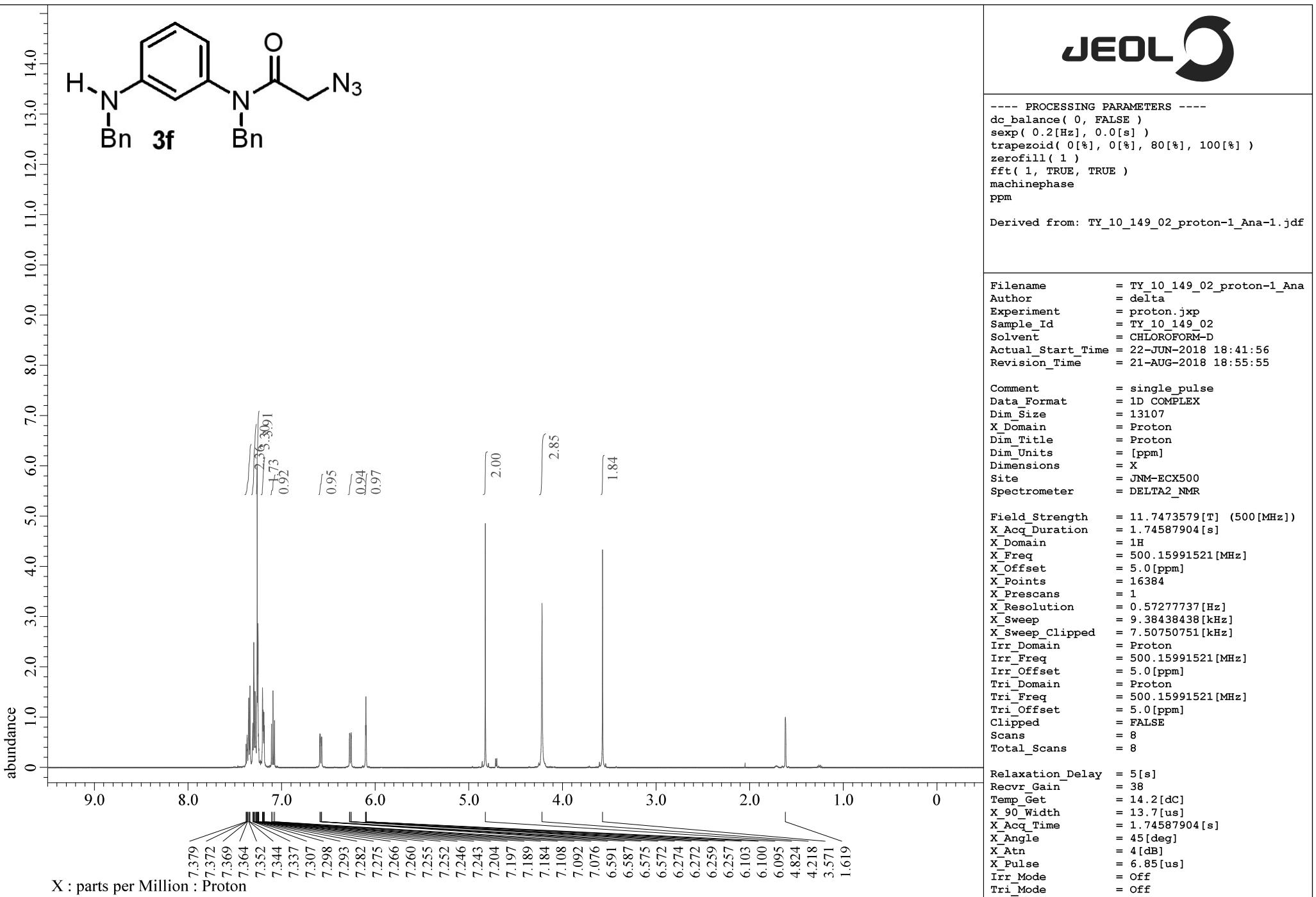


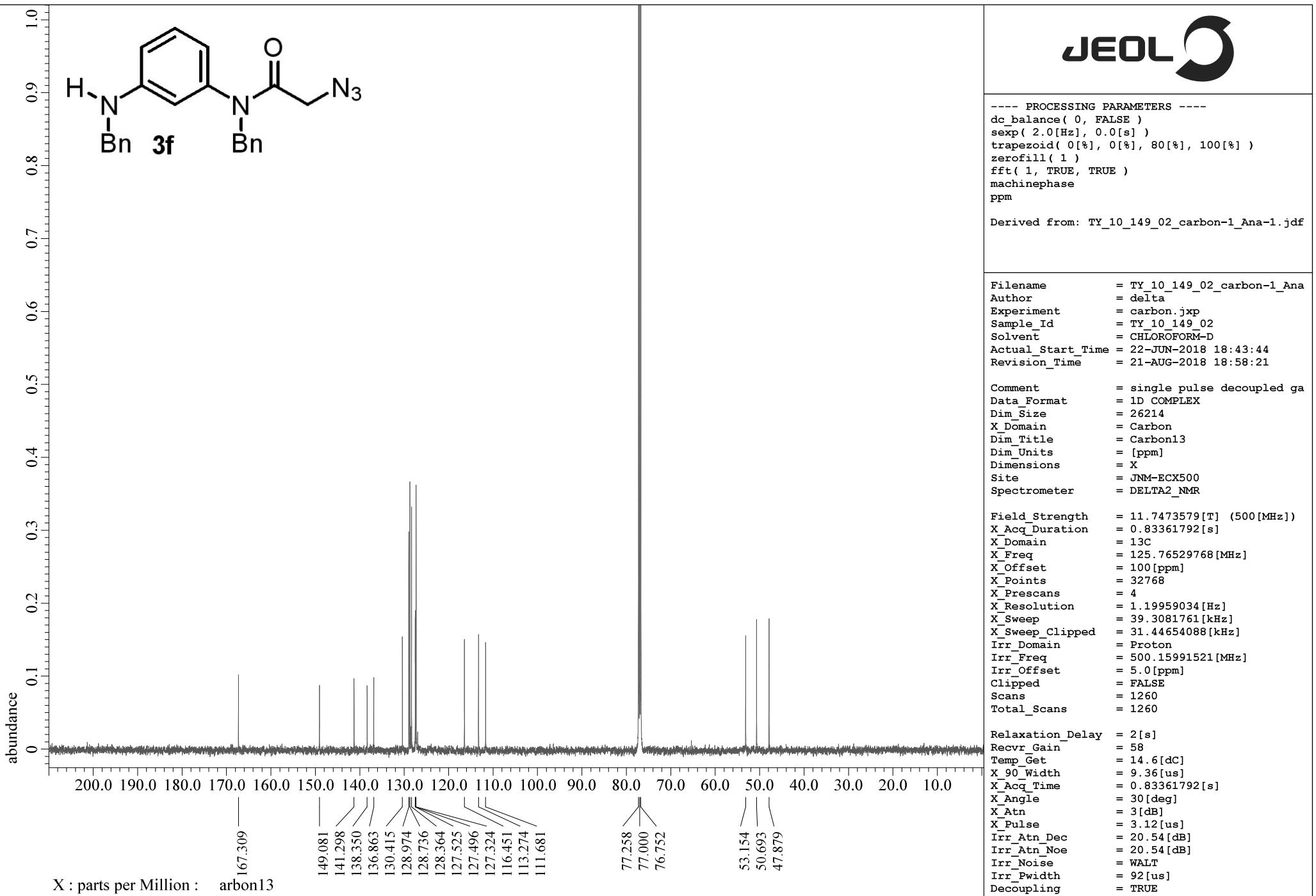


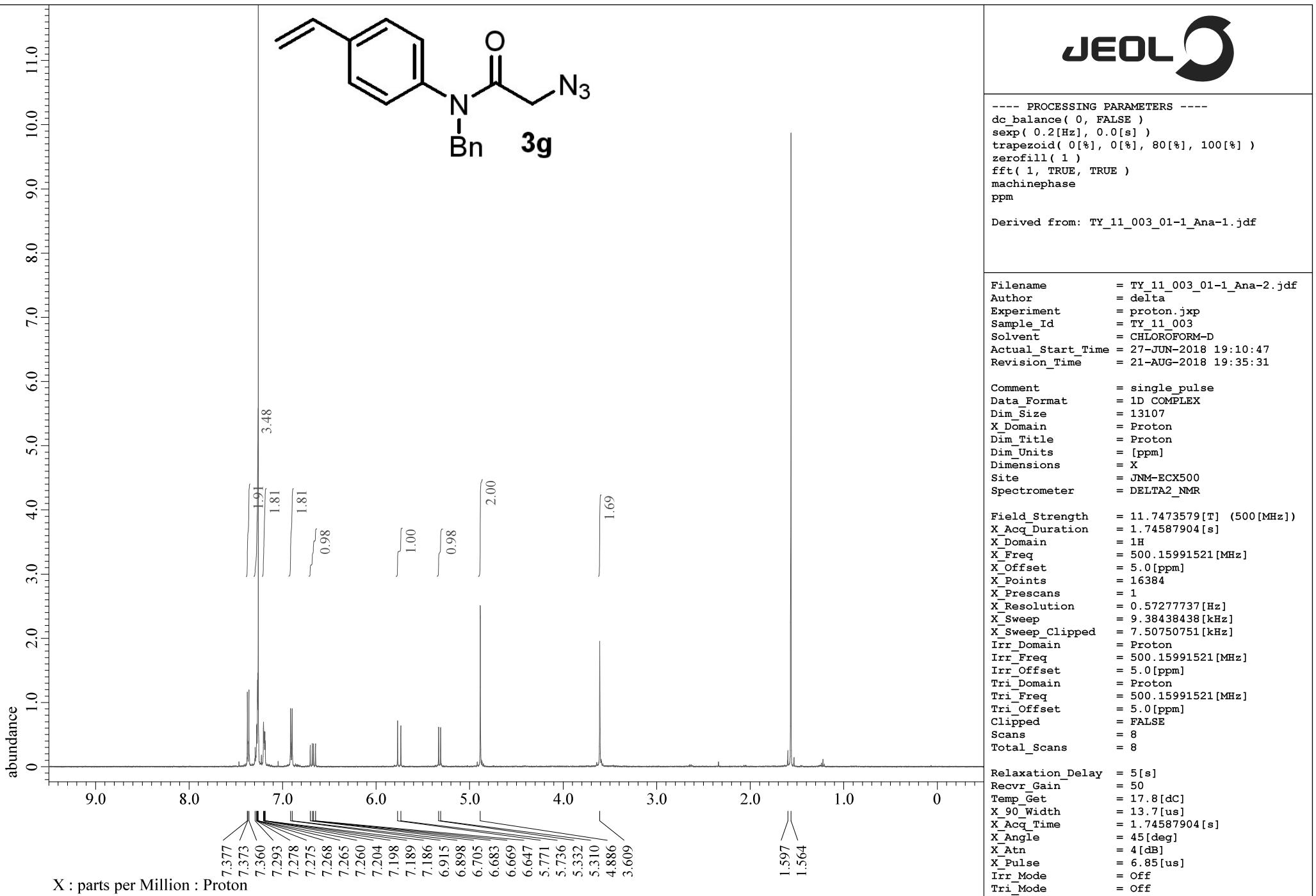
**JEOL**

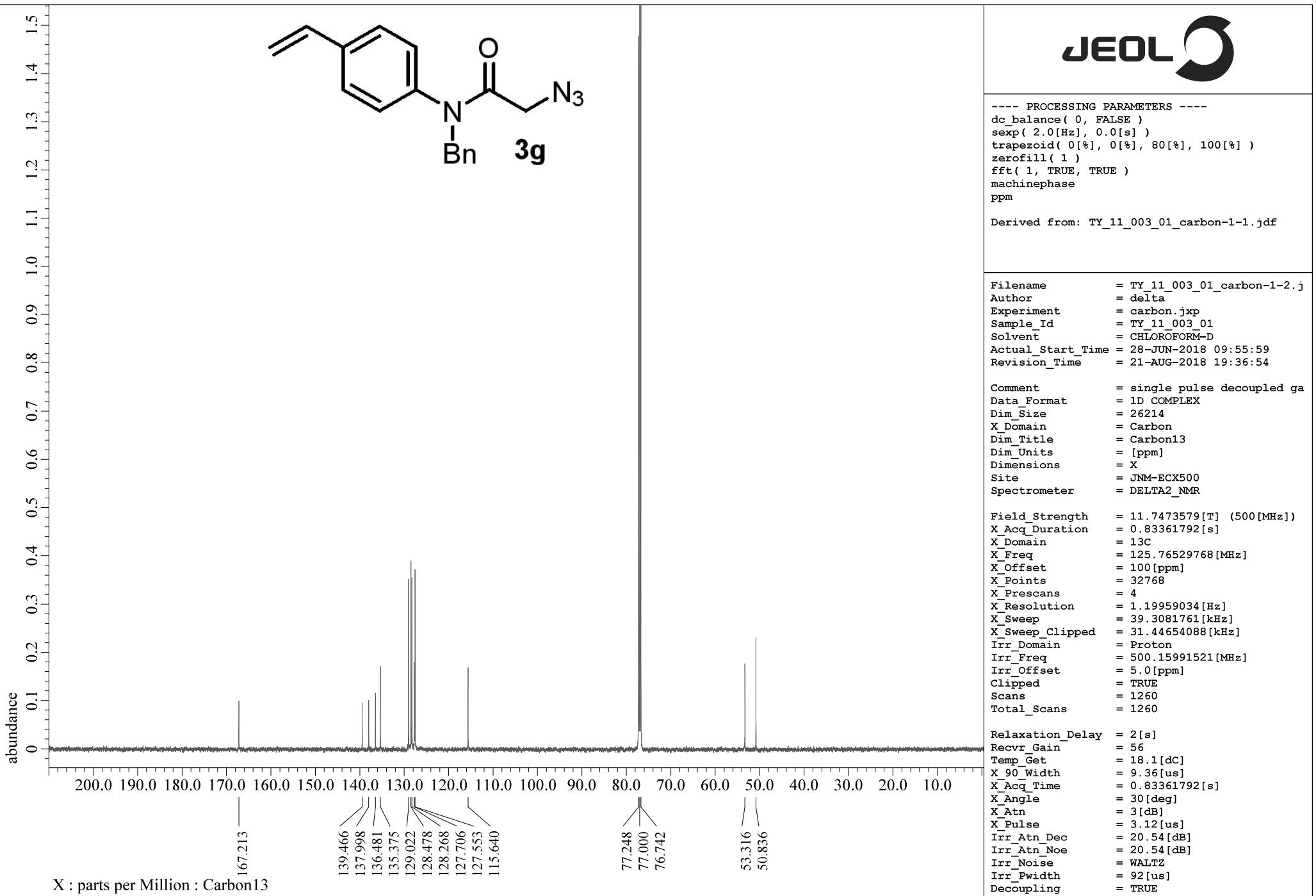
---- PROCESSING PARAMETERS ----  
dc\_balance( 0, FALSE )  
sexp( 2.0[Hz], 0.0[s] )  
trapezoid( 0[%], 0[%], 80[%], 100[%] )  
zerofill( 1 )  
fft( 1, TRUE, TRUE )  
machinephase  
ppm  
Derived from: TY\_11\_013\_01\_carbon-1\_Ana-1.jdf

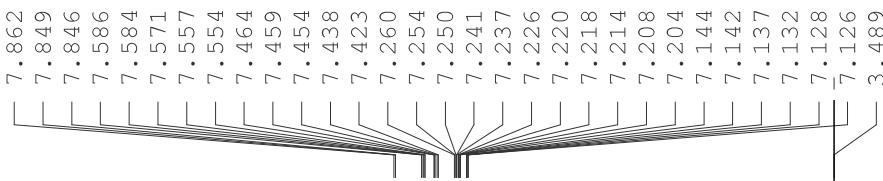
Filename = TY\_11\_013\_01\_carbon-1\_Ana  
Author = delta  
Experiment = carbon.jxp  
Sample\_Id = TY\_11\_013\_01  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 4-JUL-2018 10:00:45  
Revision\_Time = 21-AUG-2018 19:29:11  
Comment = single pulse decoupled ga  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
X\_Domain = Carbon  
Dim\_Title = Carbon13  
Dim\_Units = [ppm]  
Dimensions = X  
Site = JNM-ECX500  
Spectrometer = DELTA2\_NMR  
Field\_Strength = 11.7473579[T] (500[MHz])  
X\_Acq\_Duration = 0.83361792[s]  
X\_Domain = 13C  
X\_Freq = 125.76529768[MHz]  
X\_Offset = 100[ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 1.19959034[Hz]  
X\_Sweep = 39.3081761[kHz]  
X\_Sweep\_Clipped = 31.44654088[kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 500.15991521[MHz]  
Irr\_Offset = 5.0[ppm]  
Clipped = FALSE  
Scans = 816  
Total\_Scans = 816  
Relaxation\_Delay = 2[s]  
Recv\_Gain = 58  
Temp\_Get = 17.9[dC]  
X\_90\_Width = 9.36[us]  
X\_Acq\_Time = 0.83361792[s]  
X\_Angle = 30[deg]  
X\_Atn = 3[dB]  
X\_Pulse = 3.12[us]  
Irr\_Atn\_Dec = 20.54[dB]  
Irr\_Atn\_Noe = 20.54[dB]  
Irr\_Noise = WALTZ  
Irr\_Pwidth = 92[us]  
Decoupling = TRUE











1.95  
1.17  
1.33  
1.3602

3.00

0.30

12.5

10.0

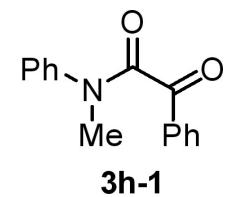
5.0

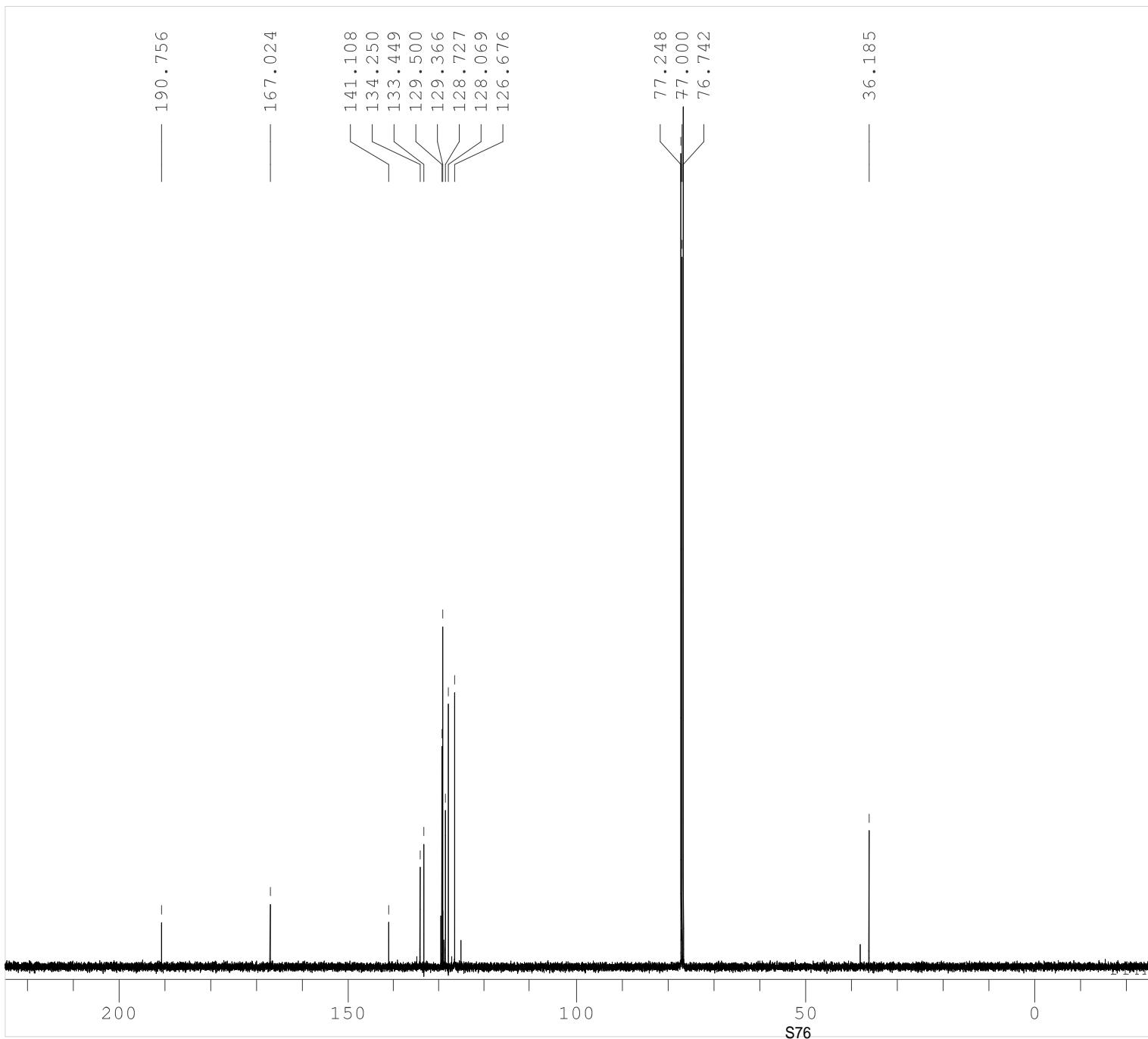
0.0

S75

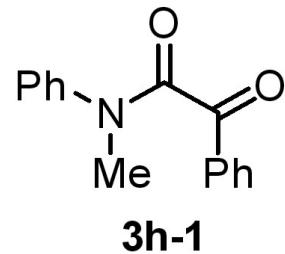
PPM

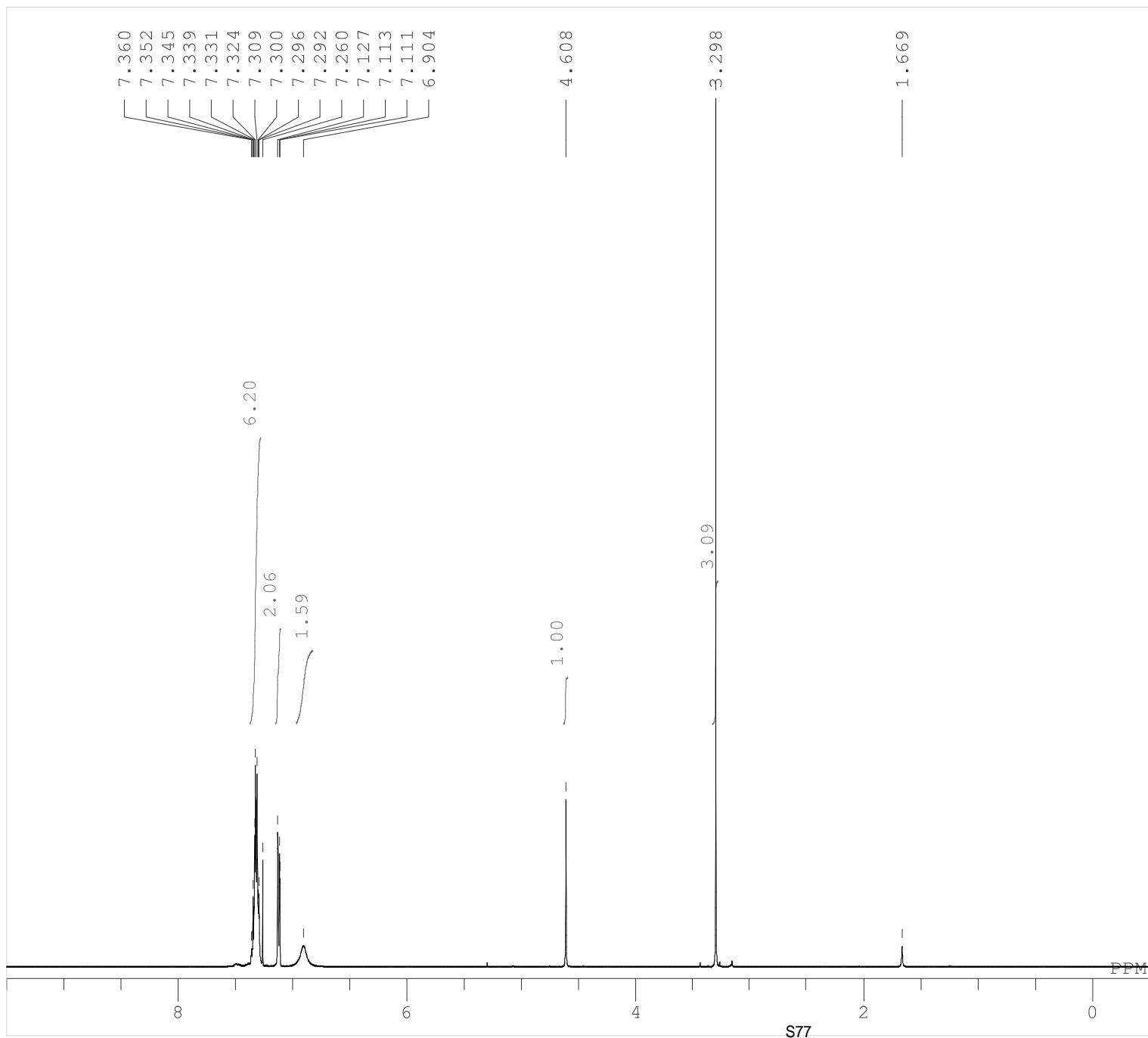
DFILE TY\_07\_097\_02\_proton-1-1.als  
 COMNT single\_pulse  
 DATIM 2016-10-13 19:17:49  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 17.7 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 38



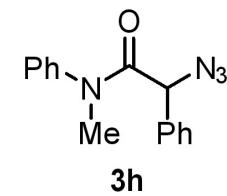


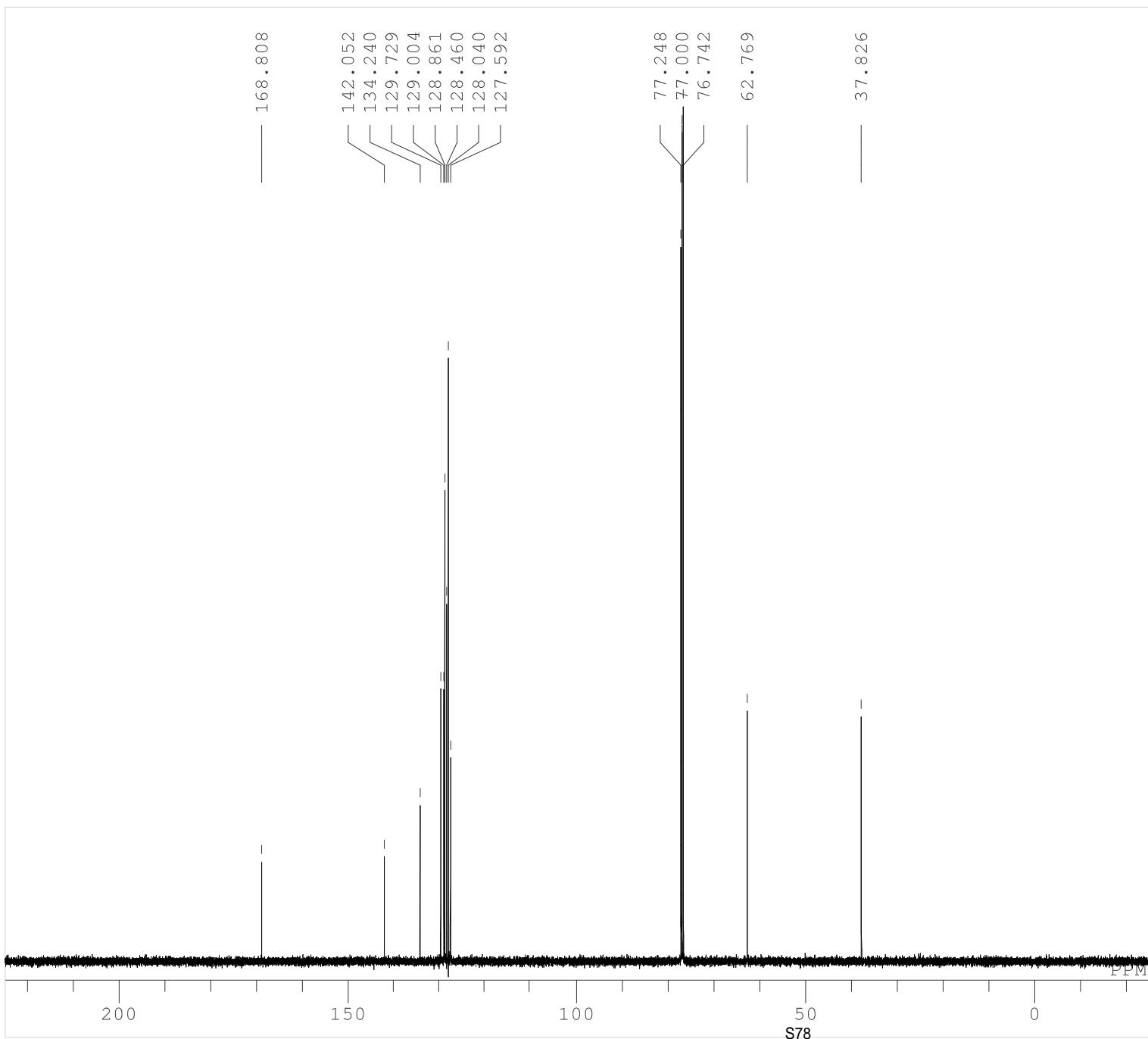
DFILE TY\_07\_097\_02\_carbon-1-1.als  
COMNT single pulse decoupled gated  
DATIM 2016-10-13 19:19:53  
OBNUC  $^{13}\text{C}$   
EXMOD carbon.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 kHz  
OBFIN 4.21 Hz  
POINT 26214  
FREQU 31446.54 Hz  
SCANS 620  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 17.4 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 56



