

*Electronic Supplementary Information for*

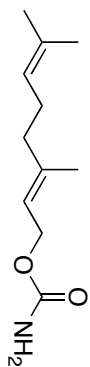
**Synthesis of Manzacidin A and C: Efficient Construction of Quaternary Stereocenters Bearing Nitrogen by Allyl Cyanate-to-isocyanate Rearrangement**

**Yoshiyasu Ichikawa,<sup>a</sup> Ken Okumura,<sup>a</sup> Yasunori Matsuda,<sup>a</sup> Tomoyuki Hasegawa,<sup>a</sup> Mitsuhiro Nakamura,<sup>b</sup> Aya Fujimoto,<sup>b</sup> Toshiya Masuda,<sup>b</sup> Hiyoshizo Kotsuki,<sup>a</sup> and Keiji Nakano<sup>a</sup>**

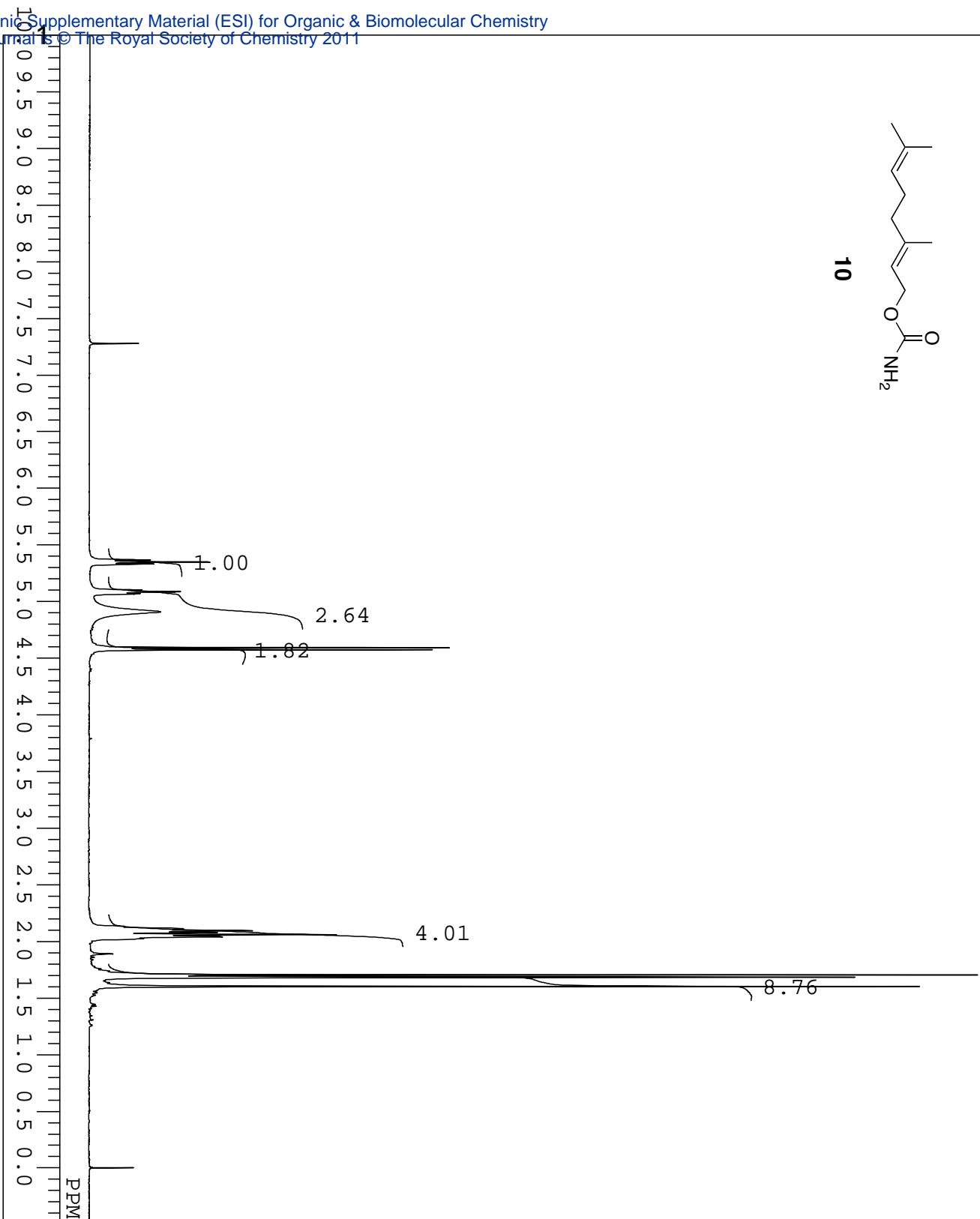
<sup>a</sup> Faculty of Science, Kochi University, Akebono-cho, Kochi 780-8520, Japan