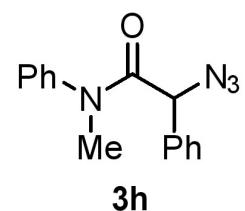


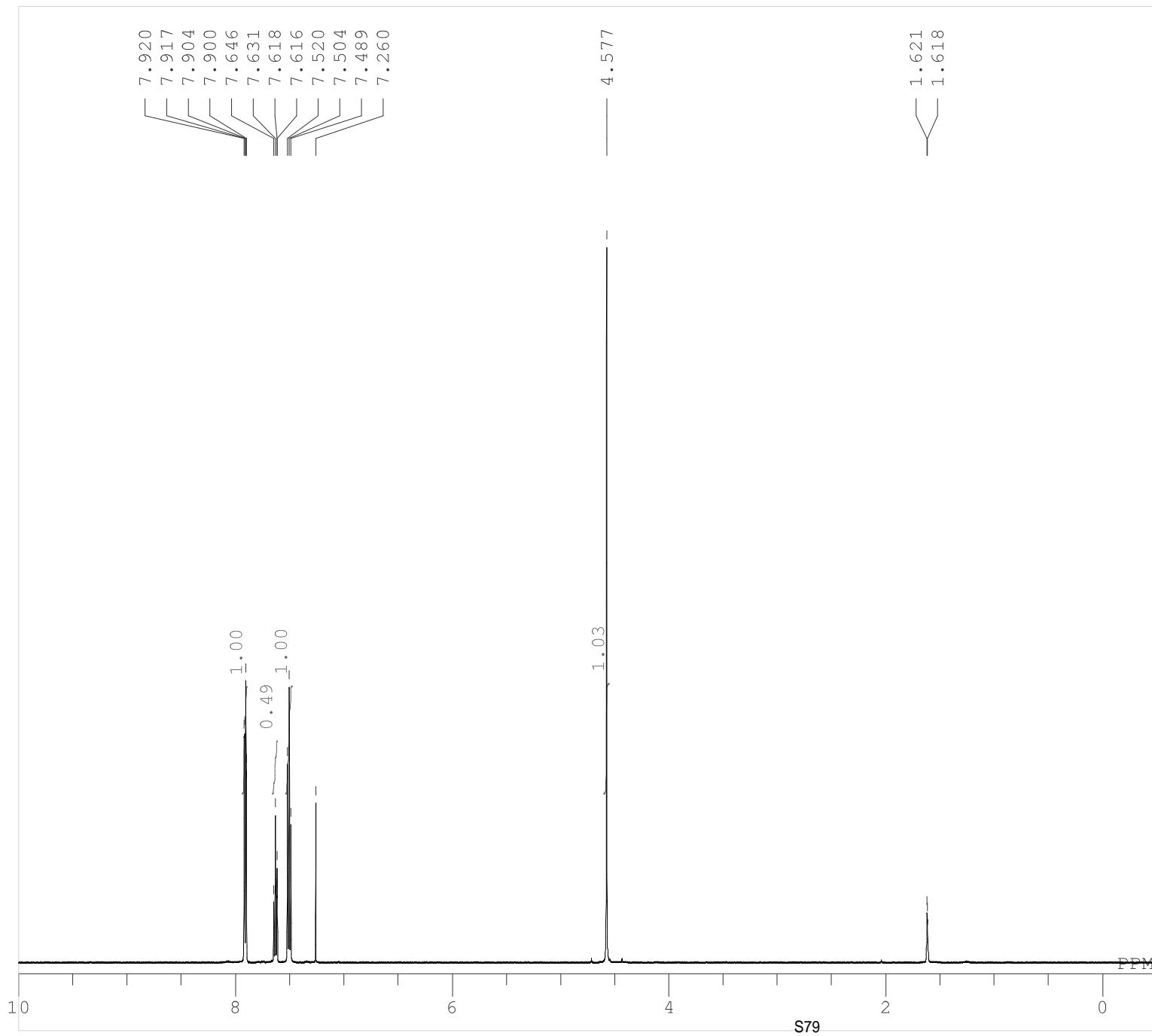
DFILE TY\_08\_026\_02\_proton-1-1.als  
 COMNT single\_pulse  
 DATIM 2016-12-09 20:16:58  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 14.5 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 36





DFILE TY\_08\_026\_02\_carbon-1-1.als  
 COMNT single pulse decoupled gated  
 DATIM 2016-12-09 20:21:10  
 OBNUC <sup>13</sup>C  
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 620  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 15.3 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60

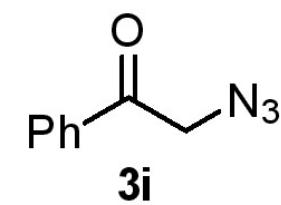


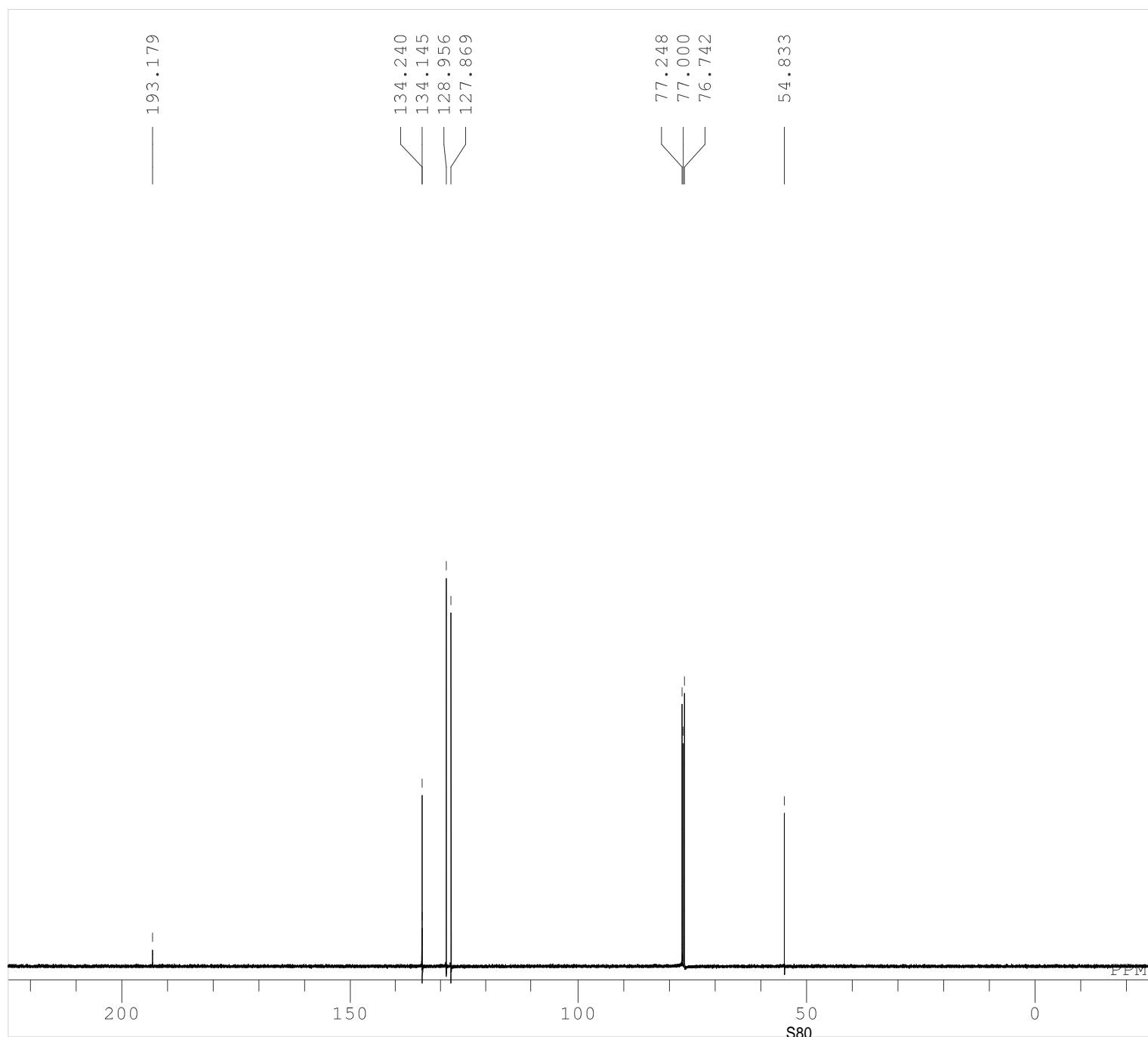


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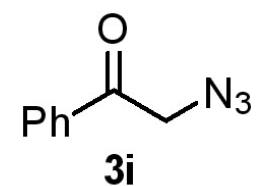
DFILE    TY_08_069_00_proton-1-1.als
COMNT    single_pulse
DATIM    2017-05-25 20:13:05
OBNUC    1H
EXMOD   proton.jxp
OBFRQ    500.16 MHz
OBSET    2.41 KHz
OBFIN    6.01 Hz
POINT    13107
FREQU   7507.51 Hz
SCANS    8
ACQTM    1.7459 sec
PD       5.0000 sec
PW1      6.85 usec
IRNUC    1H
CTEMP    13.5 c
SLVNT    CDCL3
EXREF    7.26 ppm
BF       0.10 Hz
RGAIN    40

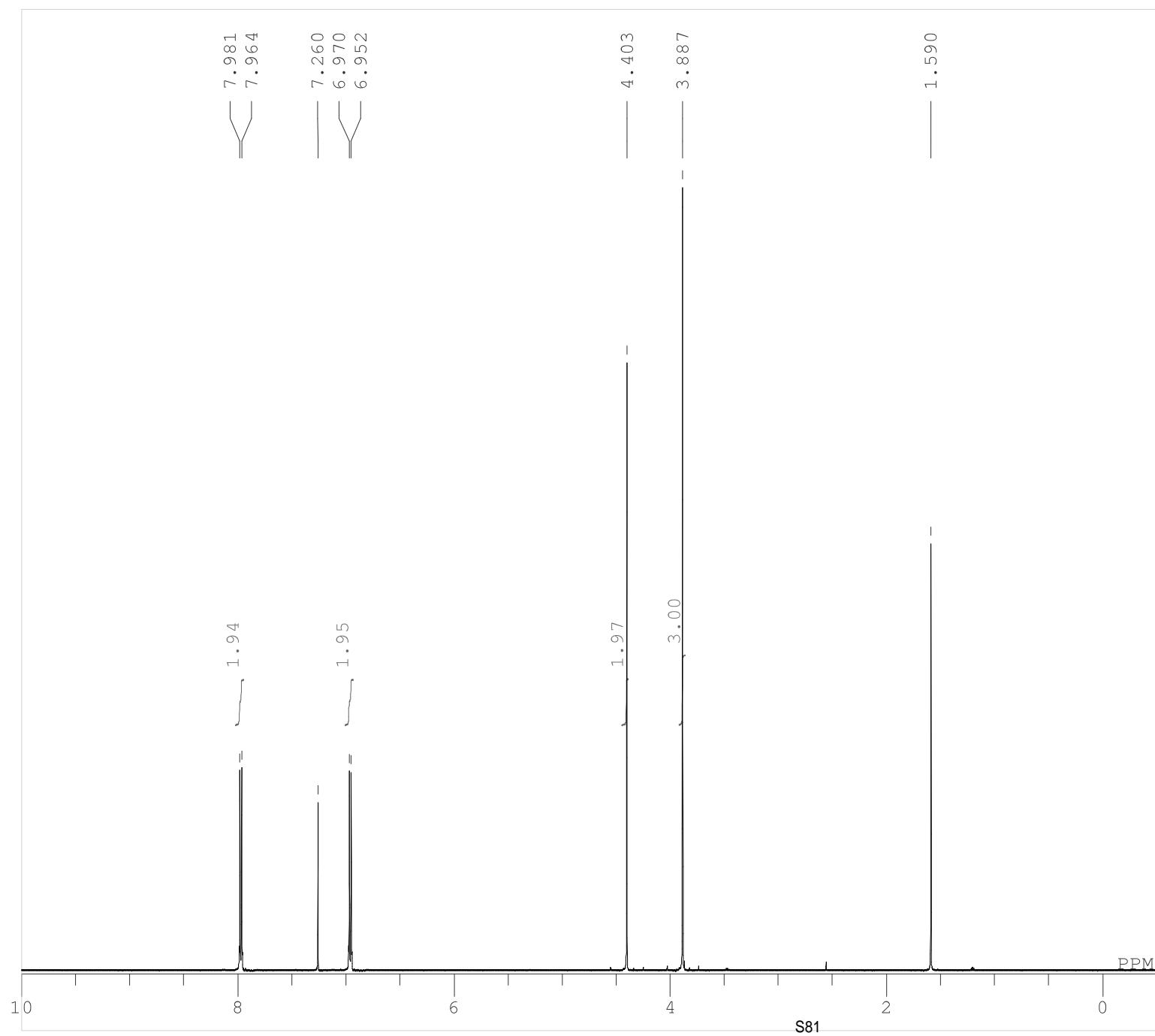
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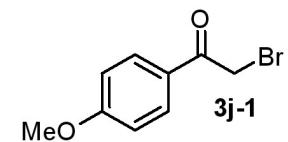


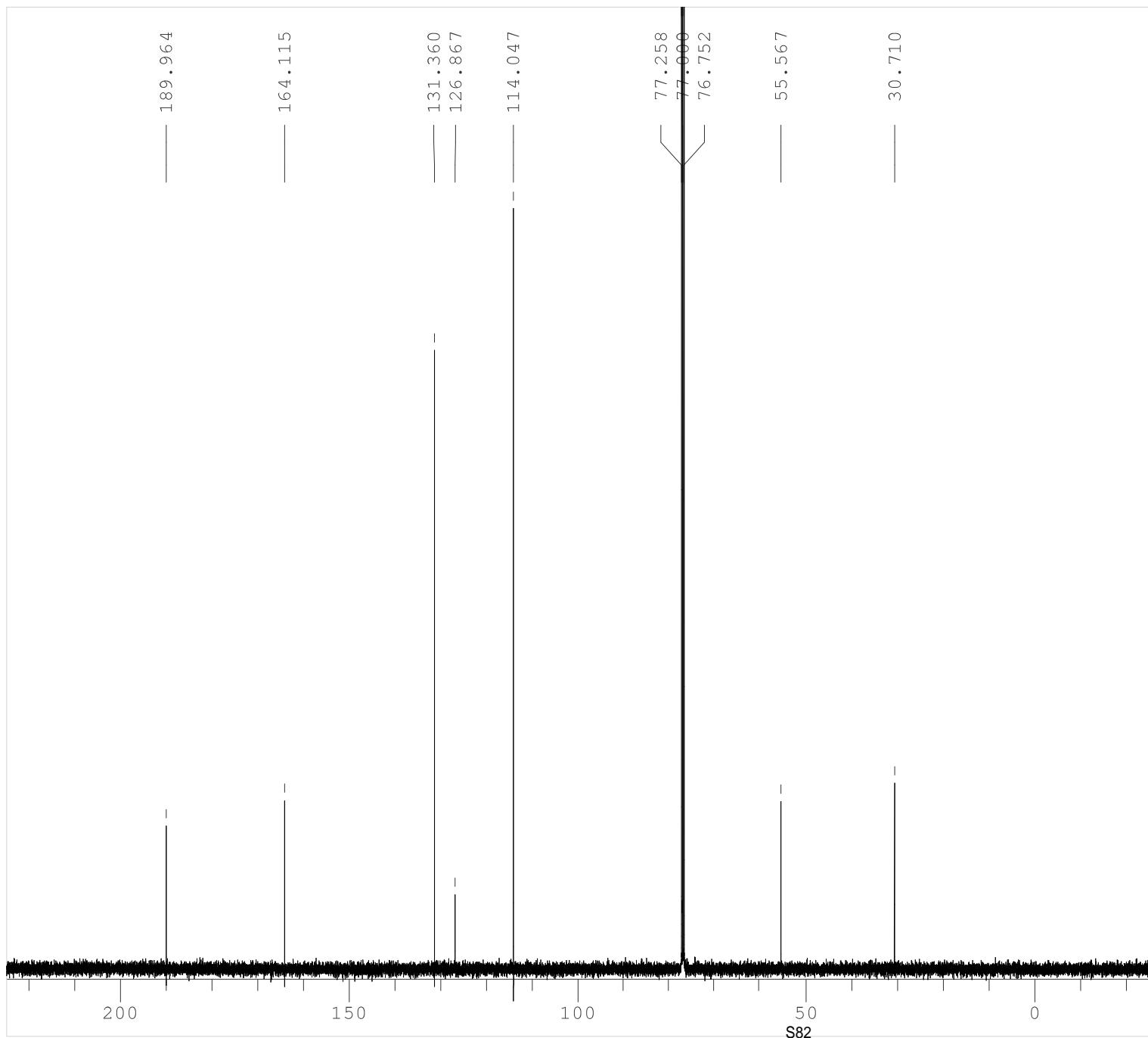
DFILE TY\_08\_069\_00\_carbn-1-1.als  
COMNT single pulse decoupled gated  
DATIM 2017-05-25 20:15:17  
OBNUC <sup>13</sup>C  
EXMOD carbn.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 kHz  
OBFIN 4.21 Hz  
POINT 26214  
FREQU 31446.54 Hz  
SCANS 840  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 14.0 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 60



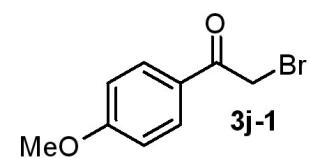


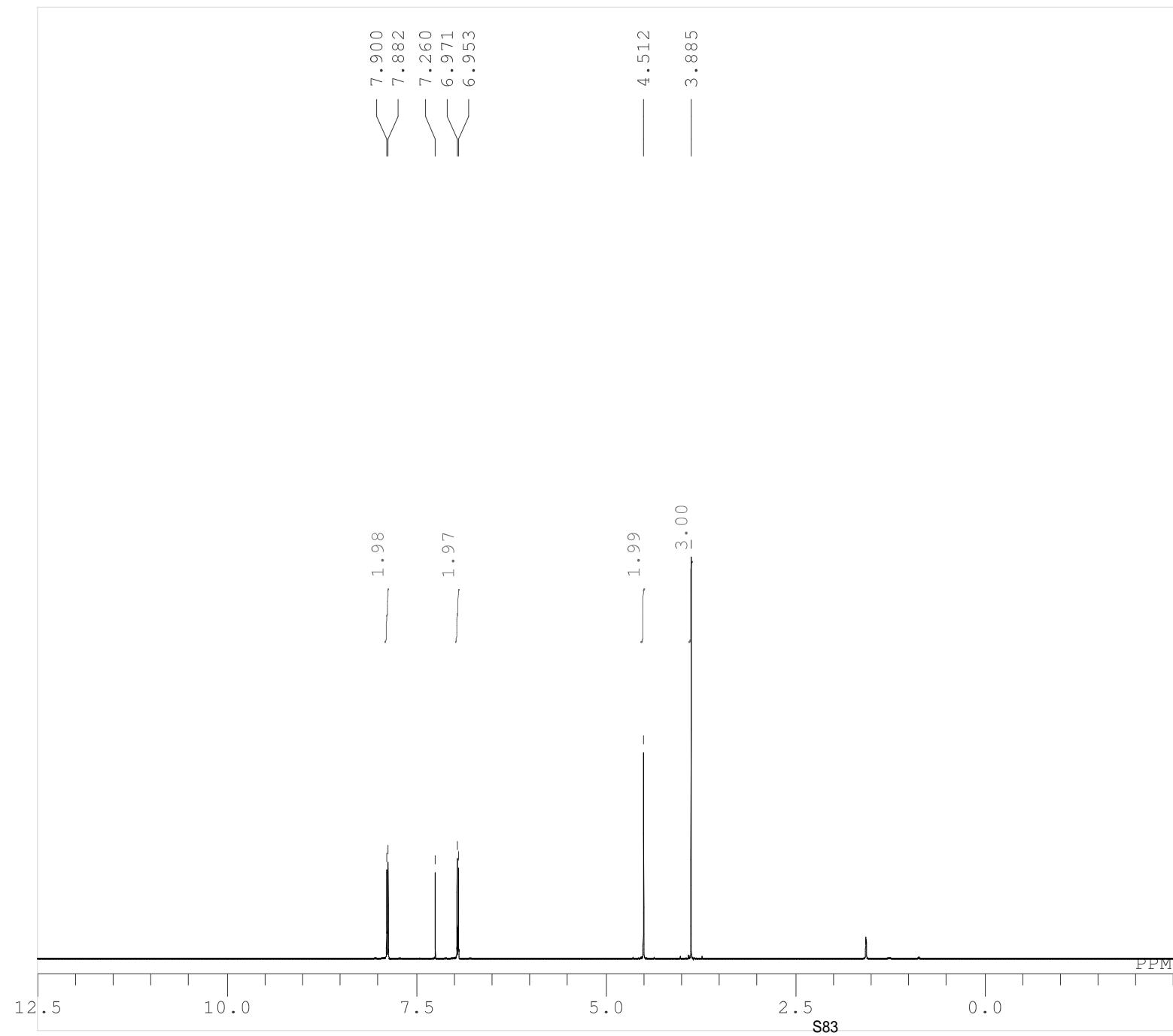
DFILE TY\_09\_020\_01\_proton-1-1.als  
COMNT single\_pulse  
DATIM 2017-07-14 16:17:33  
OBNUC 1H  
EXMOD proton.jxp  
OBFRQ 500.16 MHz  
OBSET 2.41 kHz  
OBFIN 6.01 Hz  
POINT 13107  
FREQU 7507.51 Hz  
SCANS 8  
ACQTM 1.7459 sec  
PD 5.0000 sec  
PW1 6.85 usec  
IRNUC 1H  
CTEMP 18.8 c  
SLVNT CDCL<sub>3</sub>  
EXREF 7.26 ppm  
BF 0.10 Hz  
RGAIN 44



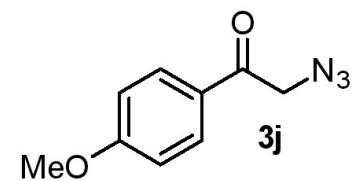


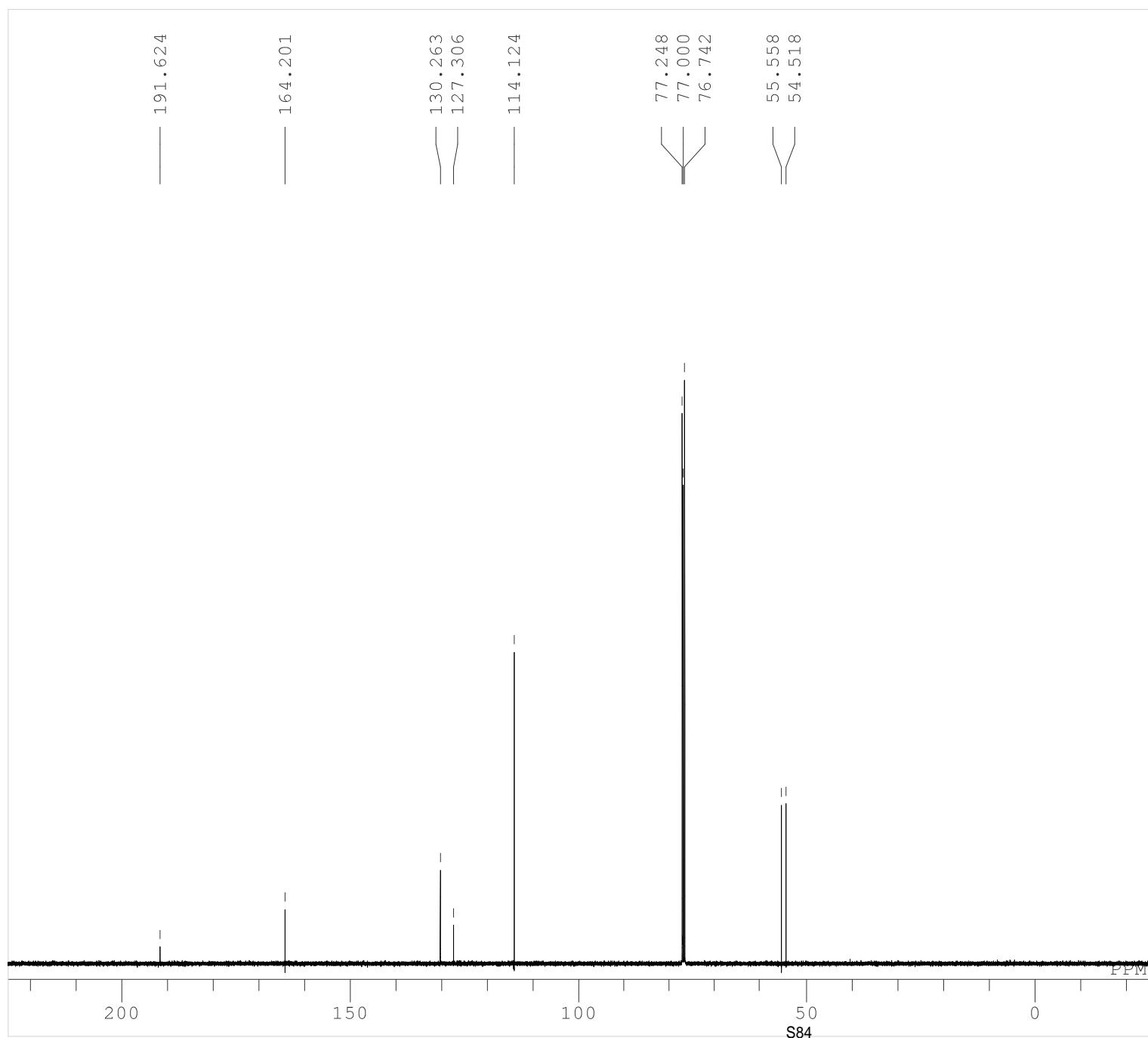
DFILE TY\_09\_020\_01\_carbn-1-1.als  
COMNT single pulse decoupled gated  
DATIM 2017-07-14 16:19:06  
OBNUC <sup>13</sup>C  
EXMOD carbn.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 kHz  
OBFIN 4.21 Hz  
POINT 26214  
FREQU 31446.54 Hz  
SCANS 1260  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 19.0 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 60



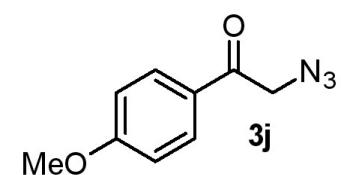


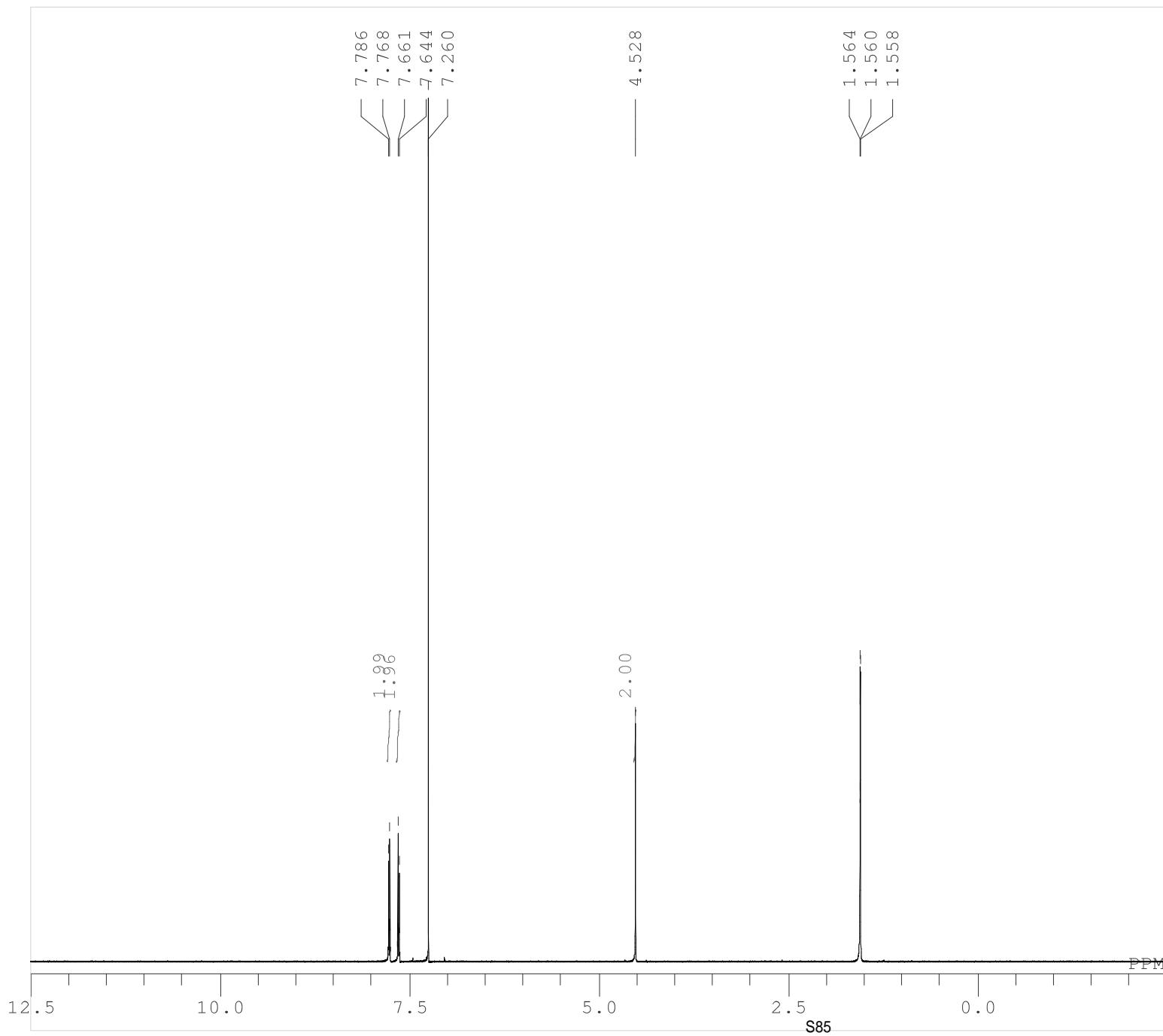
DFILE TY\_09\_022\_01\_proton-1-1.als  
 COMNT single\_pulse  
 DATIM 2017-07-19 09:54:13  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 17.7 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 46



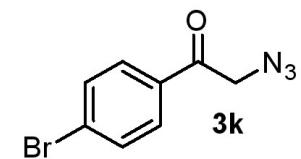


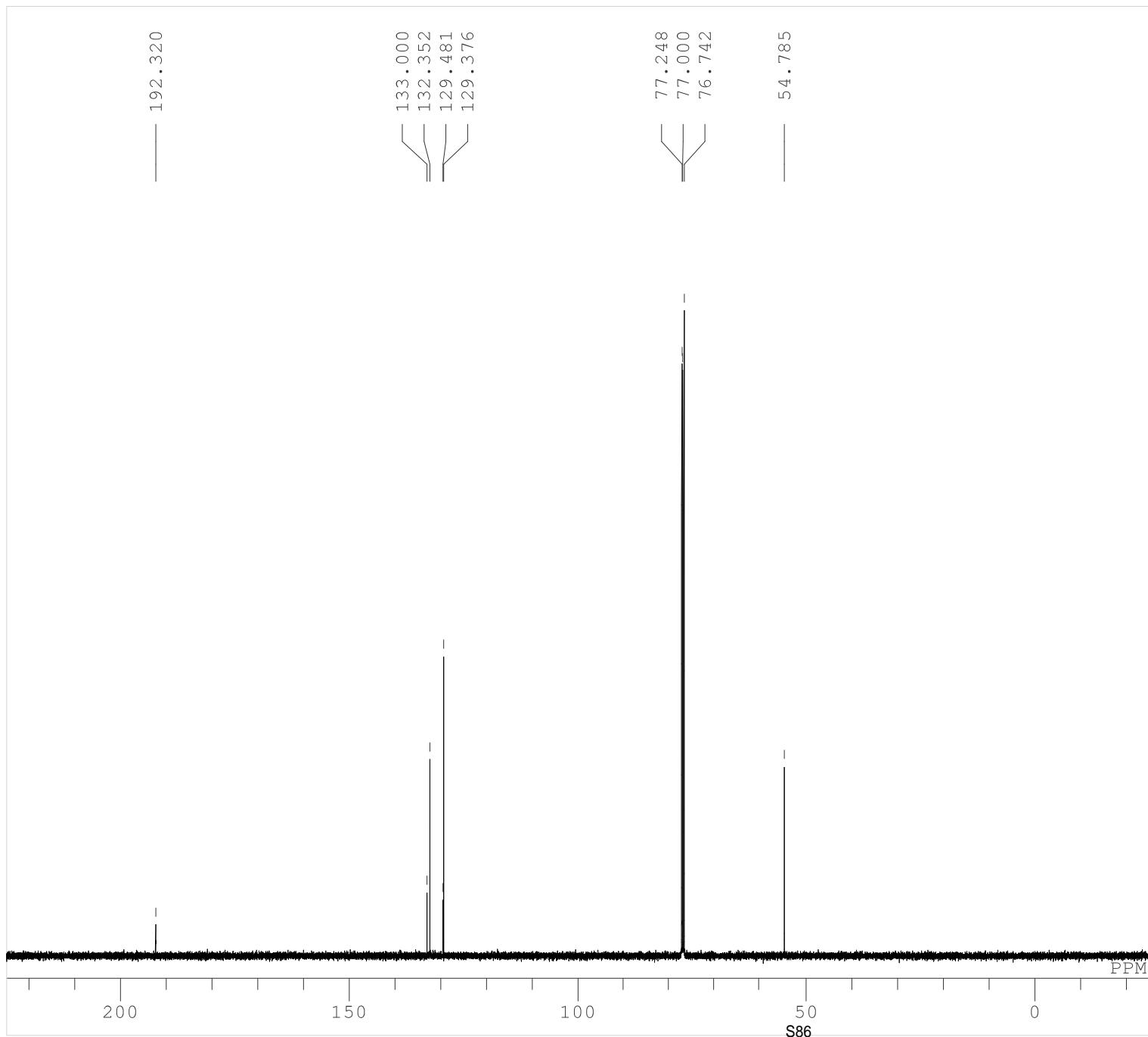
DFILE TY\_09\_022\_01\_carbn-1-1.als  
 COMNT single pulse decoupled gated  
 DATIM 2017-07-19 09:56:02  
 OBNUC <sup>13</sup>C  
 EXMOD carbn.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 1680  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 18.5 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60



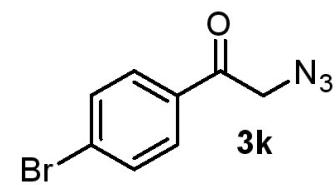


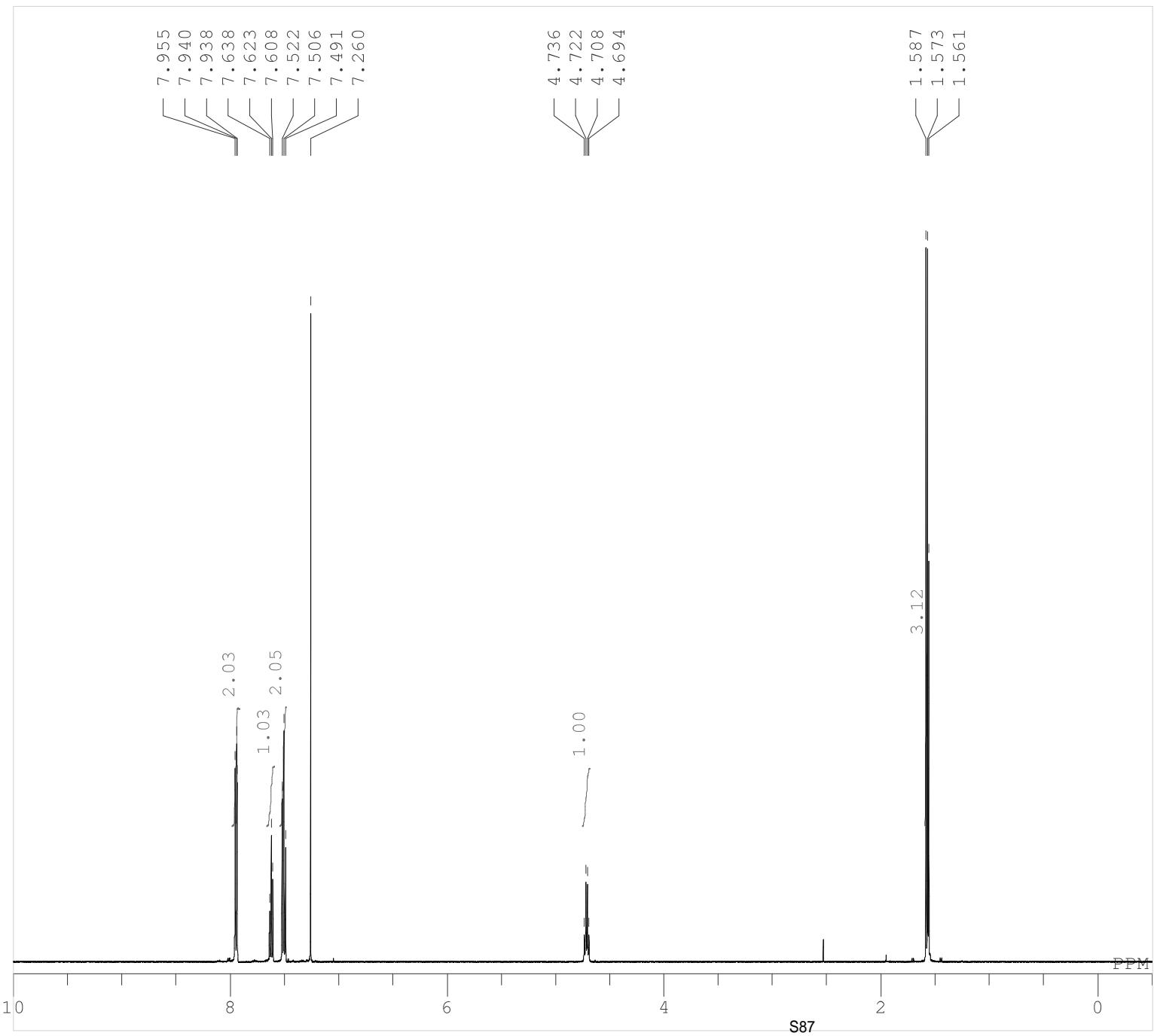
DFILE TY\_09\_048\_01-1-1.als  
 COMNT azid  
 DATIM 2017-08-01 16:34:23  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 19.0 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 50



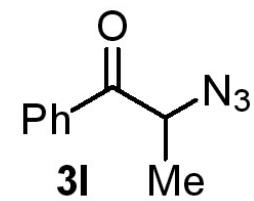


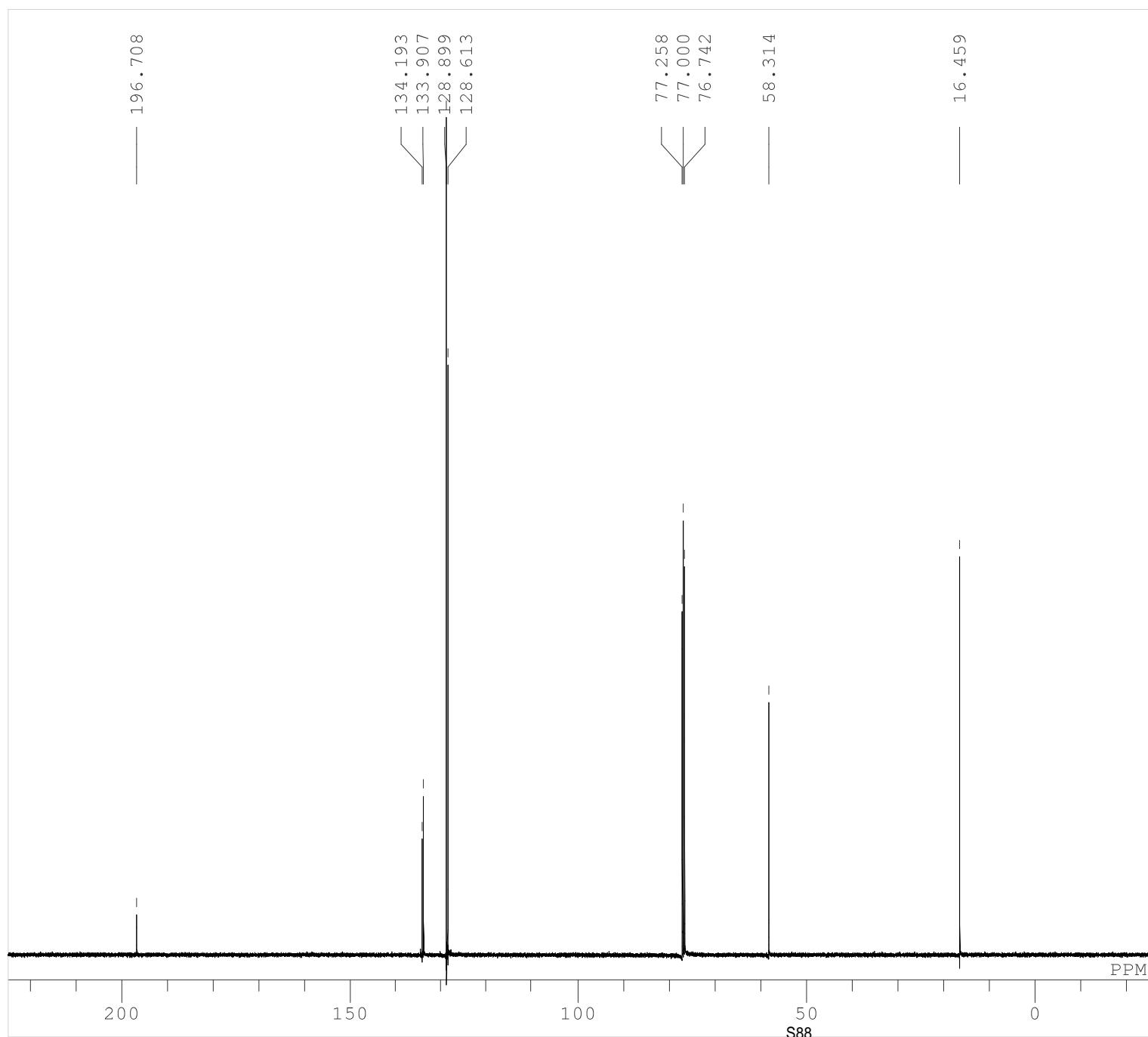
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COMNT single pulse decoupled gated  
DATIM 2017-08-01 17:44:57  
OBNUC <sup>13</sup>C  
EXMOD carbn.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 kHz  
OBFIN 4.21 Hz  
POINT 26214  
FREQU 31446.54 Hz  
SCANS 1360  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 19.0 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 60



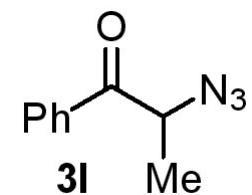


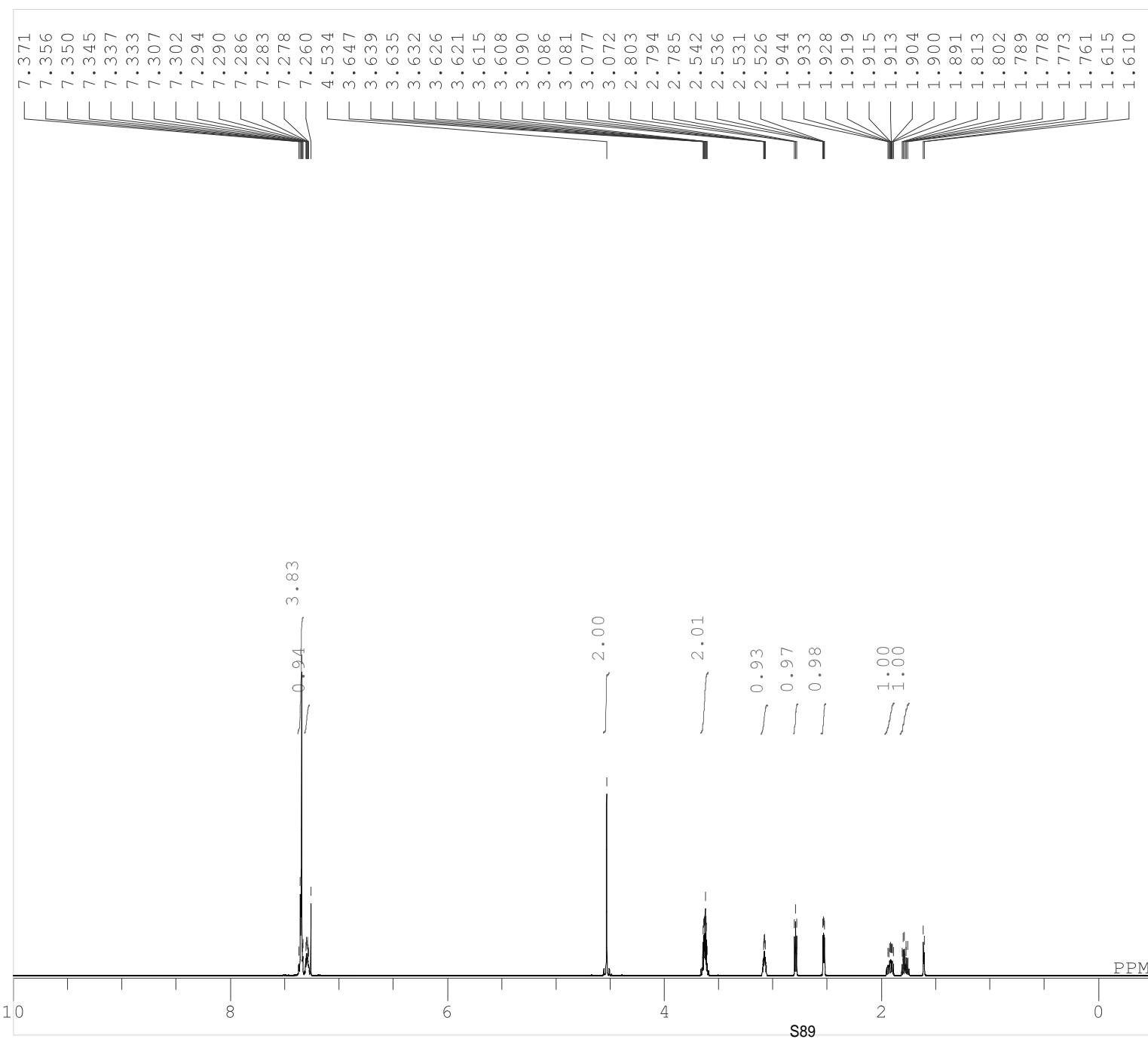
DFILE TY\_09\_033\_03-1-1.als  
 COMNT azid  
 DATIM 2017-07-20 13:55:45  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 18.5 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 48



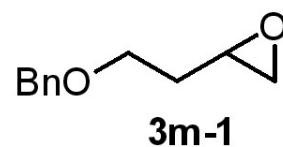


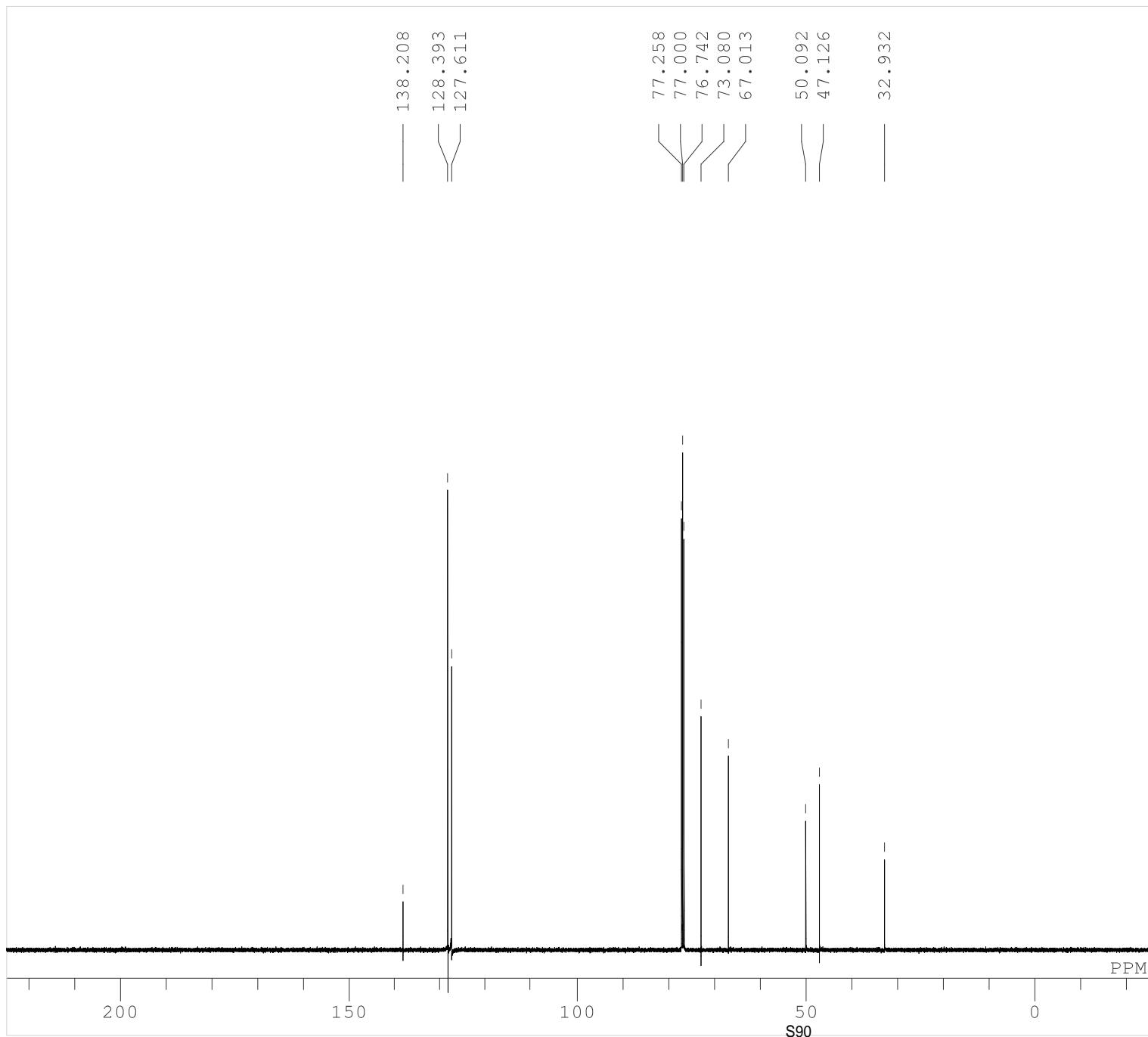
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DATIM 2017-07-20 14:16:28  
OBNUC  $^{13}\text{C}$   
EXMOD carbn.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 kHz  
OBFIN 4.21 Hz  
POINT 26214  
FREQU 31446.54 Hz  
SCANS 1260  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 19.2 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 60



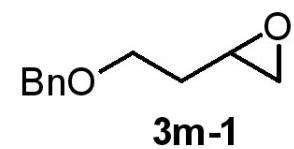


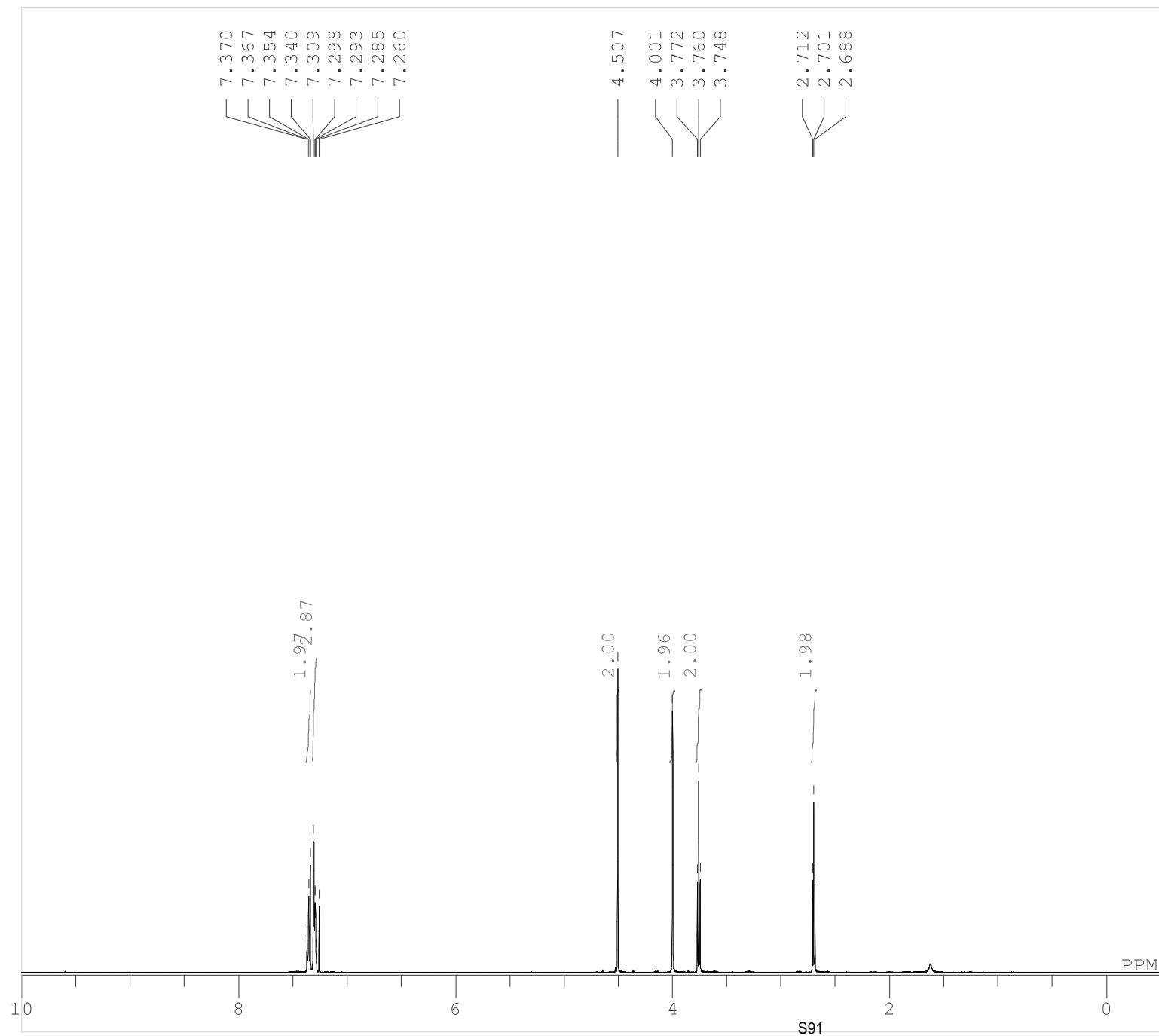
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 DATIM 2017-06-08 10:26:51  
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 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 16.3 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 38





DFILE TY\_08\_094\_01\_carbn-1-1.als  
COMNT single pulse decoupled gated  
DATIM 2017-06-08 10:29:07  
OBNUC <sup>13</sup>C  
EXMOD carbn.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 kHz  
OBFIN 4.21 Hz  
POINT 26214  
FREQU 31446.54 Hz  
SCANS 1260  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 16.6 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 60

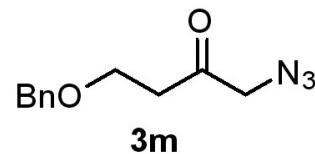


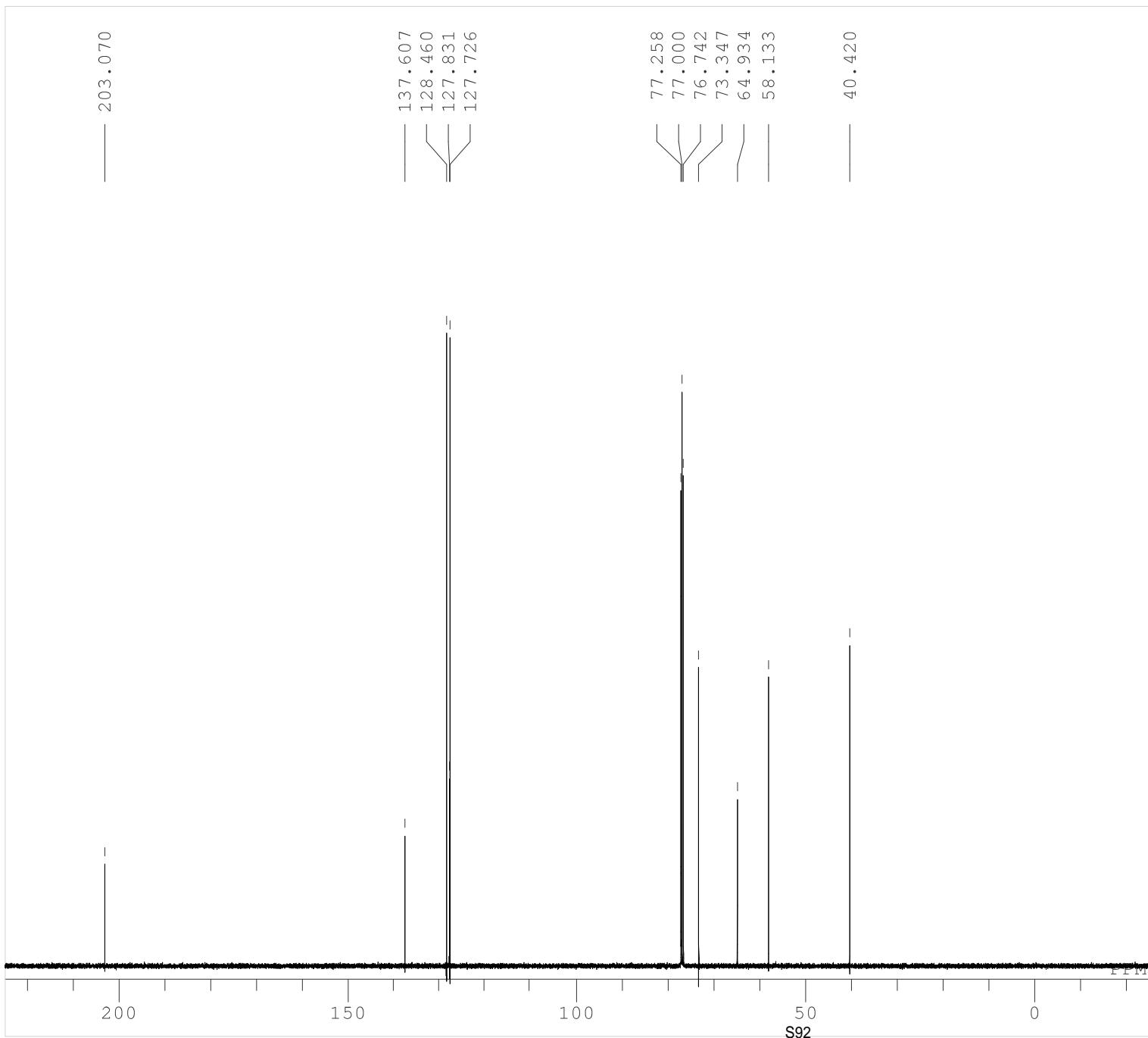


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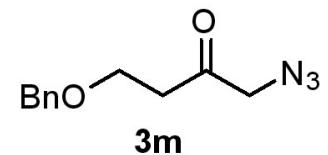
DFILE TY_08_110_01_proton-1-1.als
COMNT single_pulse
DATIM 2017-06-16 10:02:48
OBNUC 1H
EXMOD proton.jxp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 13107
FREQU 7507.51 Hz
SCANS 8
ACQTM 1.7459 sec
PD 5.0000 sec
PW1 6.85 usec
IRNUC 1H
CTEMP 13.1 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.10 Hz
RGAIN 38

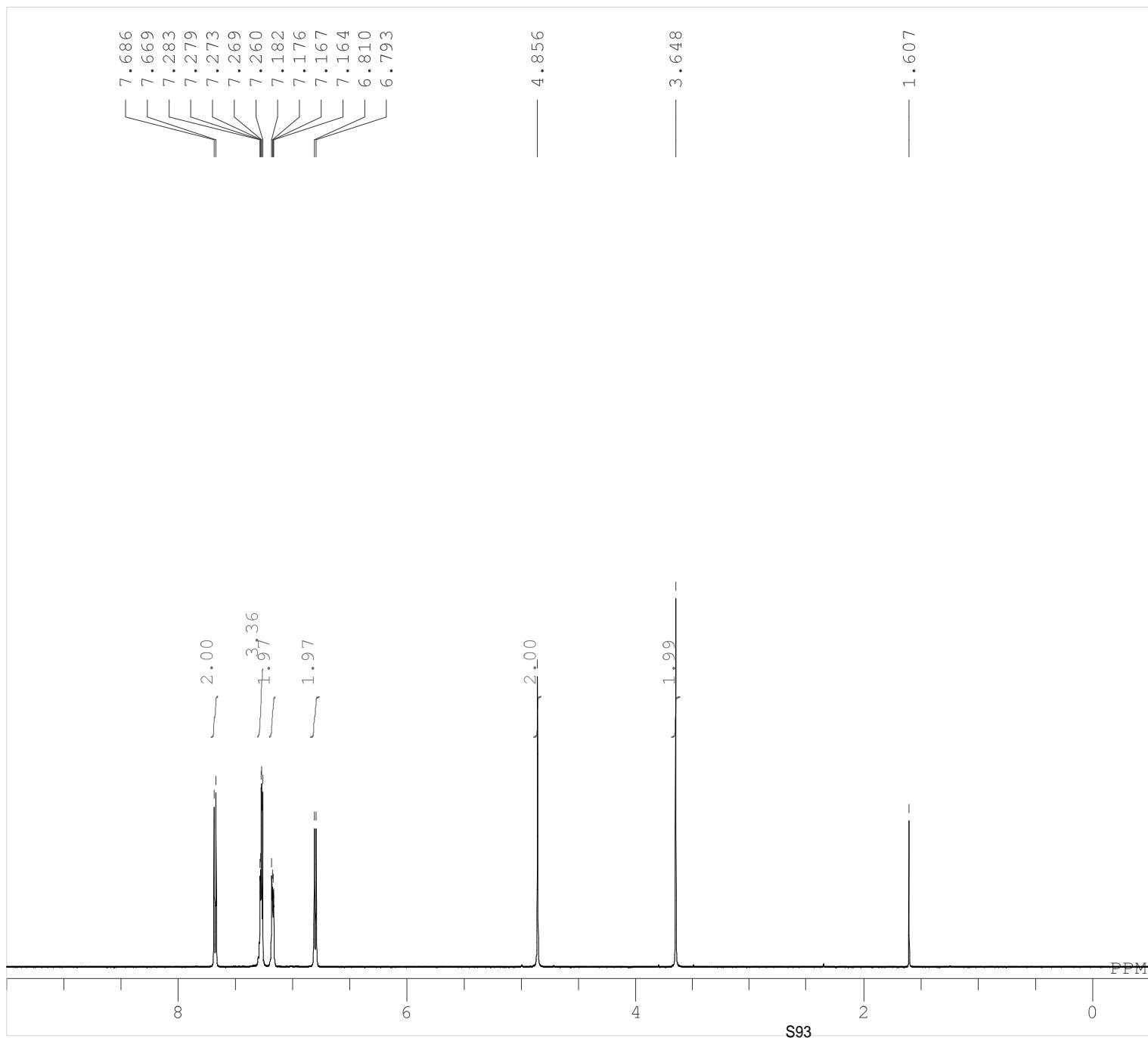
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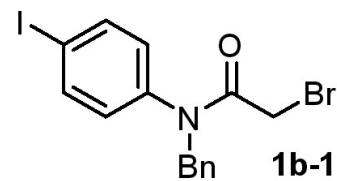


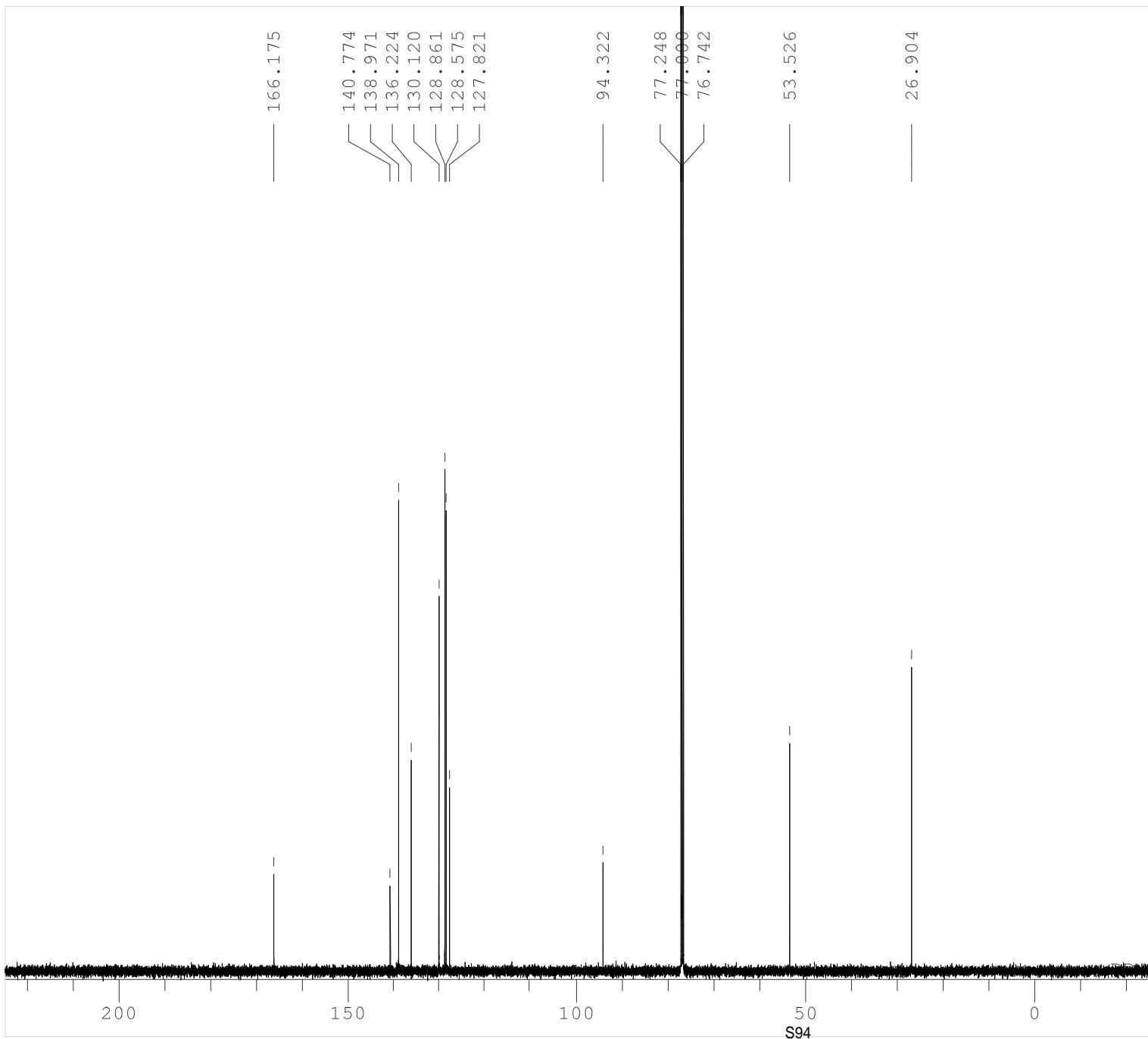
DFILE TY\_08\_110\_01\_carbn-1-1.als  
 COMNT single pulse decoupled gated  
 DATIM 2017-06-16 10:04:47  
 OBNUC <sup>13</sup>C  
 EXMOD carbn.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 1260  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC <sup>1</sup>H  
 CTEMP 13.8 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60



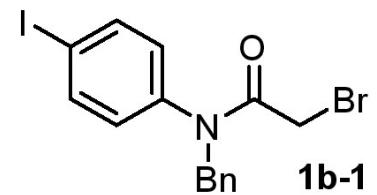


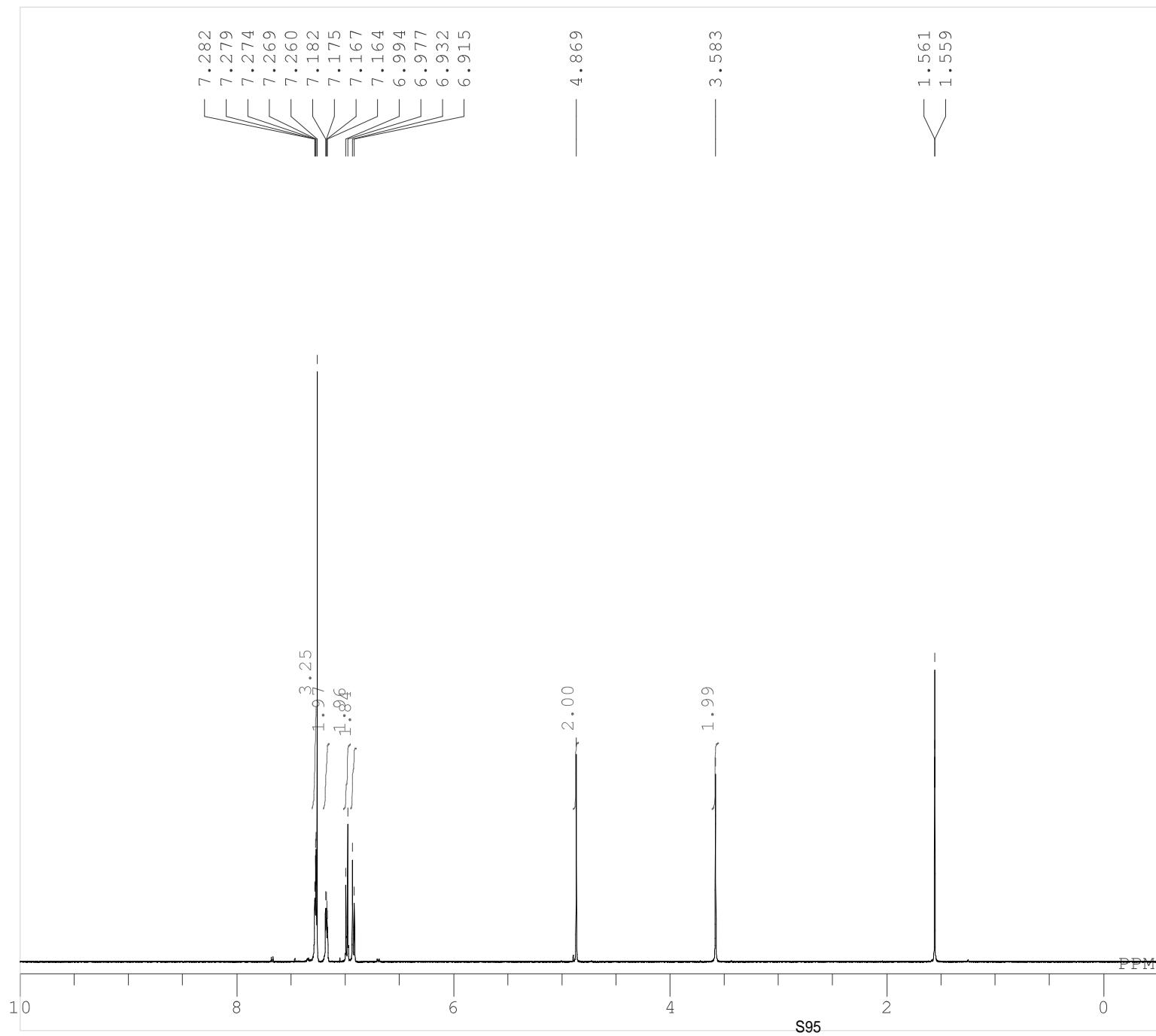
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 DATIM 2017-07-26 09:56:09  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 17.9 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 40



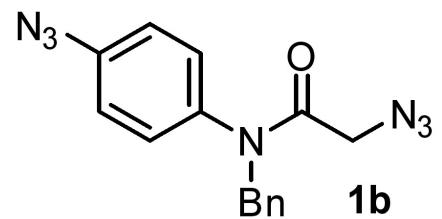


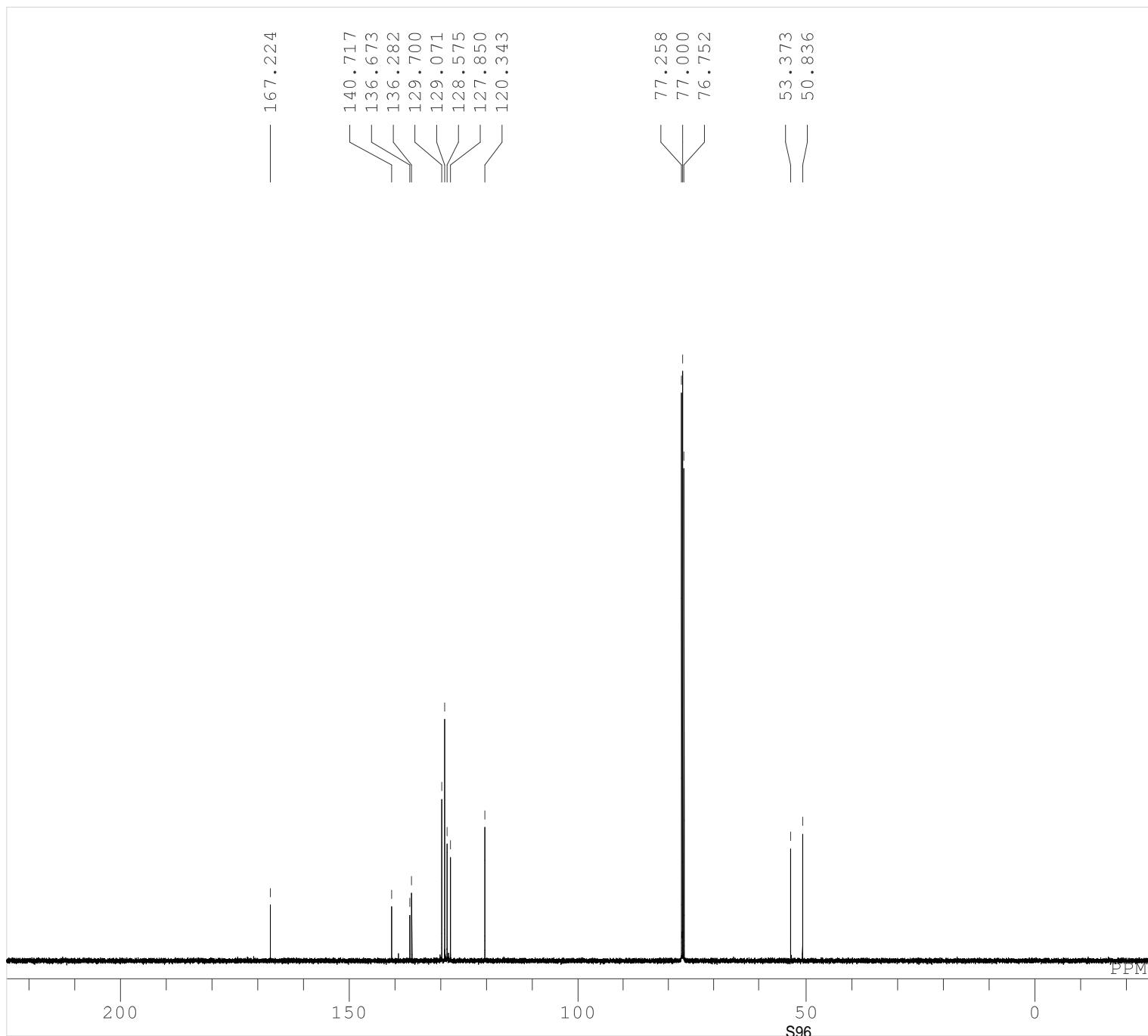
DFILE TY\_09\_041\_01\_carbn-1-1.als  
COMNT single pulse decoupled gated  
DATIM 2017-07-26 10:01:44  
OBNUC <sup>13</sup>C  
EXMOD carbn.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 kHz  
OBFIN 4.21 Hz  
POINT 26214  
FREQU 31446.54 Hz  
SCANS 1680  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 18.9 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 60



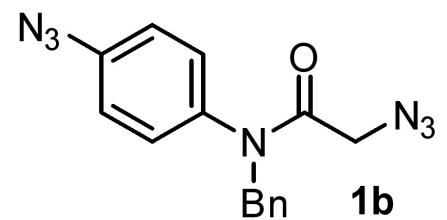


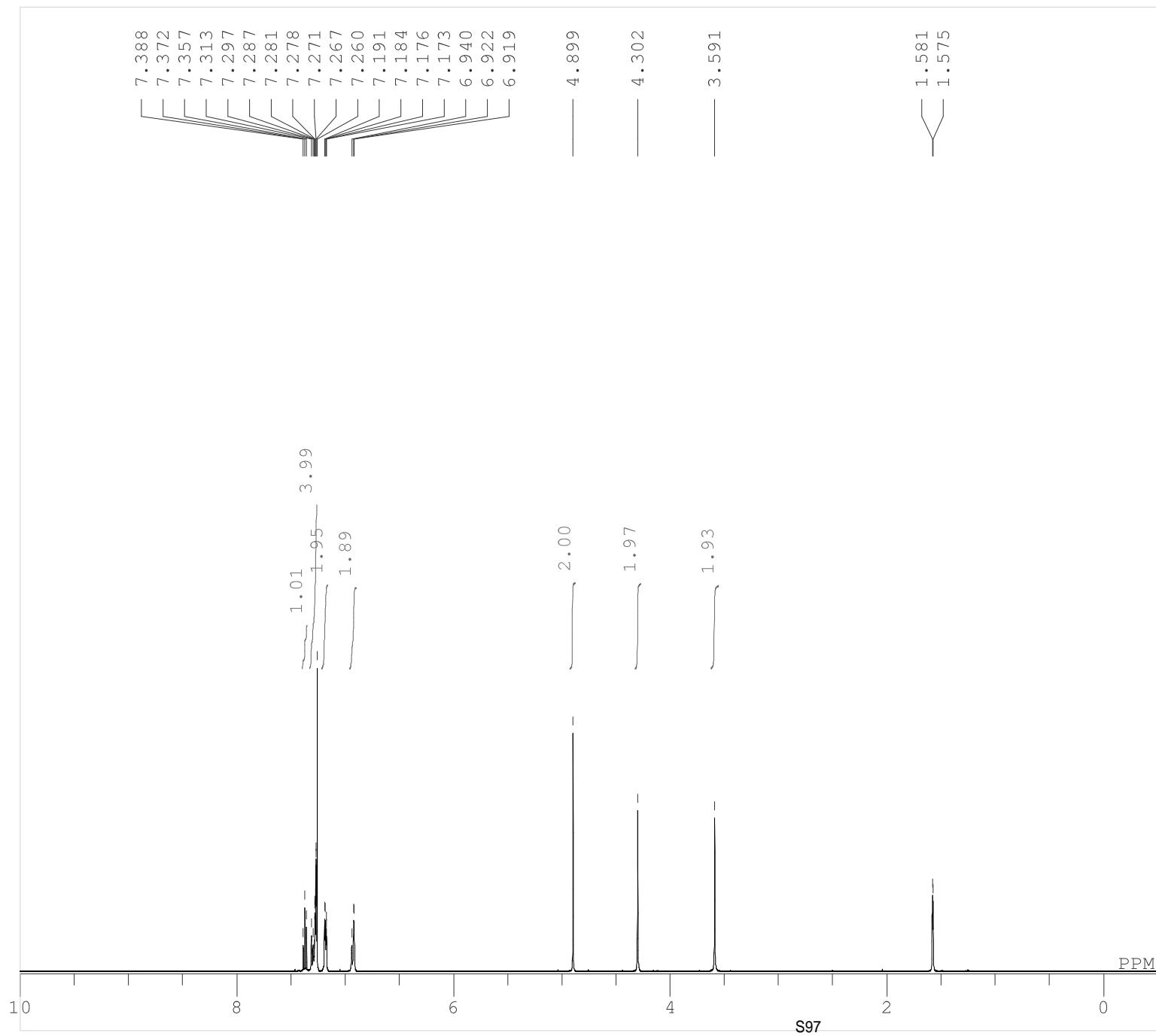
DFILE TY\_09\_042\_01-1-1.als  
 COMNT dazid  
 DATIM 2017-07-26 12:13:20  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 18.7 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 48



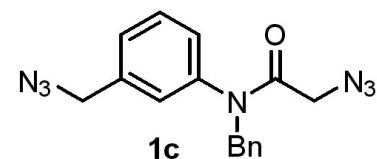


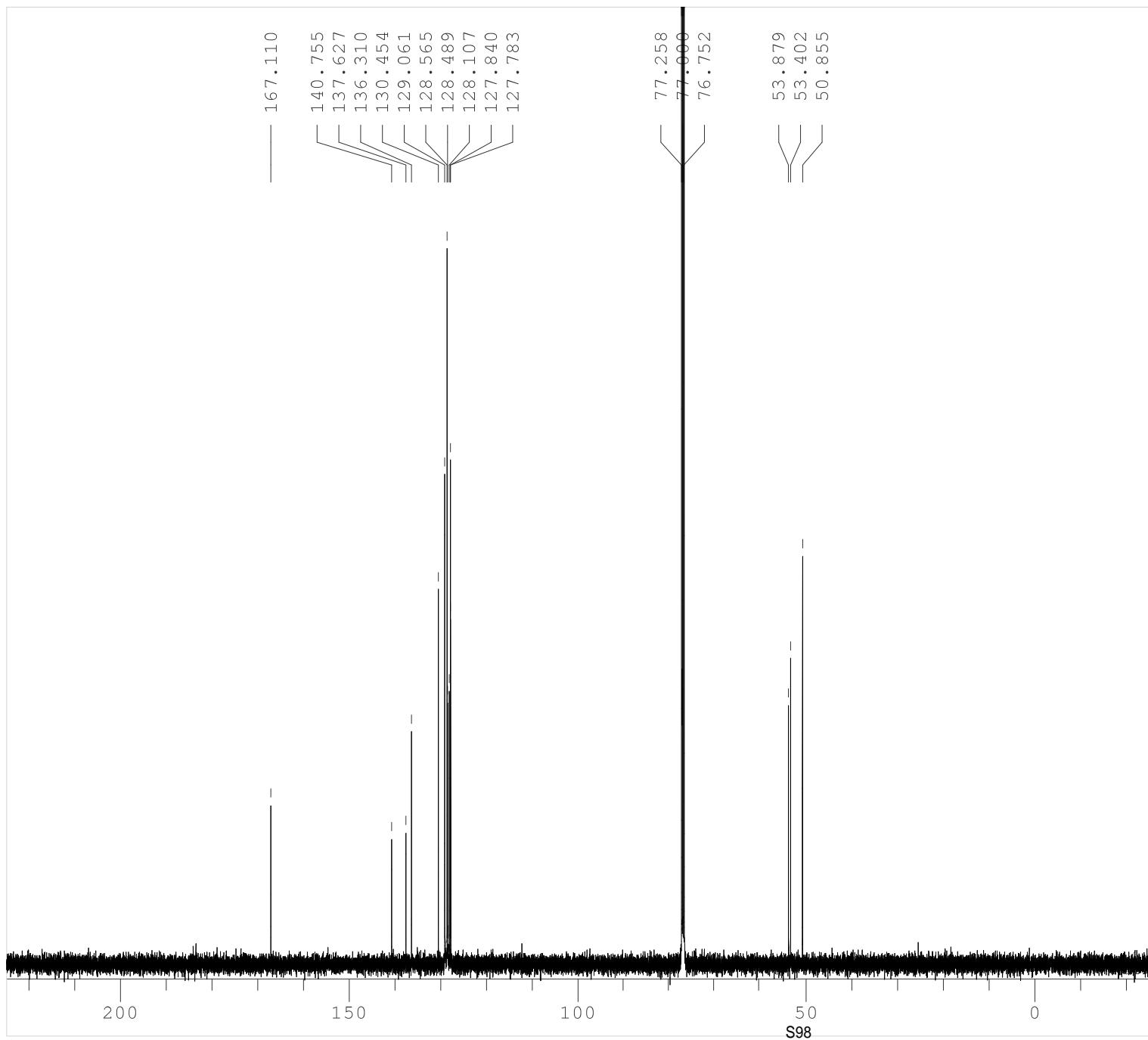
DFILE TY\_09\_042\_01\_carbon-1-1.als  
 COMNT single pulse decoupled gated  
 DATIM 2017-07-27 09:55:36  
 OBNUC <sup>13</sup>C  
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 1680  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 19.0 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60



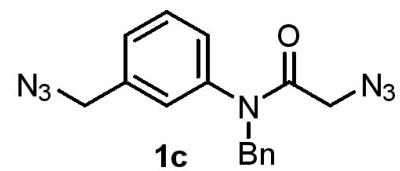


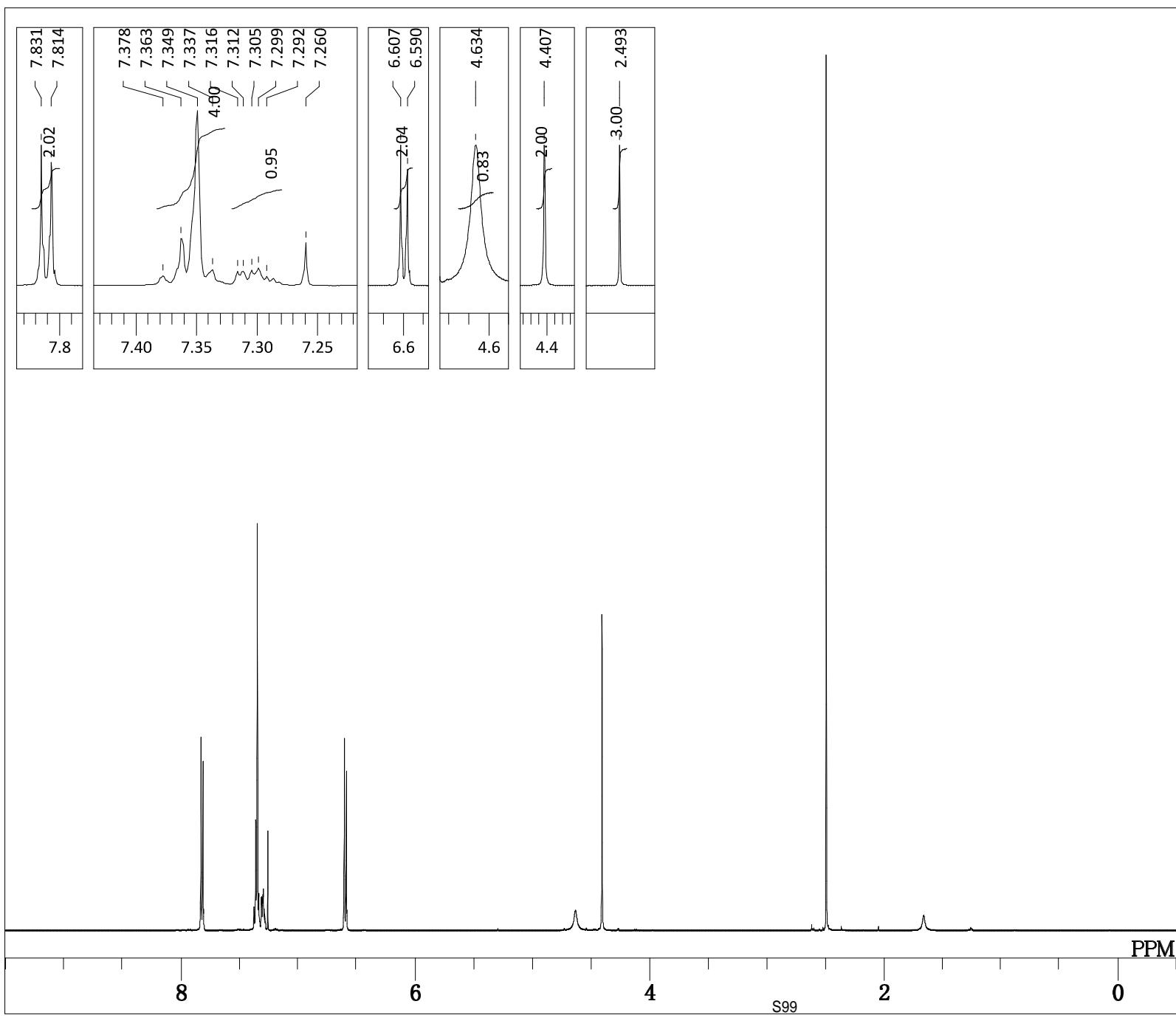
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 DATIM 2017-10-17 23:17:24  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 18.4 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 44



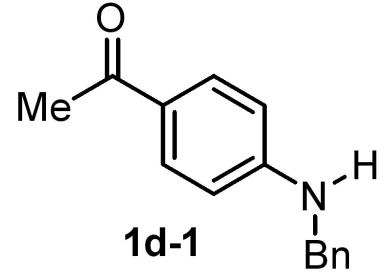


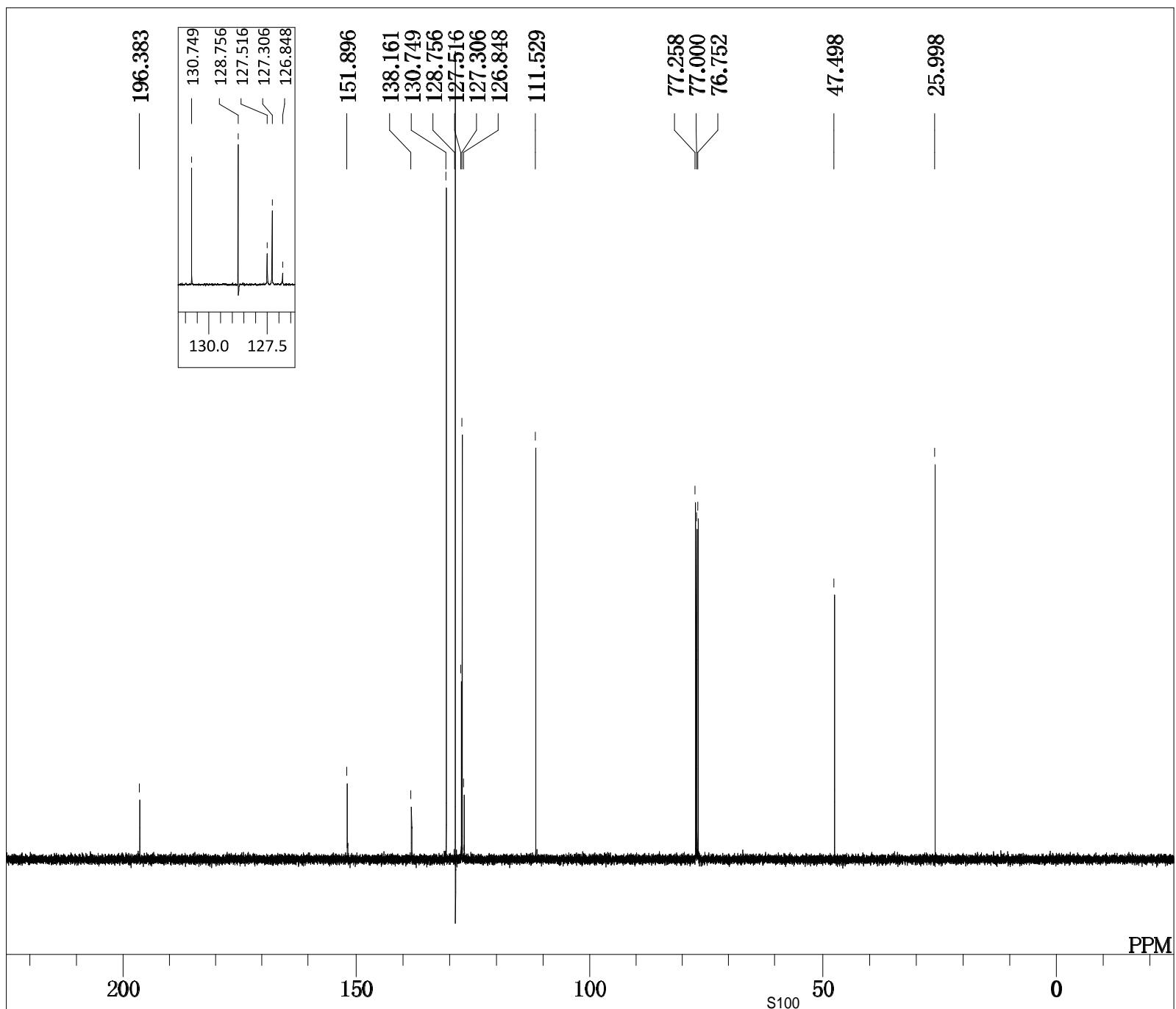
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COMNT single pulse decoupled gated  
DATIM 2017-10-17 23:19:05  
OBNUC <sup>13</sup>C  
EXMOD carbn.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 kHz  
OBFIN 4.21 Hz  
POINT 26214  
FREQU 31446.54 Hz  
SCANS 8460  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 19.2 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 60



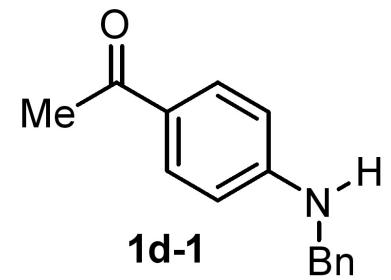


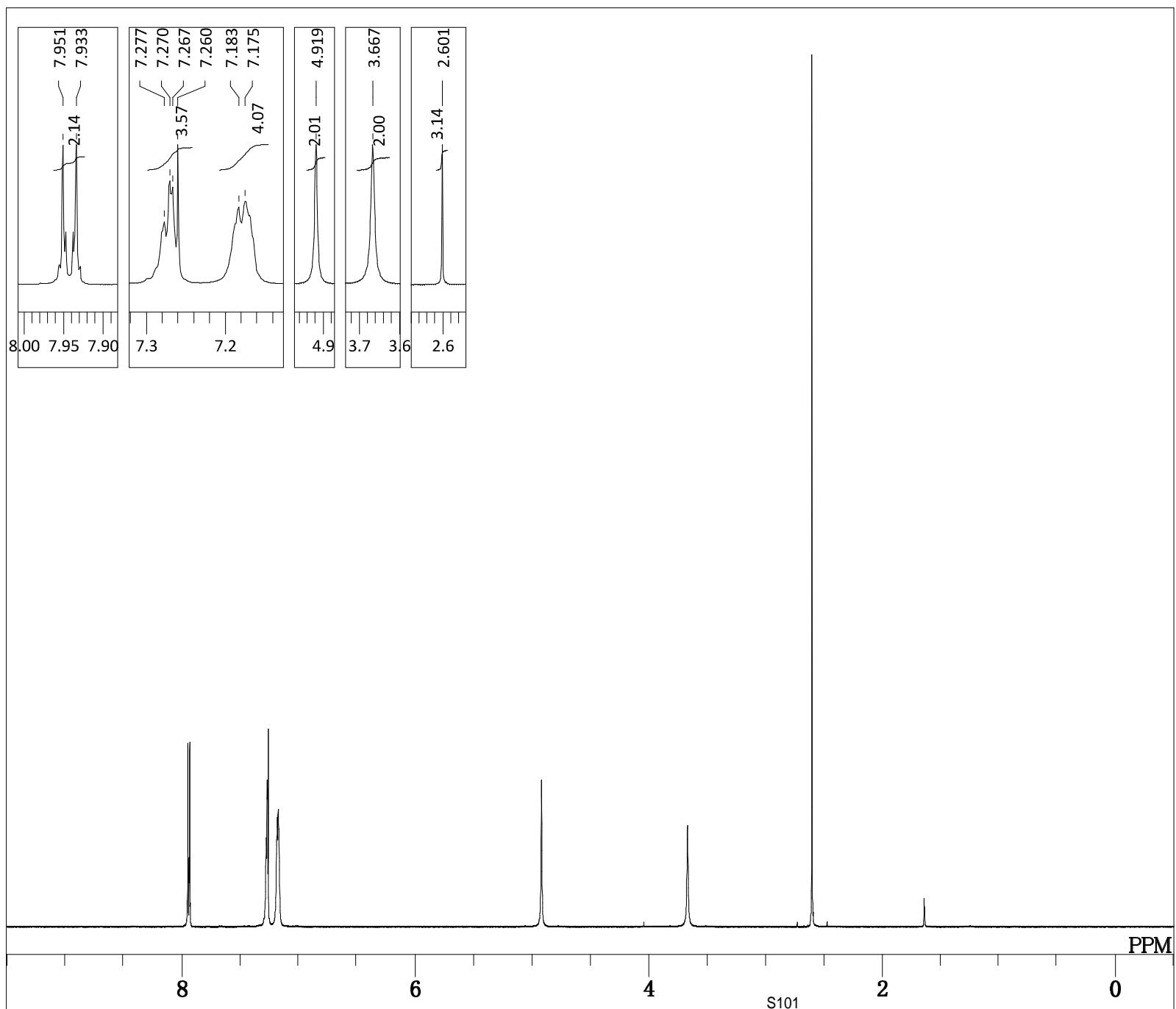
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 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 KHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 17.9 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 38



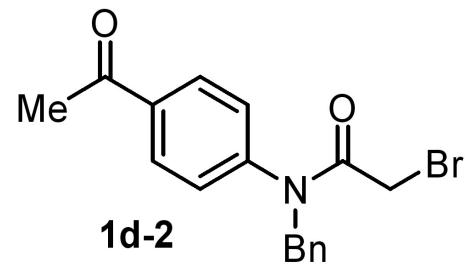


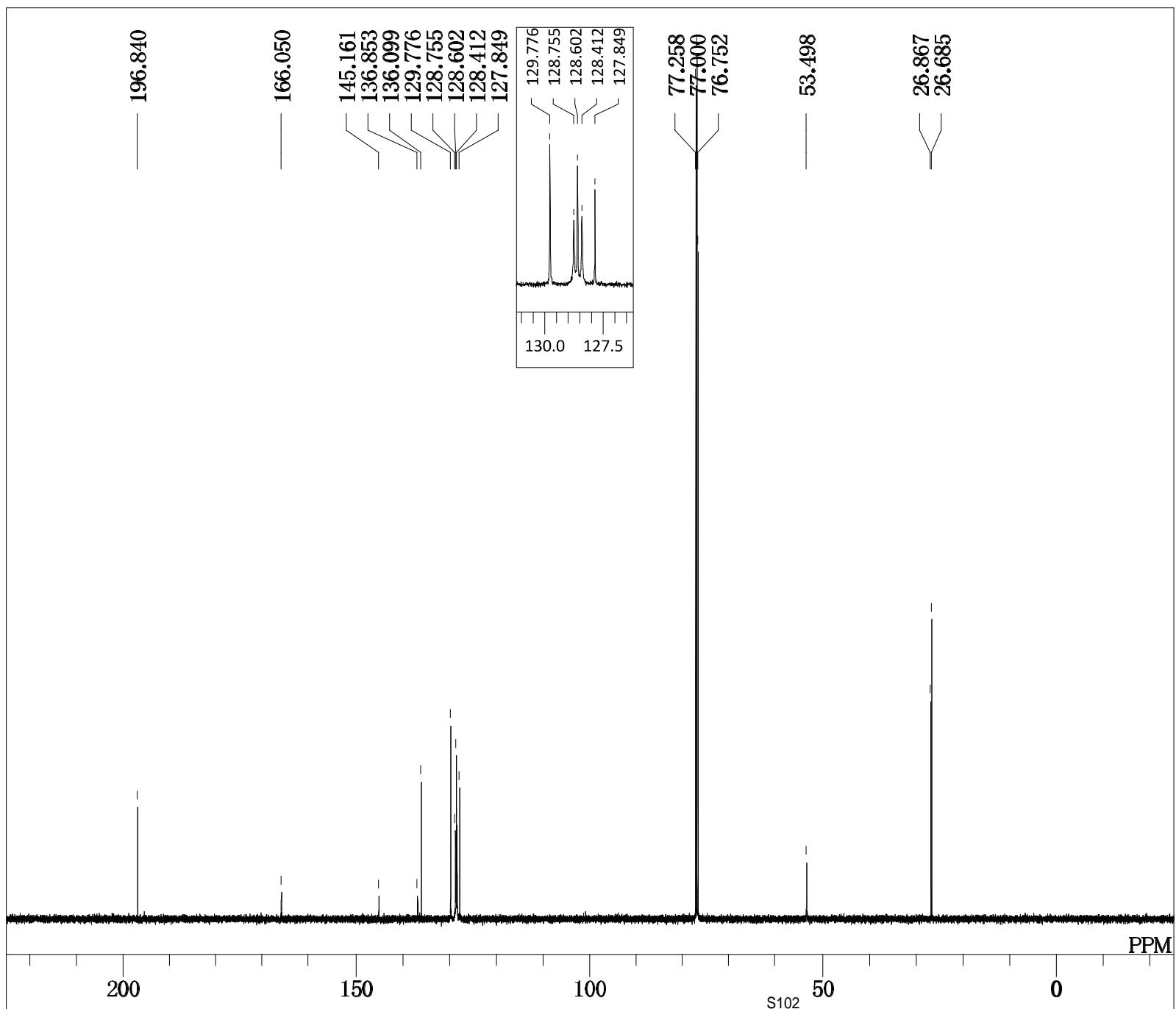
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COMNT single pulse decoupled gated NO  
DATIM 2017-08-08 15:12:13  
OBNUC 13C  
EXMOD carbon.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 KHz  
OBFIN 4.21 Hz  
POINT 26214  
FREQU 31446.54 Hz  
SCANS 256  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 18.0 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 60



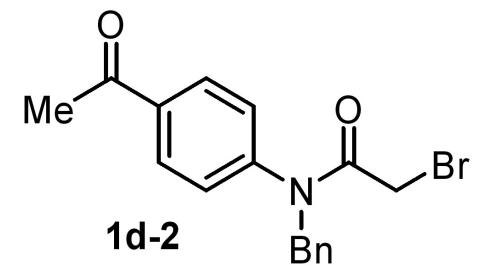


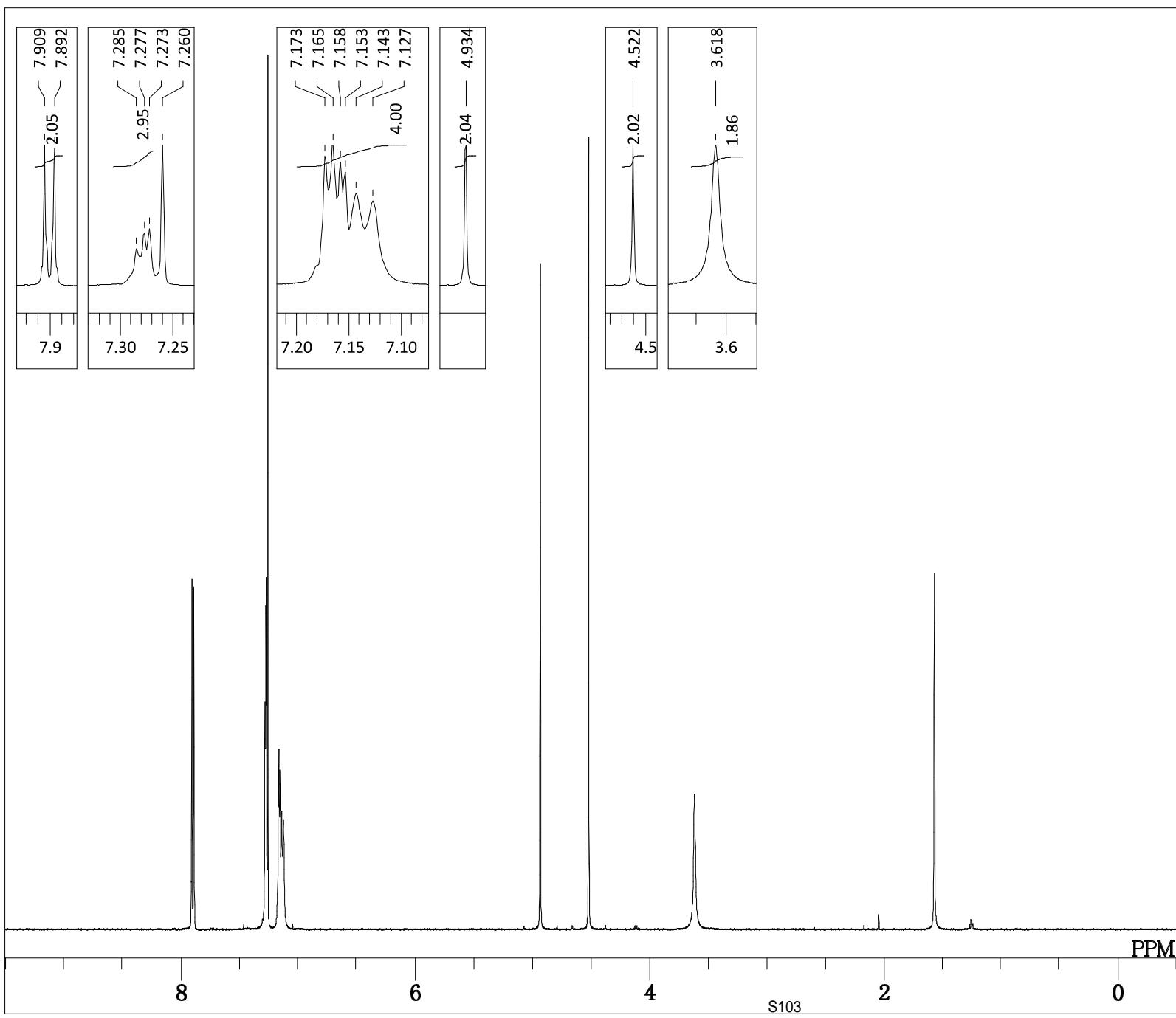
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 COMNT single\_pulse  
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 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 KHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 15.0 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 40



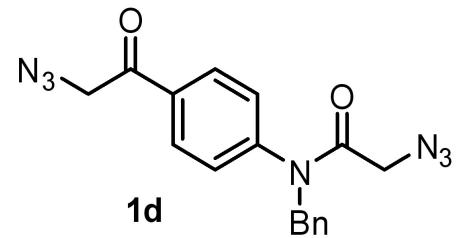


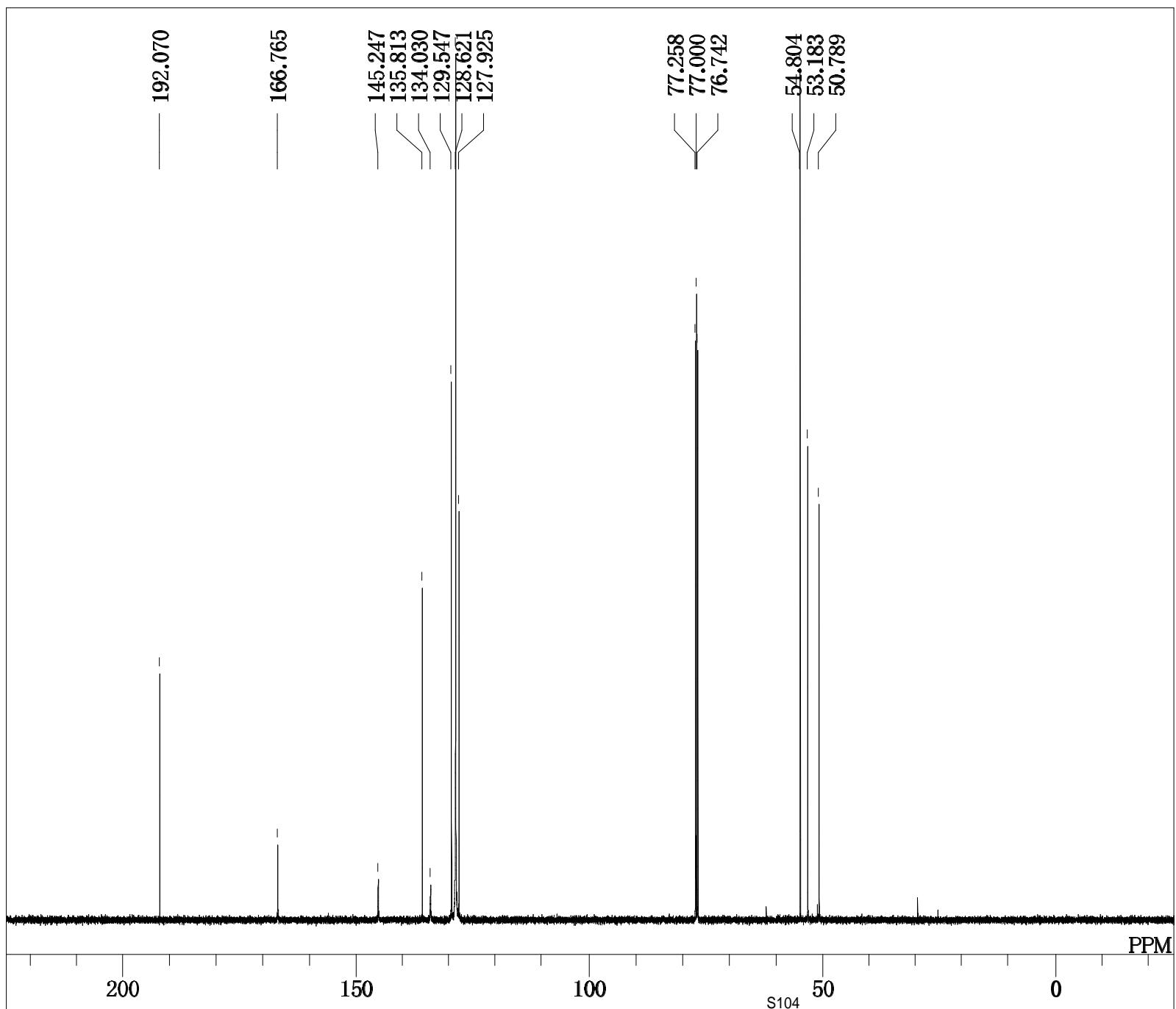
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 OBNUC 13C  
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 KHz  
 OBFIN 4.21 Hz  
 POINT 32767  
 FREQU 39308.18 Hz  
 SCANS 1024  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 14.7 c  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60



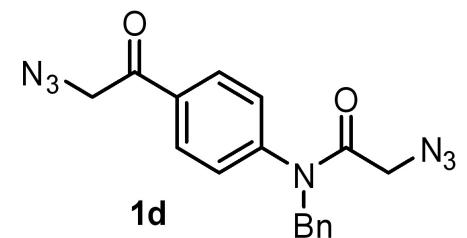


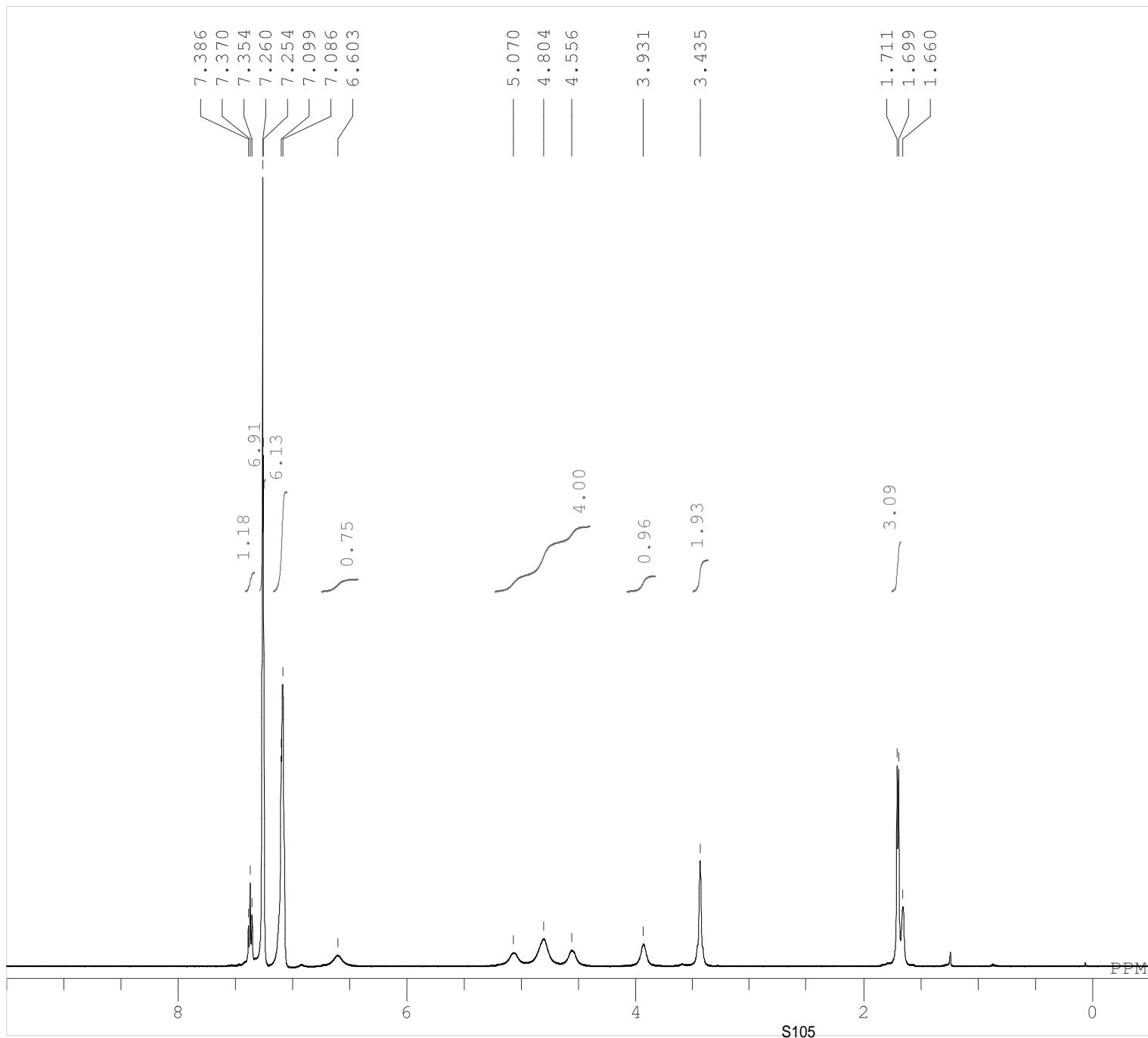
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 DATIM 2017-07-28 17:07:56  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 KHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 18.9 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 44





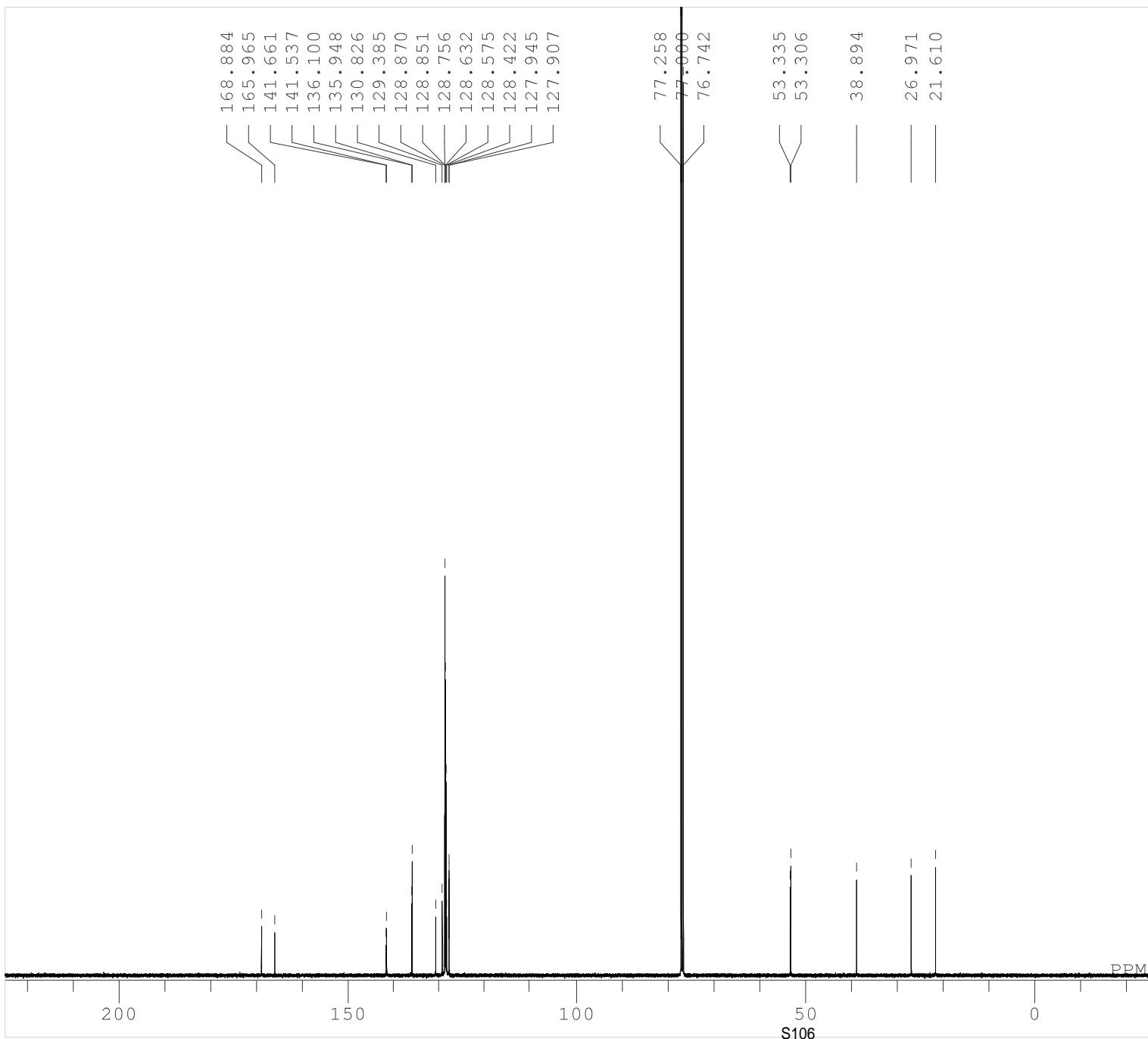
DFILE TU-02-055-2 170808\_carbon-1-  
COMNT single pulse decoupled gated NO  
DATIM 2017-08-08 19:59:57  
OBNUC 13C  
EXMOD carbon.jxp  
OBFRQ 125.77 MHz  
OBSET 7.87 KHz  
OBFIN 4.21 Hz  
POINT 32767  
FREQU 39308.18 Hz  
SCANS 1024  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 3.12 usec  
IRNUC 1H  
CTEMP 17.6 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 0.10 Hz  
RGAIN 60



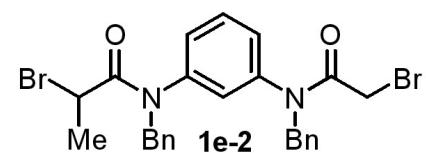


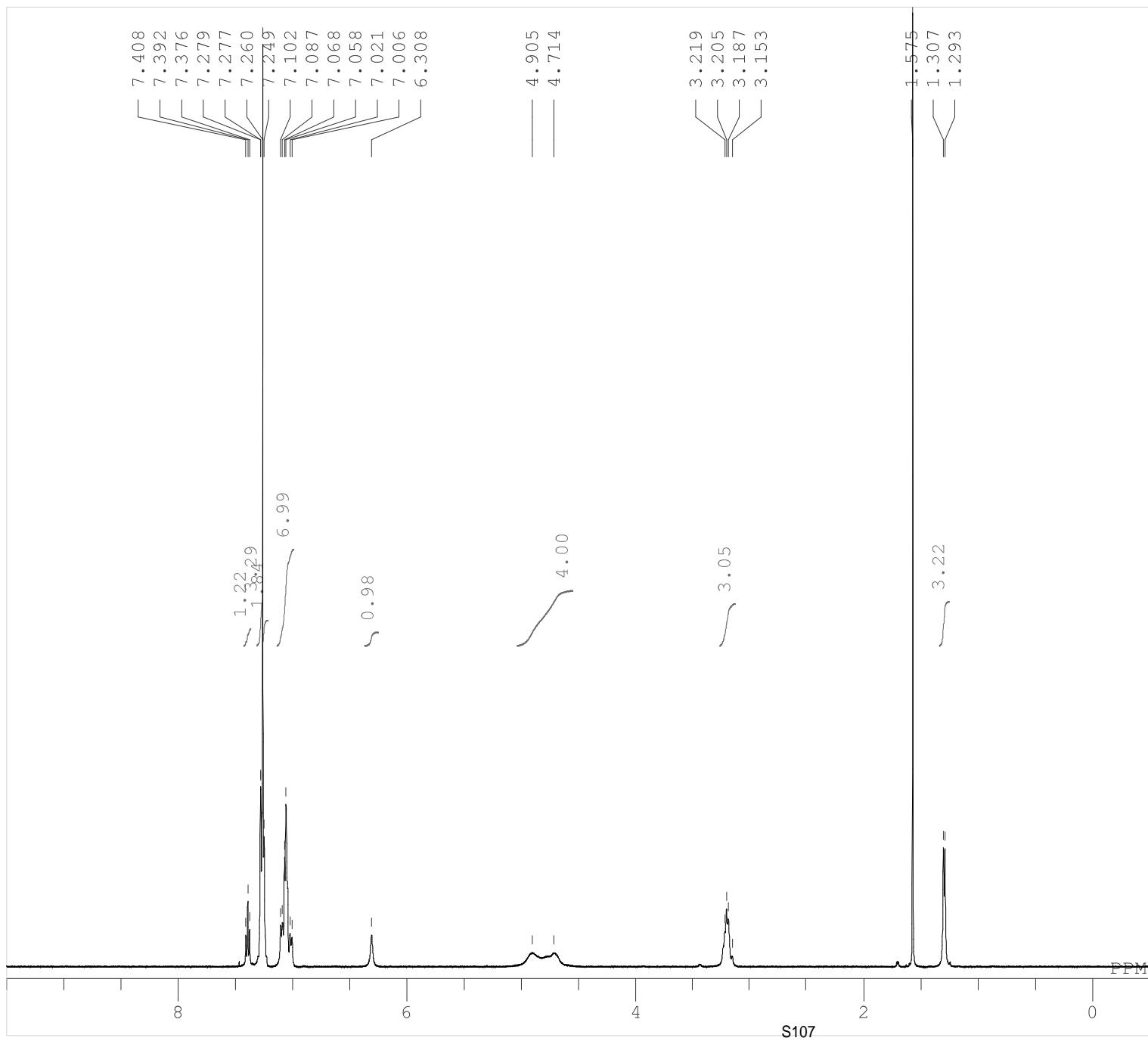
DFILE TY\_09\_106\_01\_2\_proton-1-1.als  
 COMNT single\_pulse  
 DATIM 2017-10-11 23:19:13  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 14.9 c  
 SLVNT CDCL3  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 38



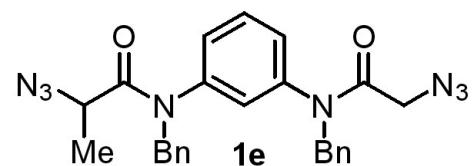


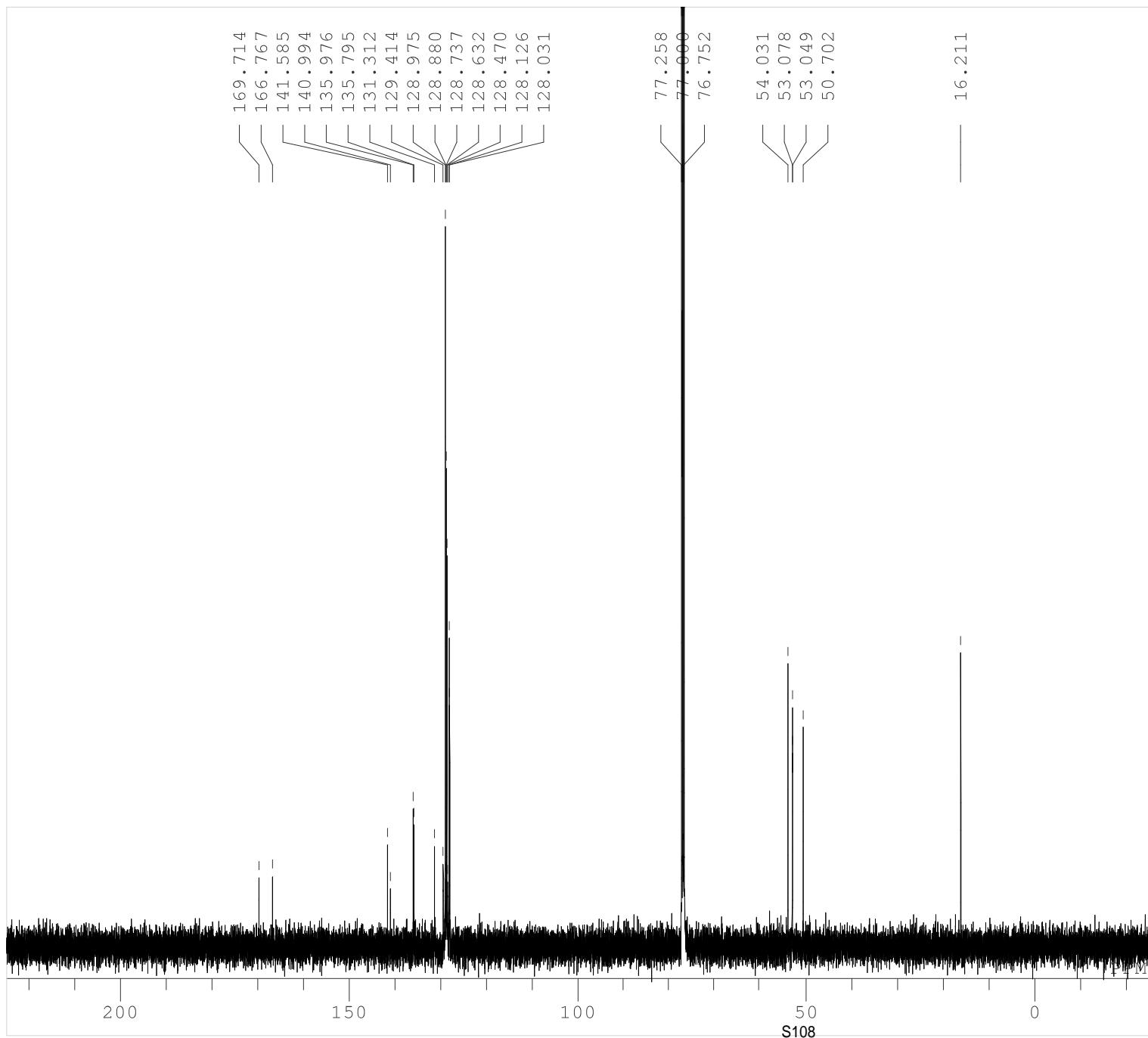
DFILE TY\_09\_106\_01\_2\_carbn-1-1.als  
 COMNT single pulse decoupledgated  
 DATIM 2017-10-11 23:20:47  
 OBNUC <sup>13</sup>C  
 EXMOD carbn.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 8840  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 14.6 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60



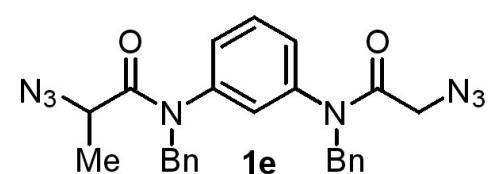


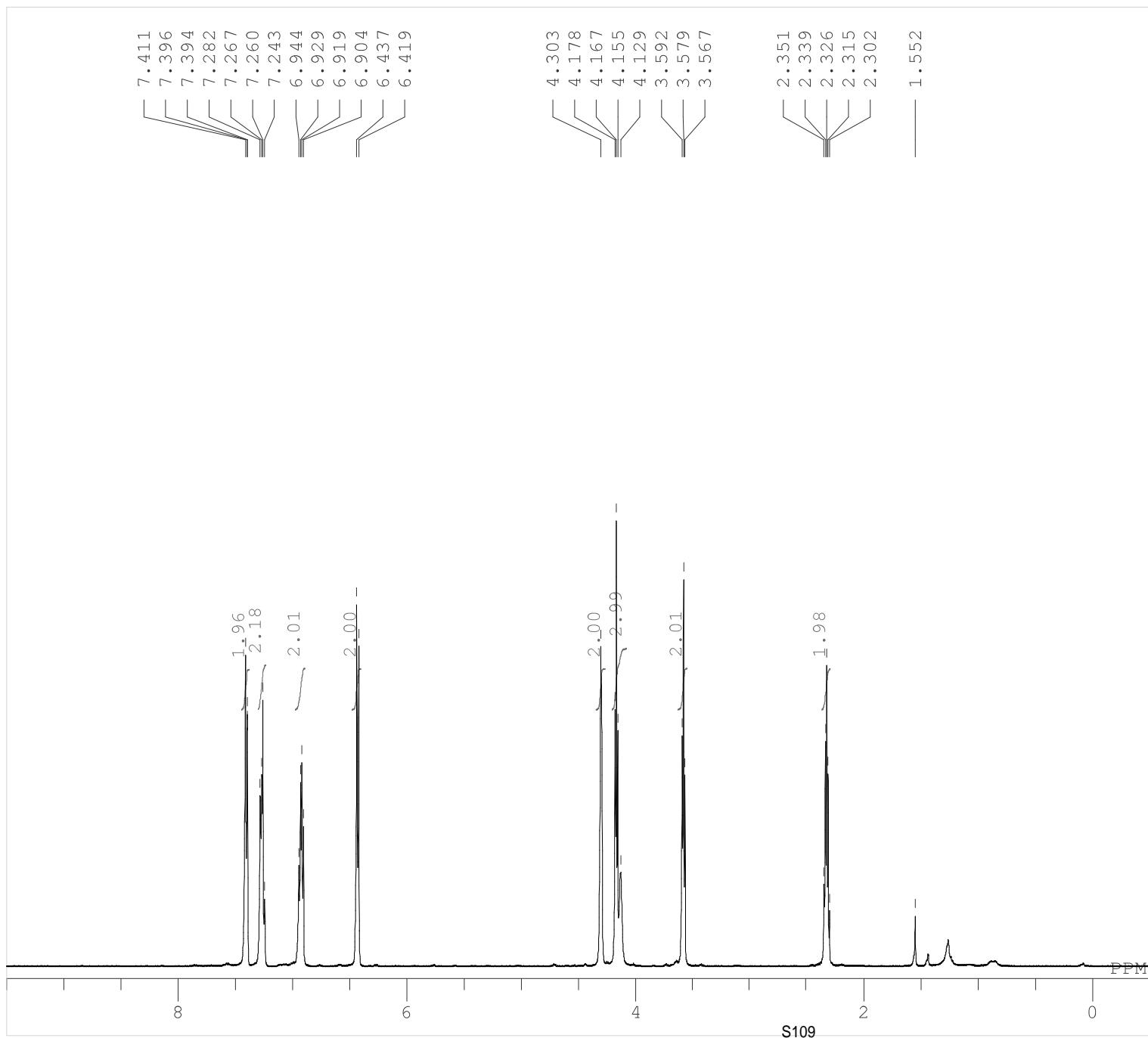
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 COMNT single\_pulse  
 DATIM 2017-10-18 23:11:59  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 17.3 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 46





DFILE TY\_09\_109\_01\_carbn-1-1.als  
 COMNT single pulse decoupledgated  
 DATIM 2017-10-18 23:13:37  
 OBNUC <sup>13</sup>C  
 EXMOD carbn.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 8680  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 18.1 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60

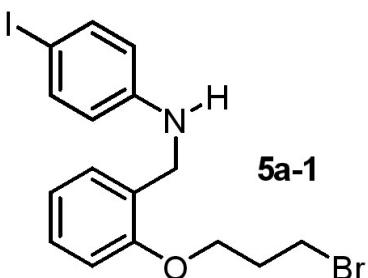


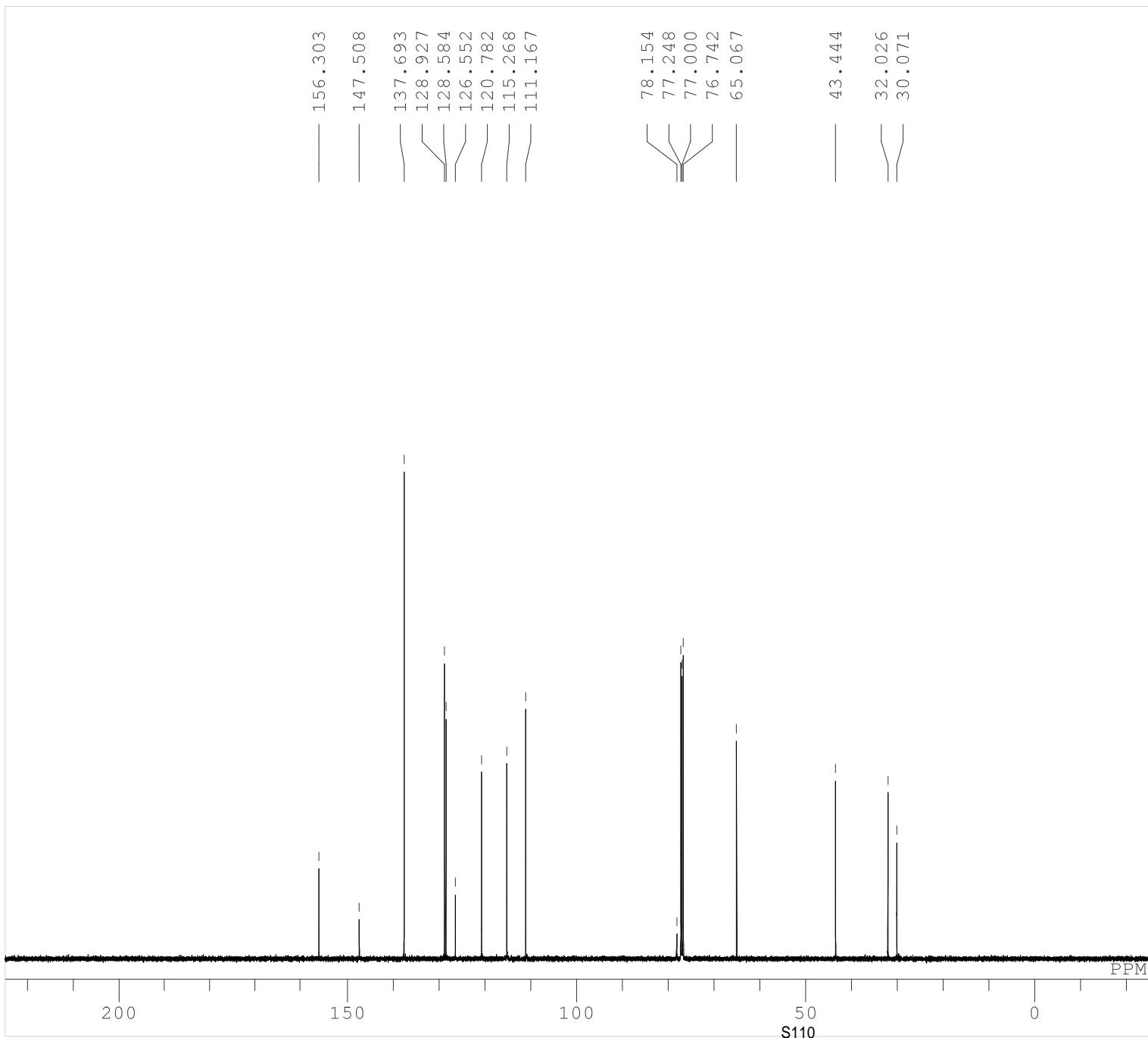


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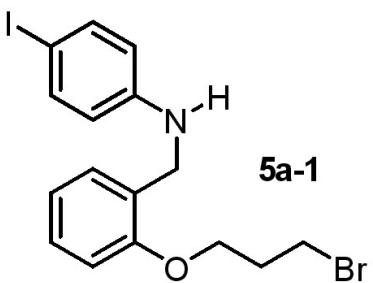
DFILE      TY_10_029_01_proton-1-1.als
COMNT      single_pulse
DATIM      2017-12-14 10:10:51
OBNUC      1H
EXMOD      proton.jxp
OBFRQ      500.16 MHz
OBSET      2.41 KHz
OBFIN      6.01 Hz
POINT      13107
FREQU     7507.51 Hz
SCANS       8
ACQTM      1.7459 sec
PD         5.0000 sec
PW1        6.85 usec
IRNUC      1H
CTEMP       19.9 c
SLVNT      CDCL3
EXREF      7.26 ppm
BF         0.10 Hz
RGAIN       36

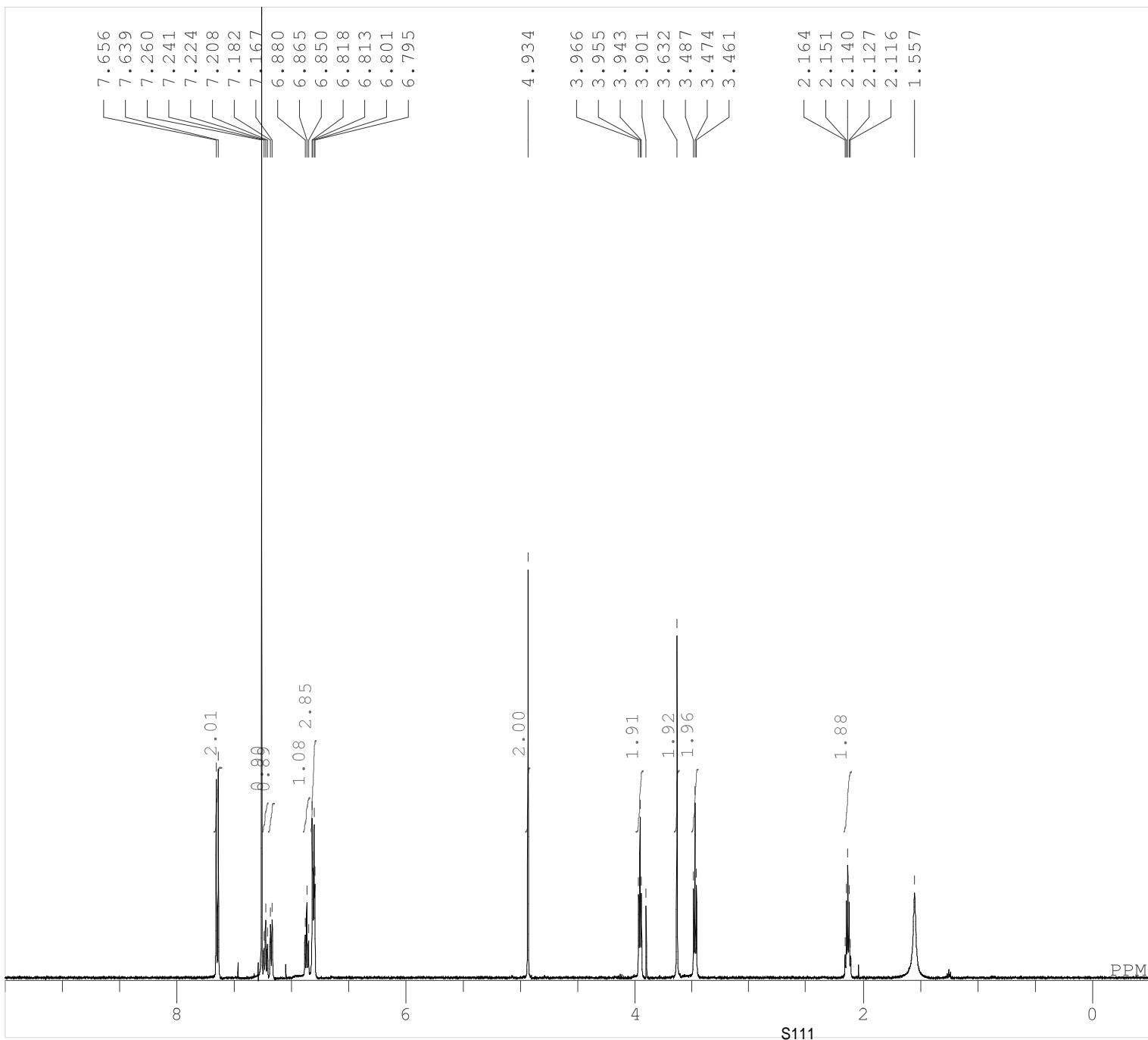
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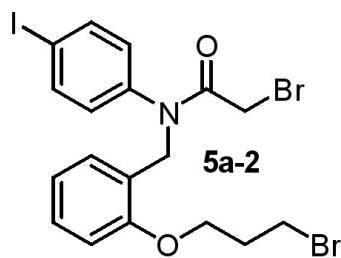


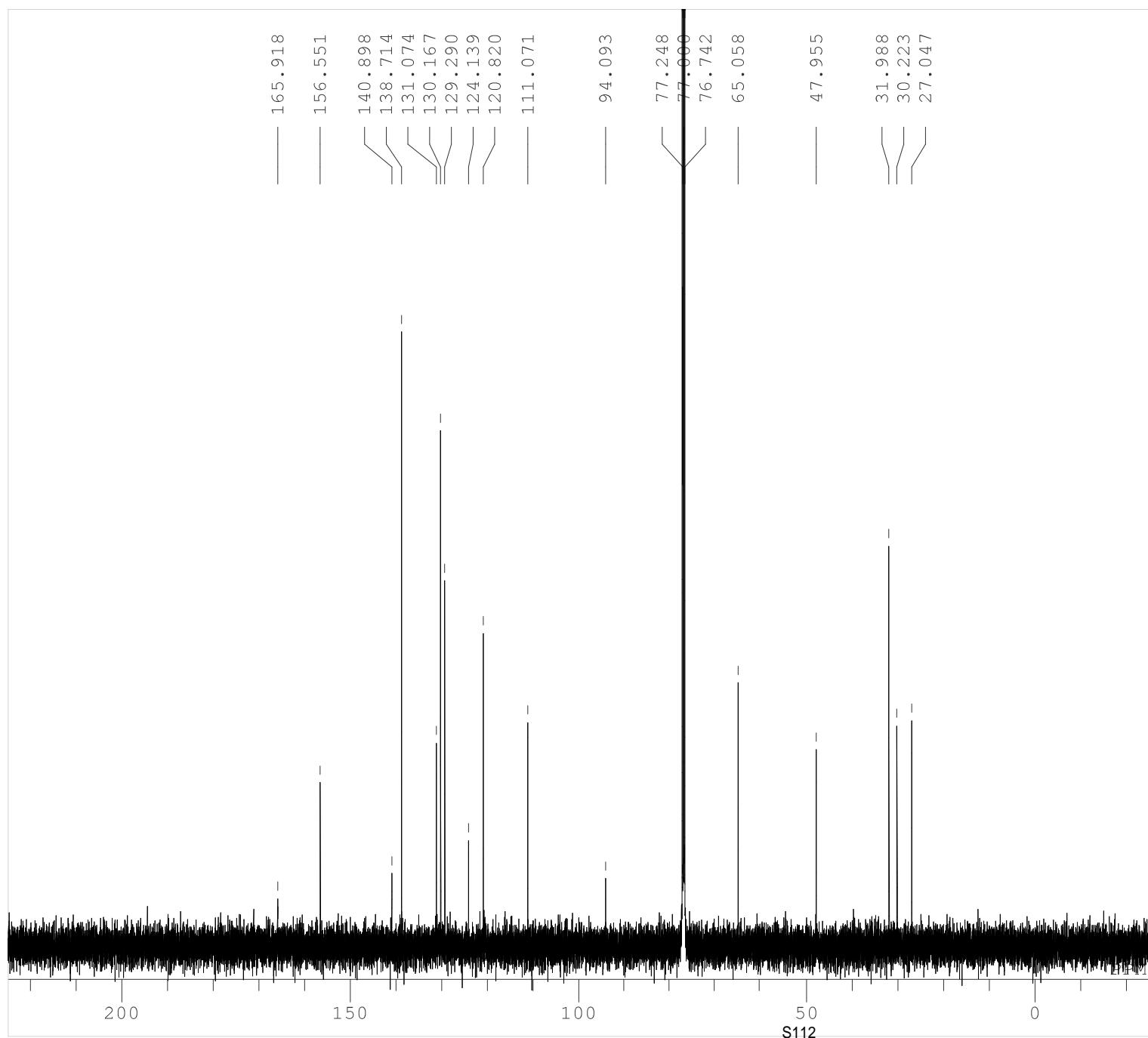
DFILE TY\_10\_029\_01\_2\_carbn-1-1.als  
 COMNT single pulse decoupledgated  
 DATIM 2018-02-13 15:52:32  
 OBNUC <sup>13</sup>C  
 EXMOD carbn.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 1256  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 16.2 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60



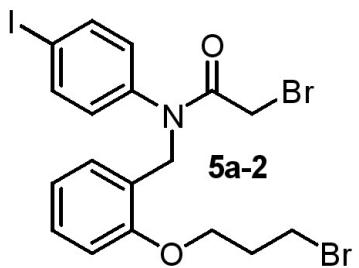


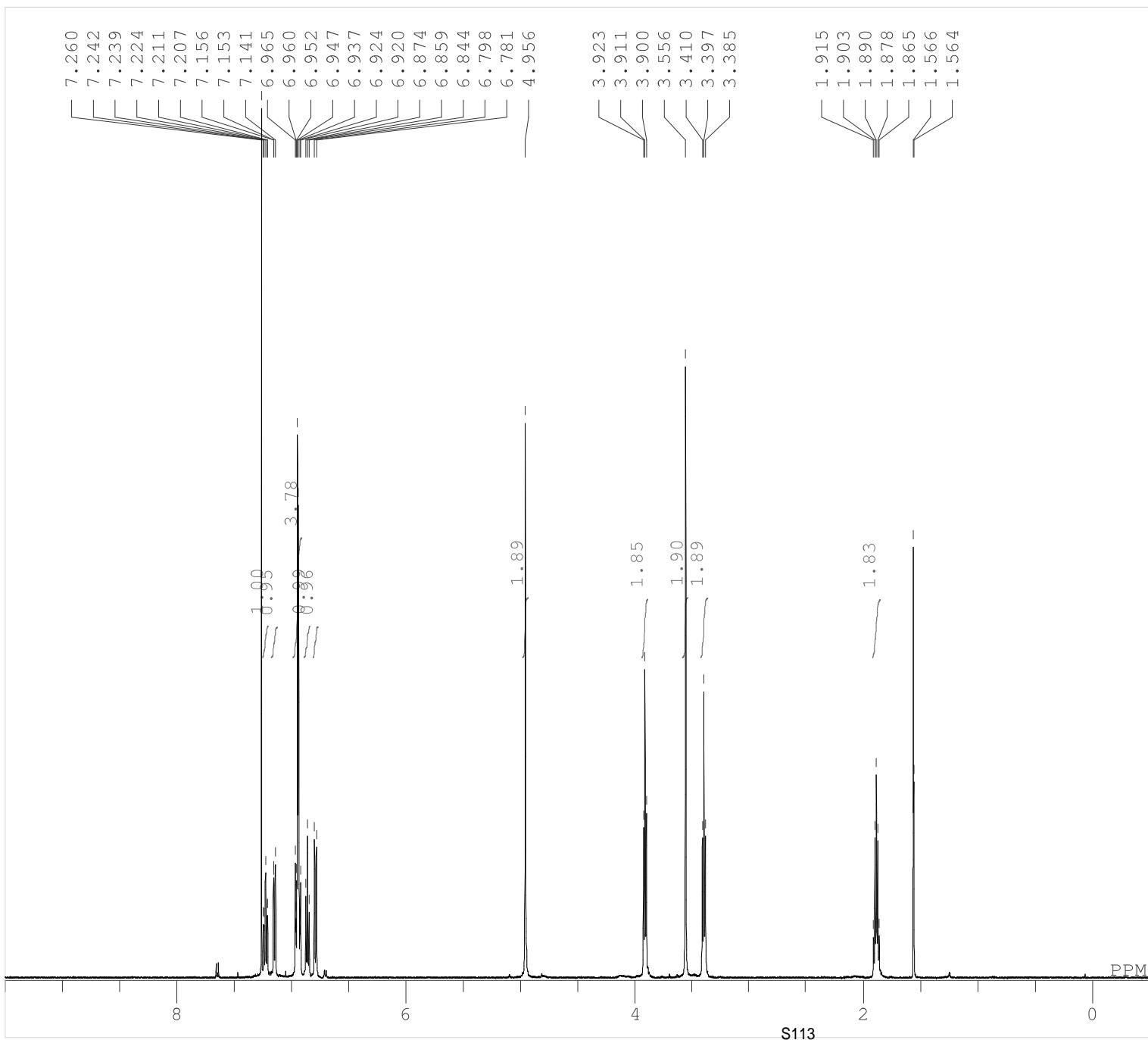
DFILE TY\_10\_038\_01\_proton-1-1.als  
 COMNT single\_pulse  
 DATIM 2017-12-21 00:50:35  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 18.4 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 50



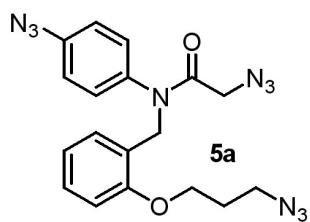


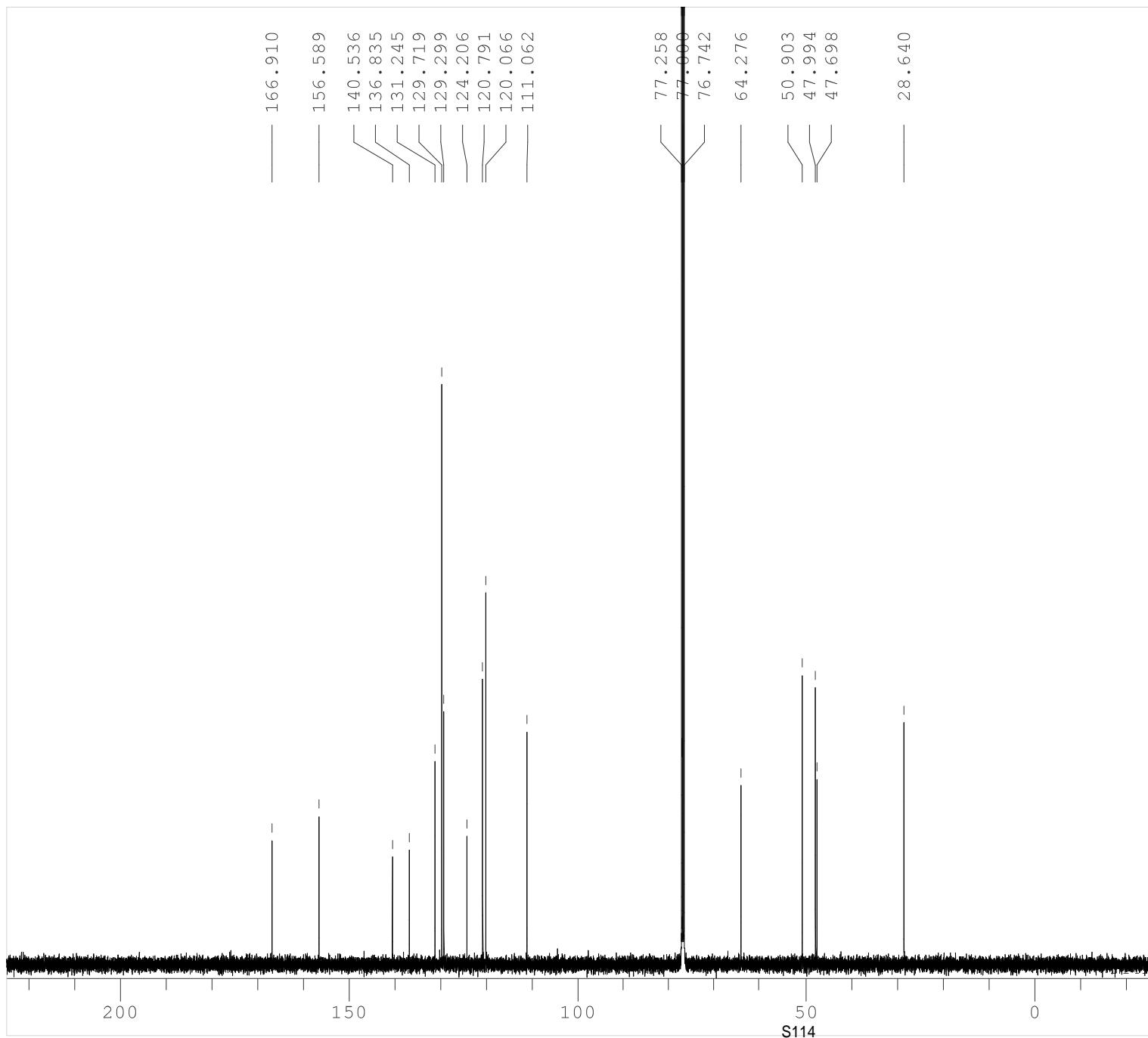
DFILE TY\_10\_038\_01\_carbn-1-1.als  
 COMNT single pulse decoupled gated  
 DATIM 2017-12-21 00:52:01  
 OBNUC <sup>13</sup>C  
 EXMOD carbn.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 6980  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 19.7 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60



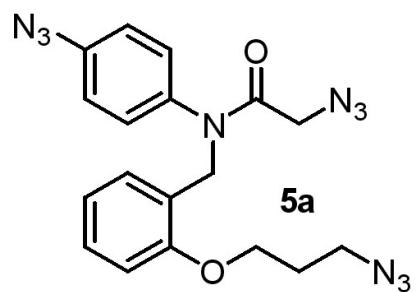


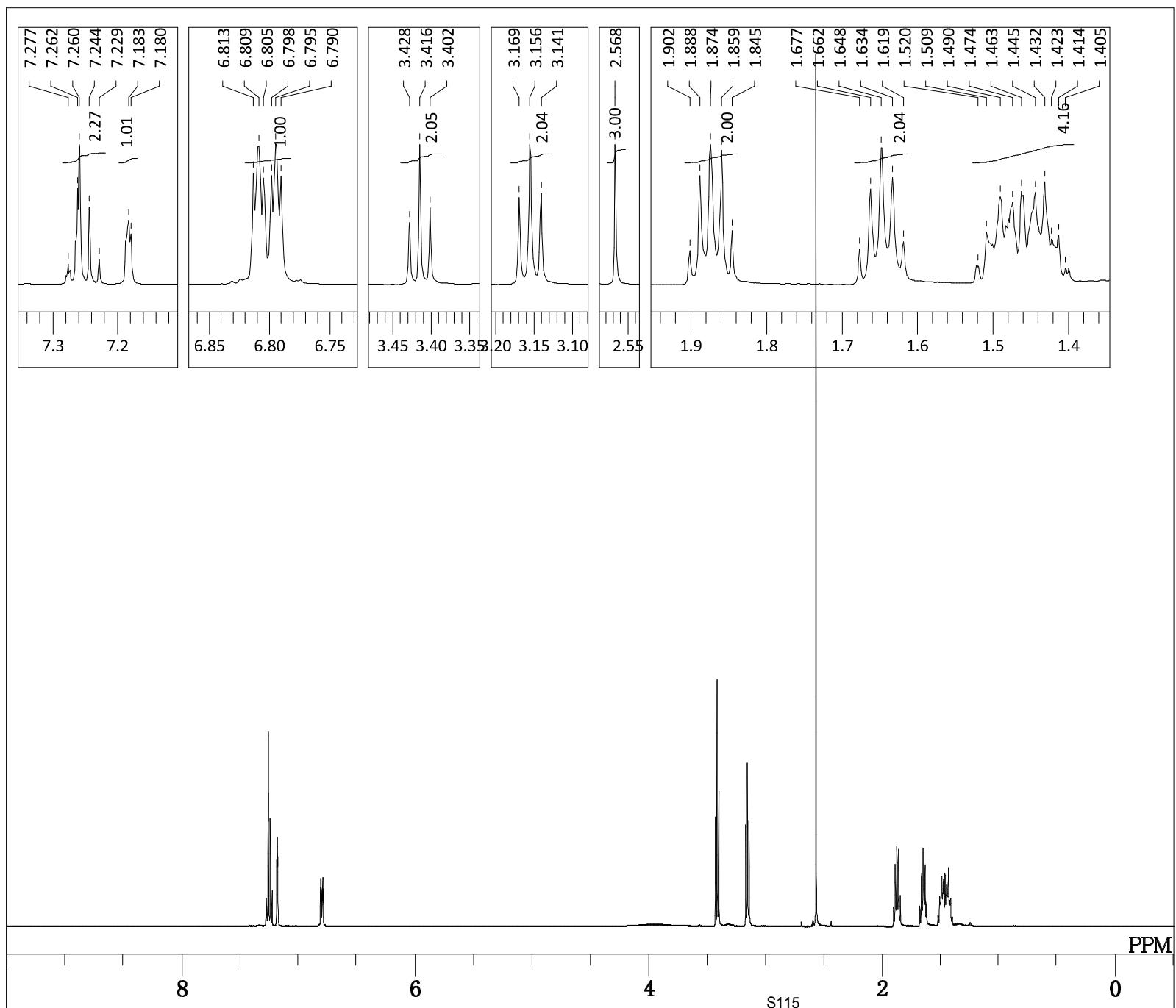
DFILE TY\_10\_039\_02\_proton-1-1.als  
 COMNT single\_pulse  
 DATIM 2017-12-21 23:12:23  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 18.5 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 48





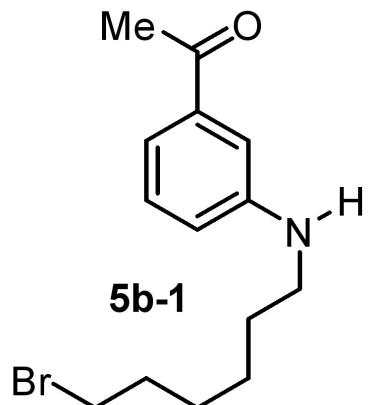
DFILE TY\_10\_039\_02\_carbn-1-1.als  
 COMNT single pulse decoupled gated  
 DATIM 2017-12-21 23:13:55  
 OBNUC <sup>13</sup>C  
 EXMOD carbn.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 8920  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 19.7 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 50

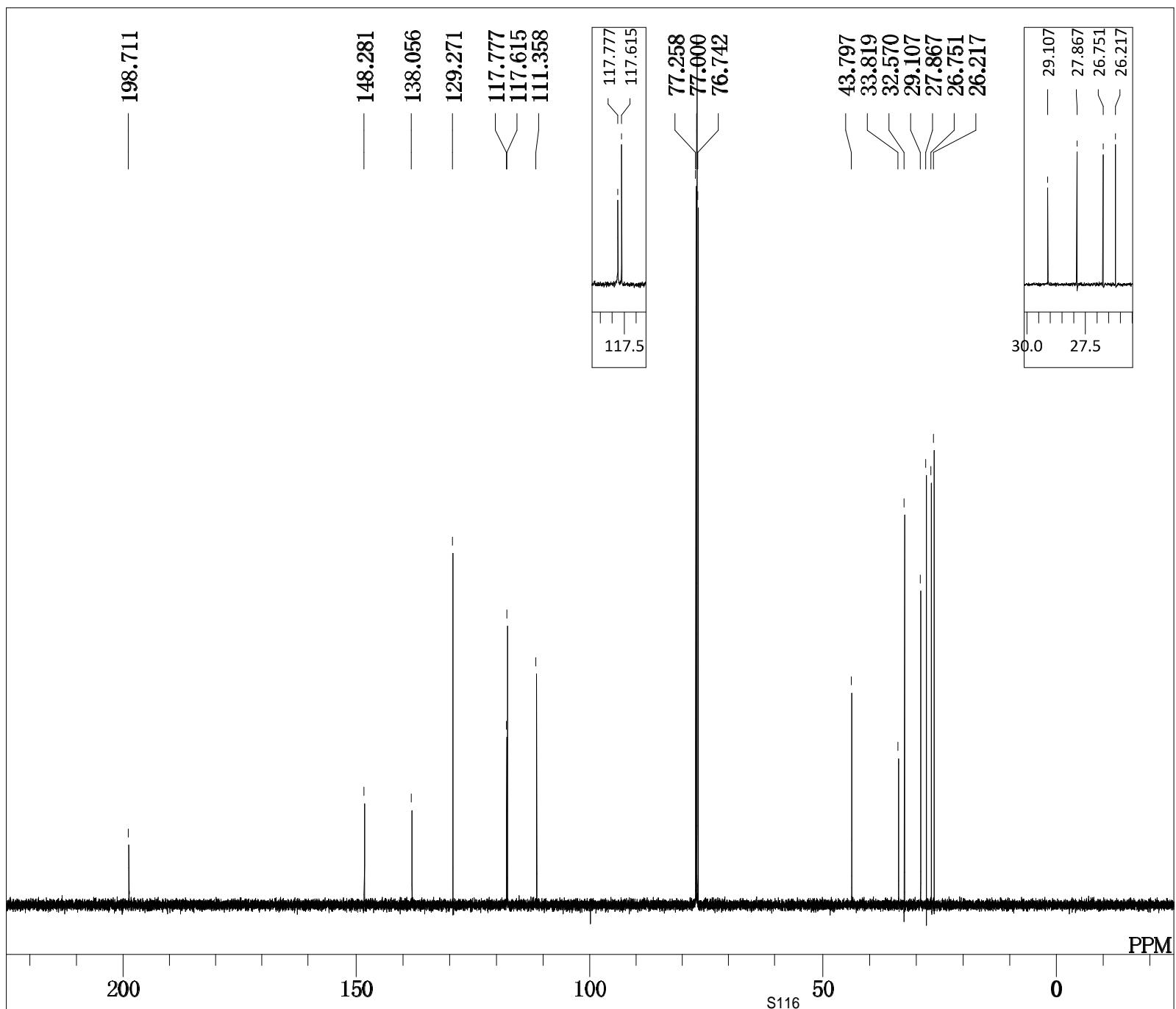




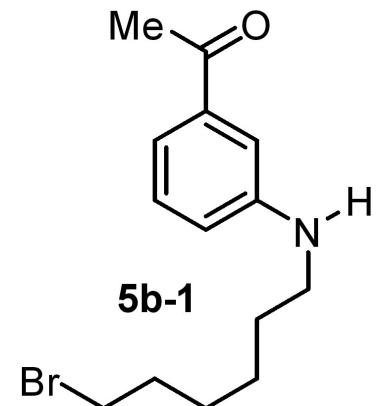
DFILE  
 COMNT  
 DATIM  
 OBNUC  
 EXMOD  
 OBFRQ  
 OBSET  
 OBFIN  
 POINT  
 FREQU  
 SCANS  
 ACQTM  
 PD  
 PW1  
 IRNUC  
 CTEMP  
 SLVNT  
 EXREF  
 BF  
 RGAIN

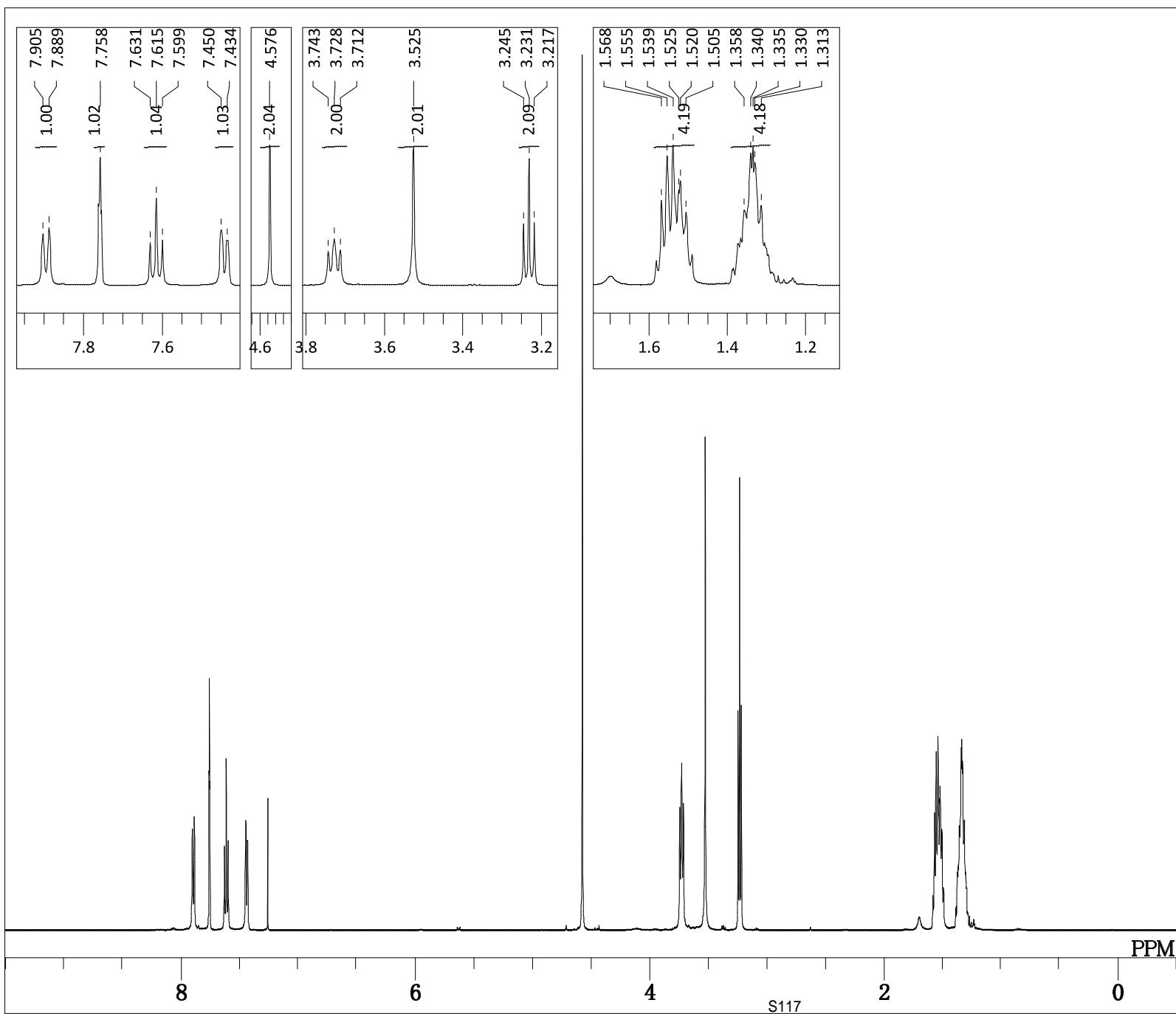
TU-02-080-2 180215\_proton-1-  
 single\_pulse  
 2018-02-15 14:43:58  
 1H  
 proton.jxp  
 500.16 MHz  
 2.41 KHz  
 6.01 Hz  
 13107  
 7507.51 Hz  
 8  
 1.7459 sec  
 5.0000 sec  
 6.85 usec  
 1H  
 15.5 c  
 CDCL<sub>3</sub>  
 7.26 ppm  
 0.10 Hz  
 34





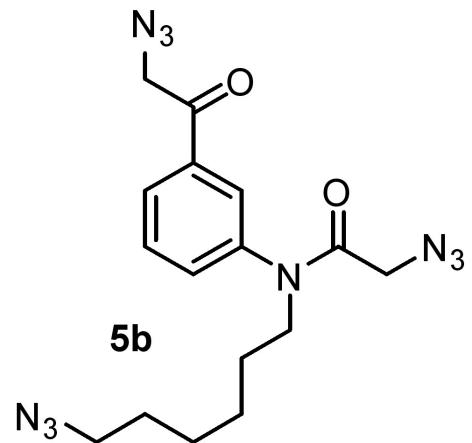
DFILE TU-02-080-2 180215\_carbon-1-  
 COMNT single pulse decoupled gated NO  
 DATIM 2018-02-15 14:45:57  
 OBNUC 13C  
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 KHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 350  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 15.9 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 58

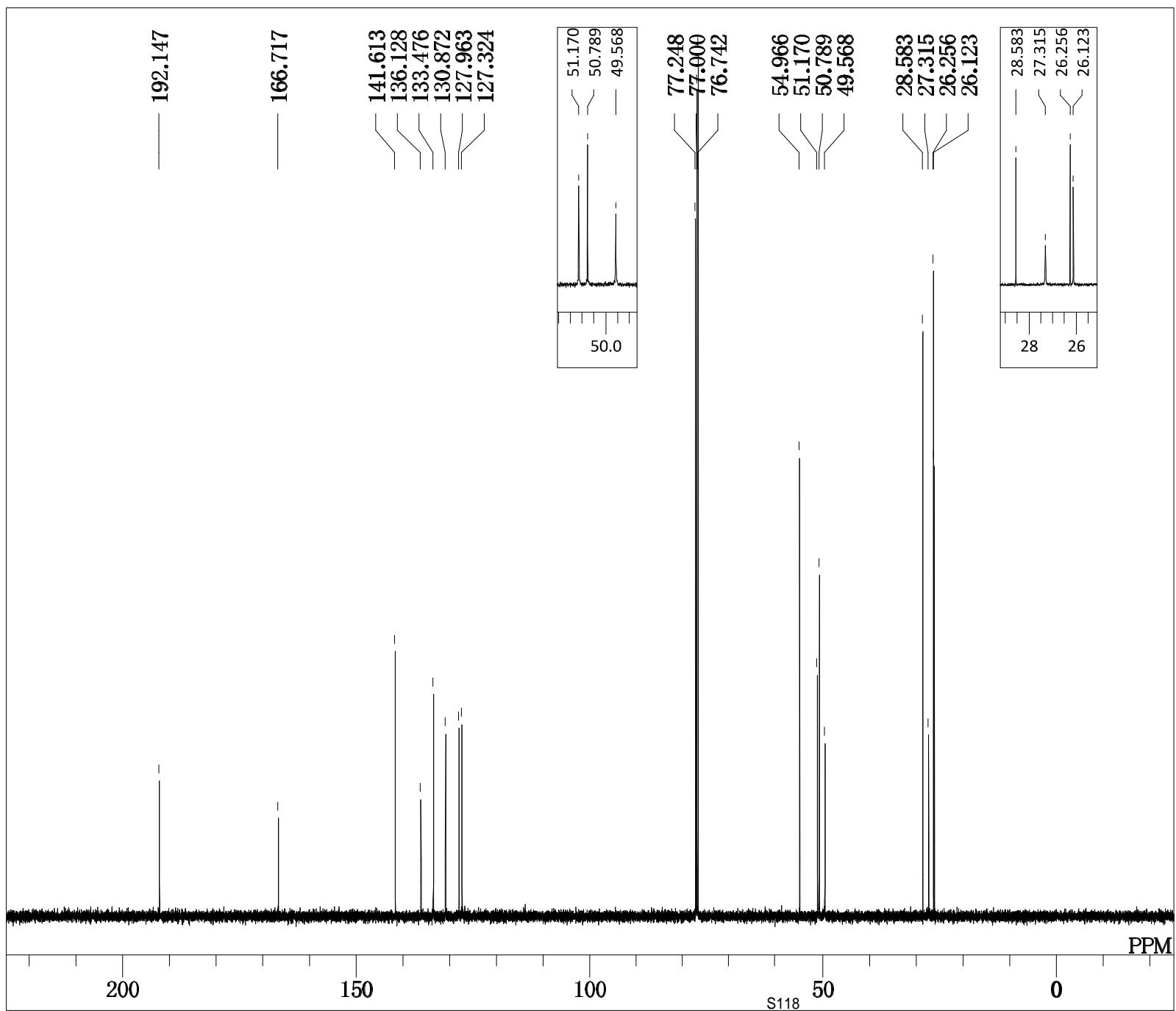




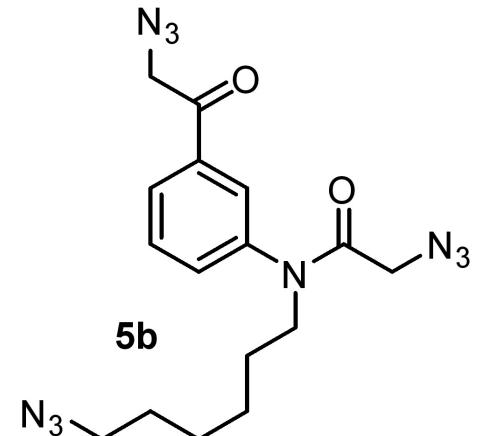
DFILE  
 COMNT  
 DATIM  
 OBNUC  
 EXMOD  
 OBFRQ  
 OBSET  
 OBFIN  
 POINT  
 FREQU  
 SCANS  
 ACQTM  
 PD  
 PW1  
 IRNUC  
 CTEMP  
 SLVNT  
 EXREF  
 BF  
 RGAIN

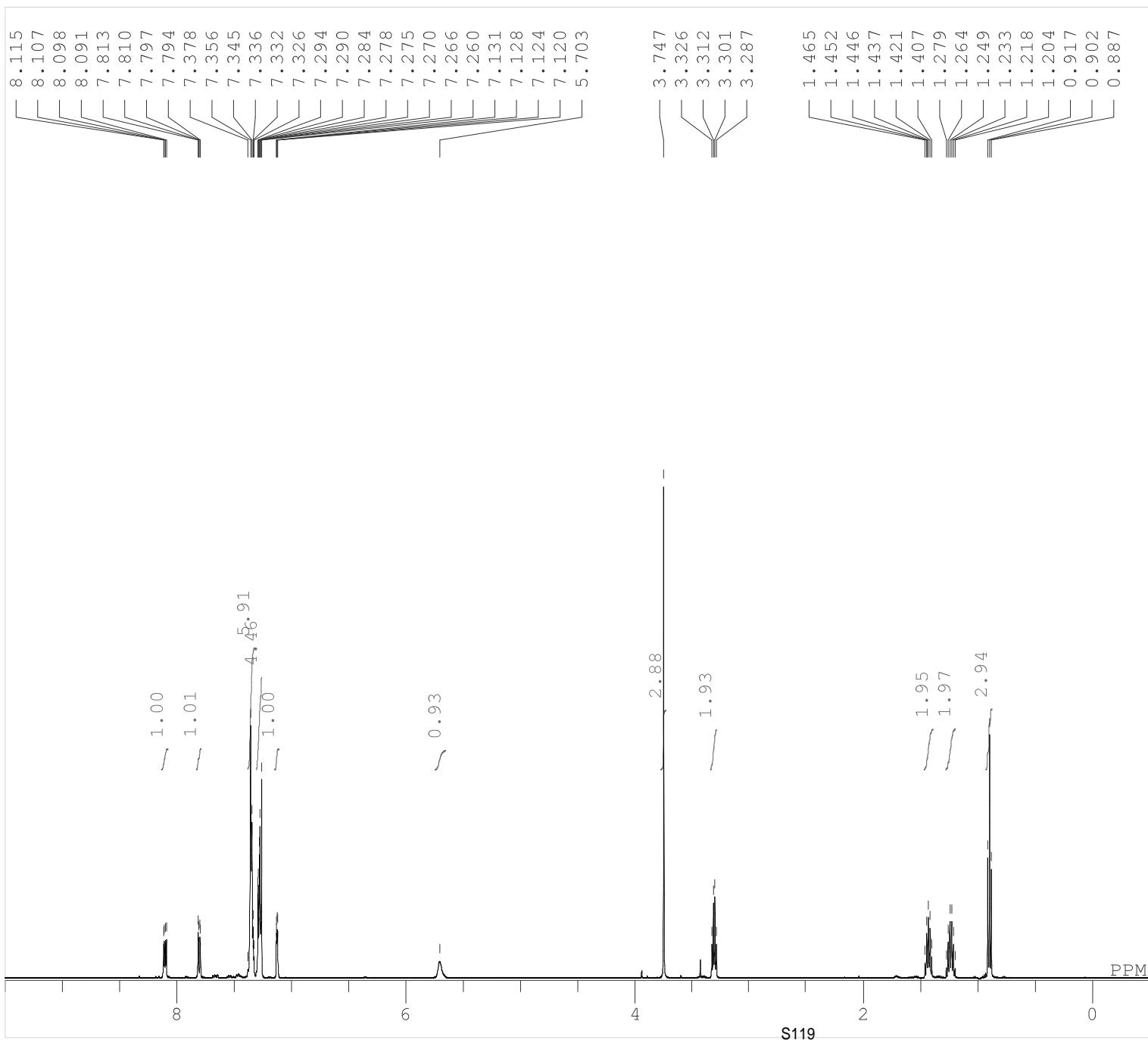
TU-02-087-2 171013\_proton-1-  
 single\_pulse  
 2017-10-13 14:28:29  
 1H  
 proton.jxp  
 500.16 MHz  
 2.41 KHz  
 6.01 Hz  
 13107  
 7507.51 Hz  
 8  
 1.7459 sec  
 5.0000 sec  
 6.85 usec  
 1H  
 15.3 c  
 CDCL3  
 7.26 ppm  
 0.10 Hz  
 32



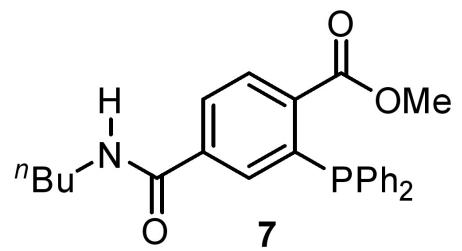


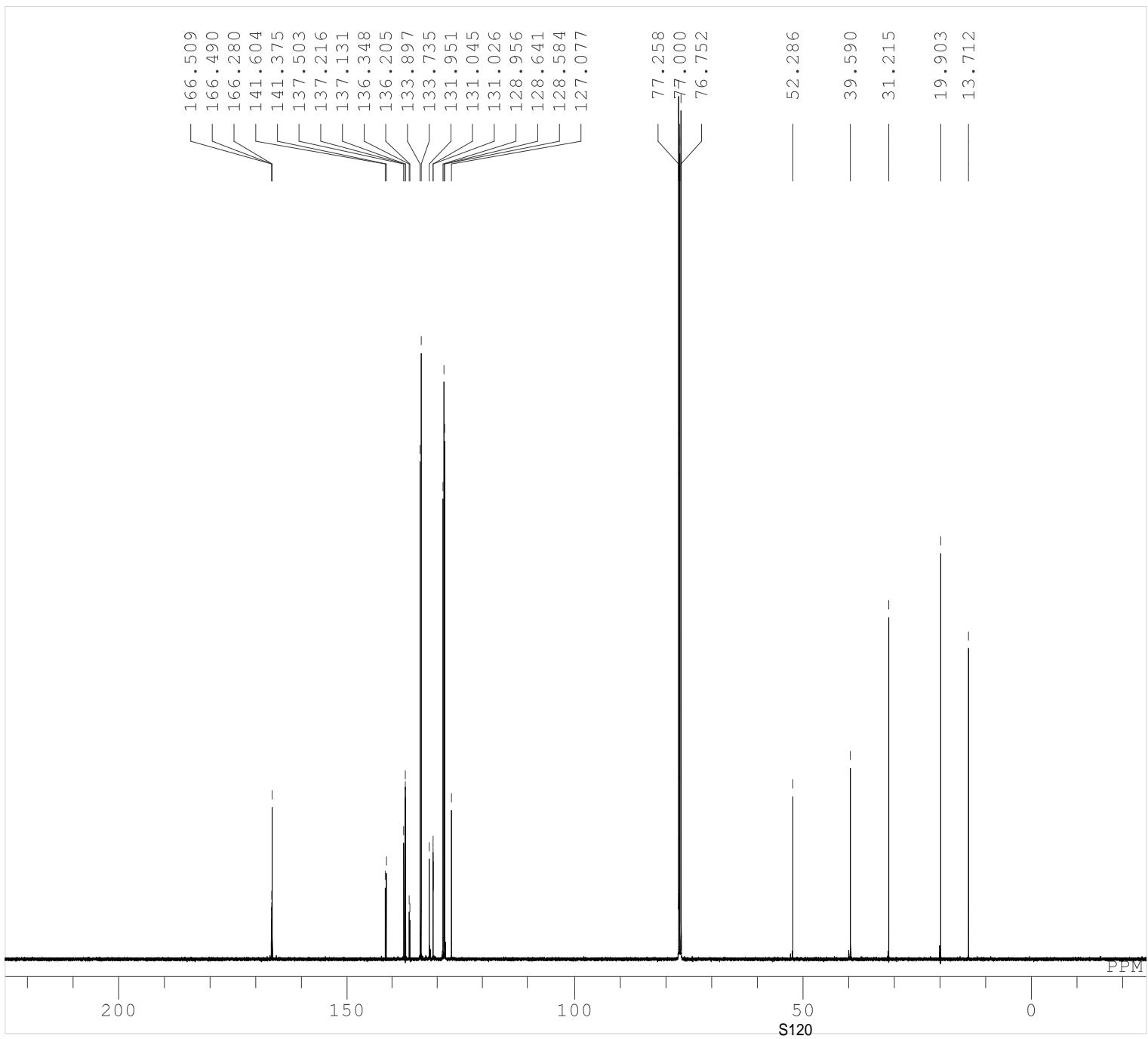
DFILE TU-02-087-2 171013\_carbon-1-  
 COMNT single pulse decoupled gated NO  
 DATIM 2017-10-13 14:30:16  
 OBNUC 13C  
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 KHz  
 OBFIN 4.21 Hz  
 POINT 32767  
 FREQU 39308.18 Hz  
 SCANS 512  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 15.5 c  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60



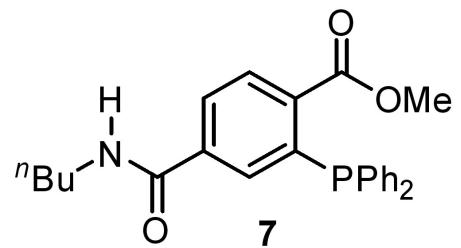


DFILE TY\_09\_080\_02\_proton-1-1.als  
 COMNT single\_pulse  
 DATIM 2018-02-20 23:12:14  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFRQ 500.16 MHz  
 OBSET 2.41 kHz  
 OBFIN 6.01 Hz  
 POINT 13107  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 1.7459 sec  
 PD 5.0000 sec  
 PW1 6.85 usec  
 IRNUC 1H  
 CTEMP 13.4 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 7.26 ppm  
 BF 0.10 Hz  
 RGAIN 34

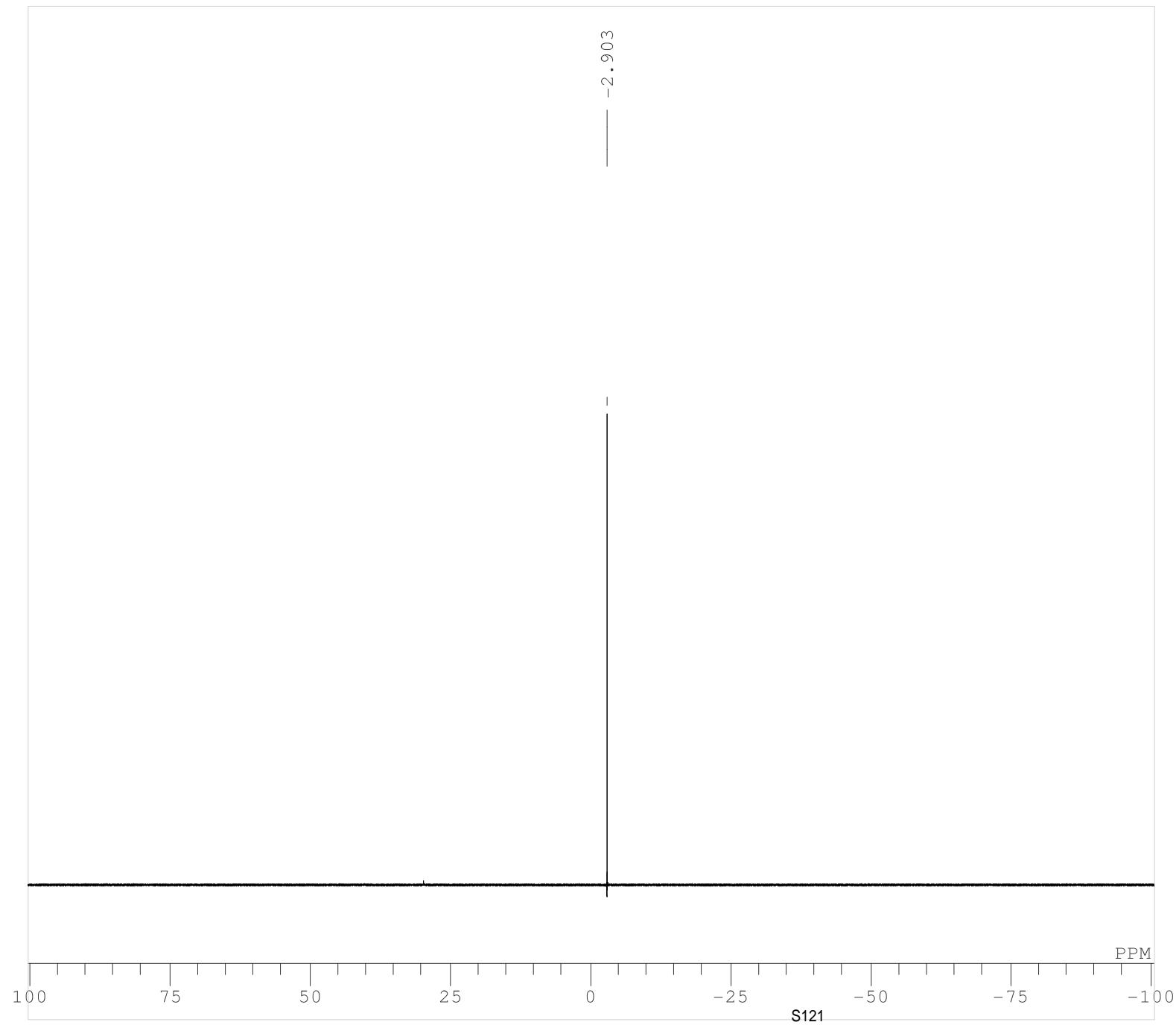
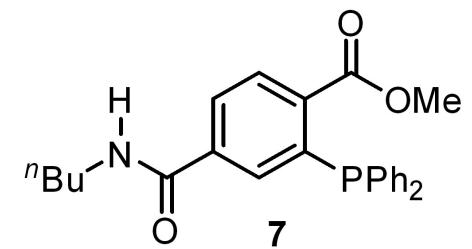




DFILE TY\_09\_080\_02\_carbon-1-1.als  
 COMNT single pulse decoupled gated  
 DATIM 2018-02-20 23:13:45  
 OBNUC  $^{13}\text{C}$   
 EXMOD carbon.jxp  
 OBFRQ 125.77 MHz  
 OBSET 7.87 kHz  
 OBFIN 4.21 Hz  
 POINT 26214  
 FREQU 31446.54 Hz  
 SCANS 9200  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 3.12 usec  
 IRNUC 1H  
 CTEMP 15.2 c  
 SLVNT CDCL<sub>3</sub>  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 60

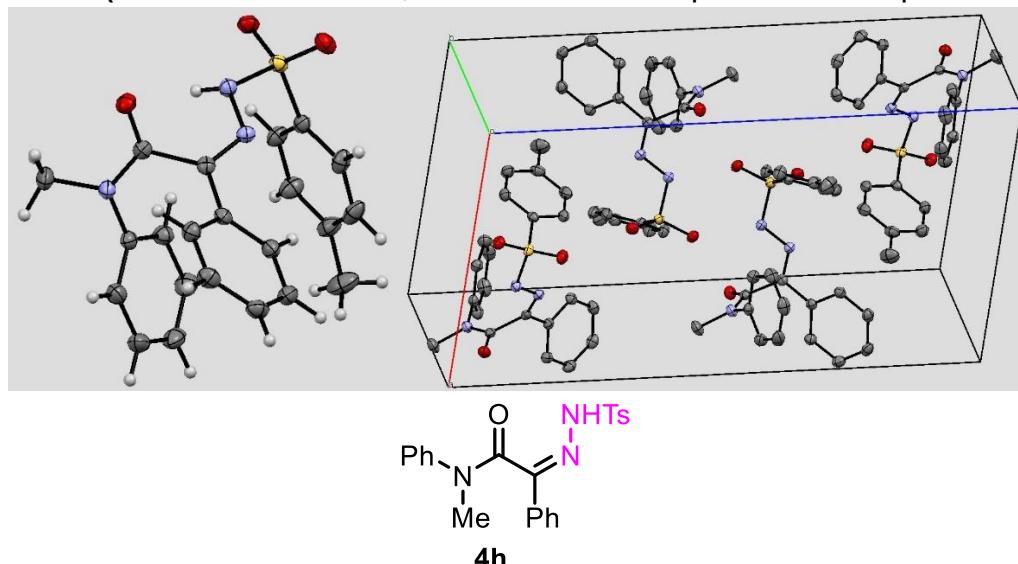


DFILE TY\_09\_080\_02\_phosphorus-1-1.a  
 COMNT single pulse decoupled gated  
 DATIM 2018-02-22 15:50:30  
 OBNUC 31P  
 EXMOD carbon.jxp  
 OBFRQ 202.46 MHz  
 OBSET 8.31 kHz  
 OBFIN 0.75 Hz  
 POINT 26214  
 FREQU 40650.41 Hz  
 SCANS 35  
 ACQTM 0.6449 sec  
 PD 2.0000 sec  
 PW1 3.88 usec  
 IRNUC 1H  
 CTEMP 15.2 c  
 SLVNT C6D6  
 EXREF 0.00 ppm  
 BF 0.10 Hz  
 RGAIN 56



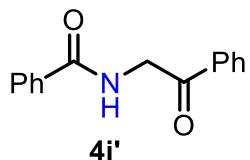
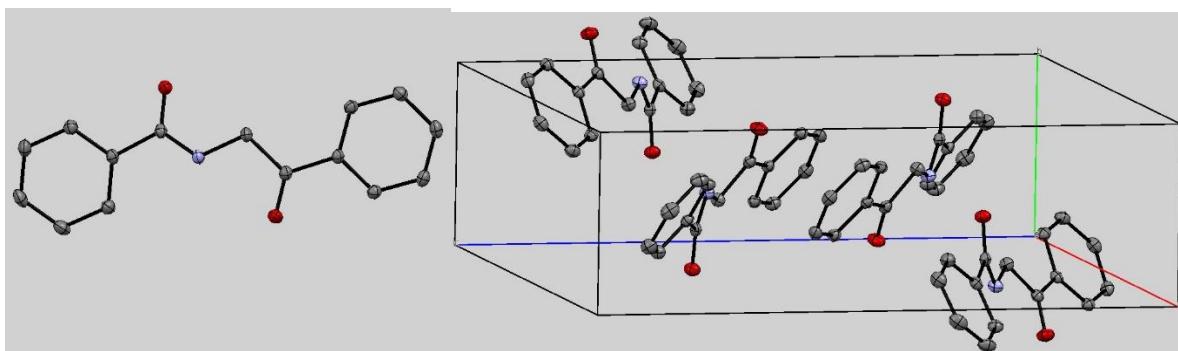
# X-ray Crystallographic Analysis Information

(1) Hydrazone 4h (CCDC No. 1839202, ORTEP thermal ellipsoids at 50% probability)



Empirical formula	C <sub>22</sub> H <sub>21</sub> N <sub>3</sub> O <sub>3</sub> S
Formula weight	407.49
Temperature	-150 ± 1 °C
Wavelength	MoKα ( $\lambda = 0.71075 \text{ \AA}$ )
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /c (#14)
Unit cell dimensions	a = 10.37797(19) Å b = 9.68067(18) Å   β = 98.126(7) ° c = 20.4861(4) Å
Volume	V = 2037.48(7) Å <sup>3</sup>
Z	4
Density (calculated)	1.328 g/cm <sup>3</sup>
2θ <sub>max</sub>	55.0 °
Absorption coefficient μ for Mo-Kα	1.873 cm <sup>-1</sup>
F(000)	856.00
Crystal size	0.120 x 0.090 x 0.020 mm
No. of reflection collected	Total: 33730 Unique: 4683 ( $R_{\text{int}} = 0.0325$ ) min: 0.834, max: 0.996
Transmission factor	Full-matrix least-squares on F <sup>2</sup>
Refinement method	
Goodness-of-fit on F <sup>2</sup>	1.041
Final R indices [ $I > 2\sigma(I)$ ]	R <sub>1</sub> = 0.0380
R indices (all data)	R <sub>1</sub> = 0.0463      wR <sub>2</sub> = 0.0948
Largest diff. peak and hole	-0.35 and 0.45 e·Å <sup>-3</sup>

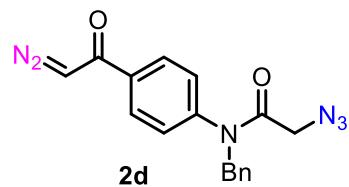
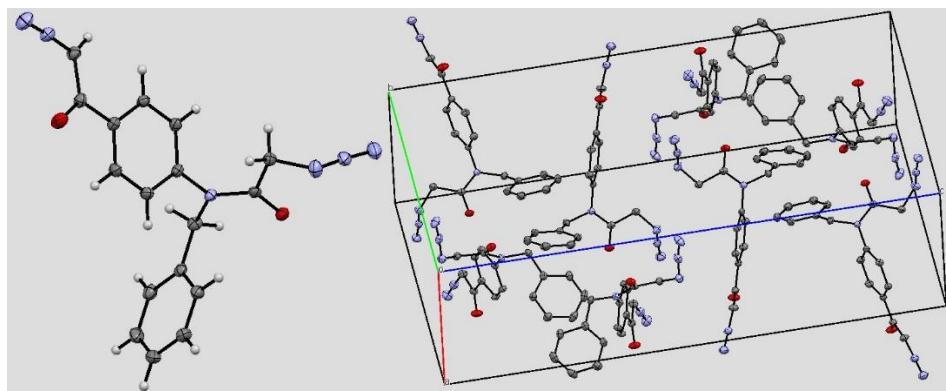
(2) Dimeric Amide **4i'** (CCDC No. 1839204, ORTEP thermal ellipsoids at 50% probability)



Empirical formula	C <sub>15</sub> H <sub>13</sub> NO <sub>2</sub>	
Formula weight	239.27	
Temperature	-170 ± 1 °C	
Wavelength	MoKα ( $\lambda = 0.71075 \text{ \AA}$ )	
Crystal system	monoclinic	
Space group	P2 <sub>1</sub> /c (#14)	
Unit cell dimensions	$a = 12.9092(4) \text{ \AA}$ $b = 5.32654(15) \text{ \AA}$ $\beta = 98.180(7)^\circ$ $c = 17.0164(5) \text{ \AA}$	
Volume	$V = 1158.17(6) \text{ \AA}^3$	
Z	4	
Density (calculated)	1.372 g/cm <sup>3</sup>	
$2\theta_{\max}$	55.0 °	
Absorption coefficient $\mu$ for Mo-Kα	0.915 cm <sup>-1</sup>	
$F(000)$	504.00	
Crystal size	0.200 x 0.130 x 0.060 mm	
No. of reflection collected	Total: 10780 Unique: 2643 ( $R_{\text{int}} = 0.0160$ )	
Transmission factor	min: 0.902, max: 0.995	
Refinement method	Full-matrix least-squares on $F^2$	
Goodness-of-fit on $F^2$	1.049	
Final R indices [ $I > 2\sigma(I)$ ]	$R_1 = 0.0361$	
R indices (all data)	$R_1 = 0.0397$	wR <sub>2</sub> = 0.0973
Largest diff. peak and hole	0.41 and -0.16 e·Å <sup>-3</sup>	

(3)  $\alpha$ -Diazoo Ketone Possessing  $\alpha$ -Azido amido moiety **2d**

(CCDC No.1839203, ORTEP thermal ellipsoids at 50% probability)



Empirical formula	C <sub>17</sub> H <sub>14</sub> N <sub>6</sub> O <sub>2</sub>
Formula weight	334.34
Temperature	-170 ± 1 °C
Wavelength	MoKα ( $\lambda = 0.71075 \text{ \AA}$ )
Crystal system	orthorhombic
Space group	Pbca (#61)
Unit cell dimensions	$a = 8.17797(15) \text{ \AA}$ $b = 14.6247(3) \text{ \AA}$ $c = 27.2033(5) \text{ \AA}$
Volume	$V = 3253.52(10) \text{ \AA}^3$
Z	8
Density (calculated)	1.365 g/cm <sup>3</sup>
$2\theta_{\max}$	55.0 °
Absorption coefficient $\mu$ for Mo-Kα	0.951 cm <sup>-1</sup>
$F(000)$	1392.00
Crystal size	0.190 x 0.060 x 0.030 mm
No. of reflection collected	Total: 52120 Unique: 3740 ( $R_{\text{int}} = 0.0341$ )
Transmission factor	min: 0.890, max: 0.997
Refinement method	Full-matrix least-squares on $F^2$
Goodness-of-fit on $F^2$	1.034
Final R indices [ $\Delta > 2\sigma(\Delta)$ ]	$R_1 = 0.0367$
R indices (all data)	$R_1 = 0.0432$ $wR_2 = 0.0897$
Largest diff. peak and hole	-0.22 and 0.35 e·Å <sup>-3</sup>