<sup>b</sup> Faculty of Integrated Arts and Sciences, University of Tokushima, Tokushima 770-8502, Japan

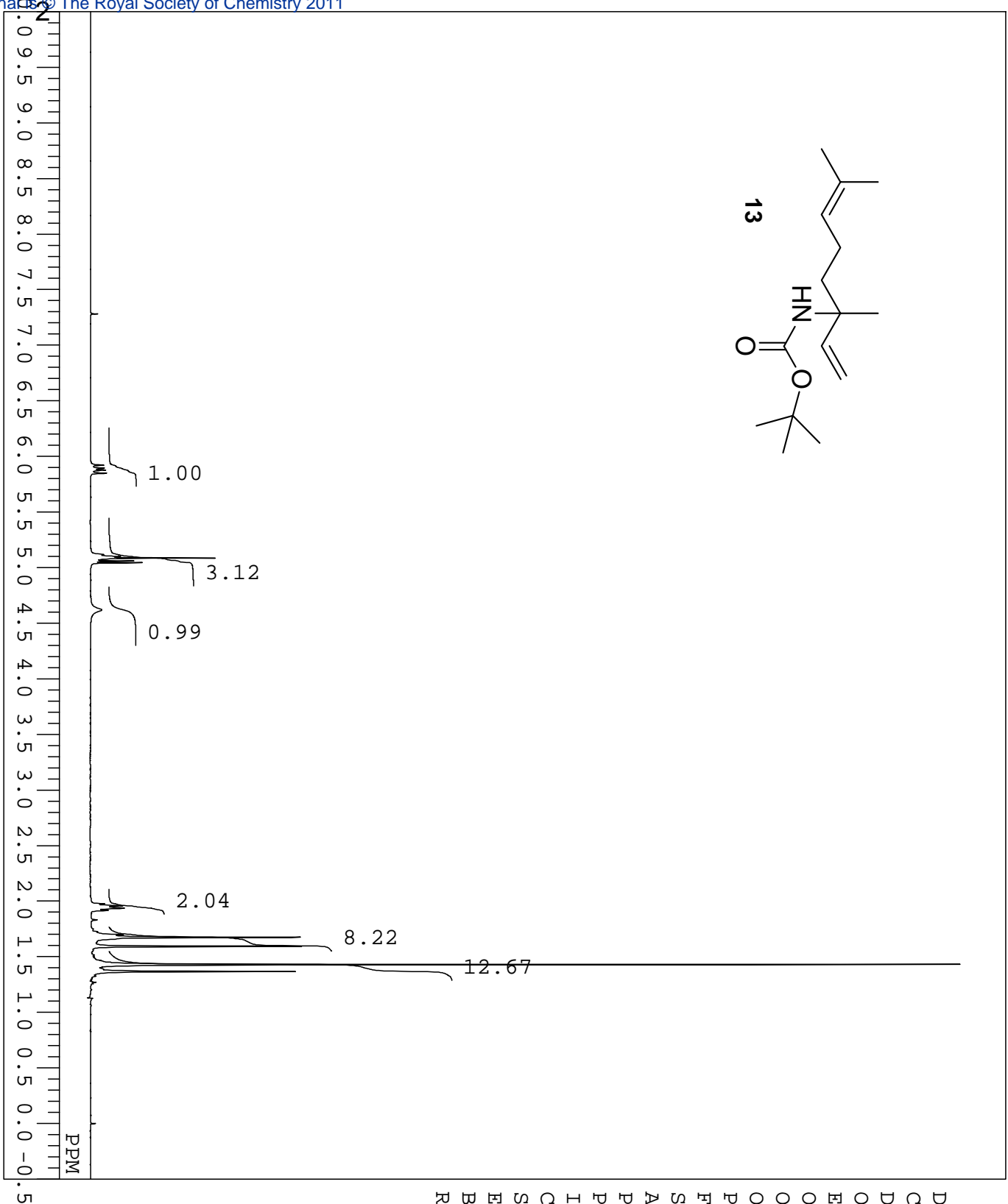
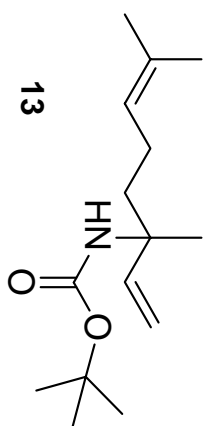
<sup>1</sup>H and <sup>13</sup>C NMR Spectra for All Relevant Compounds



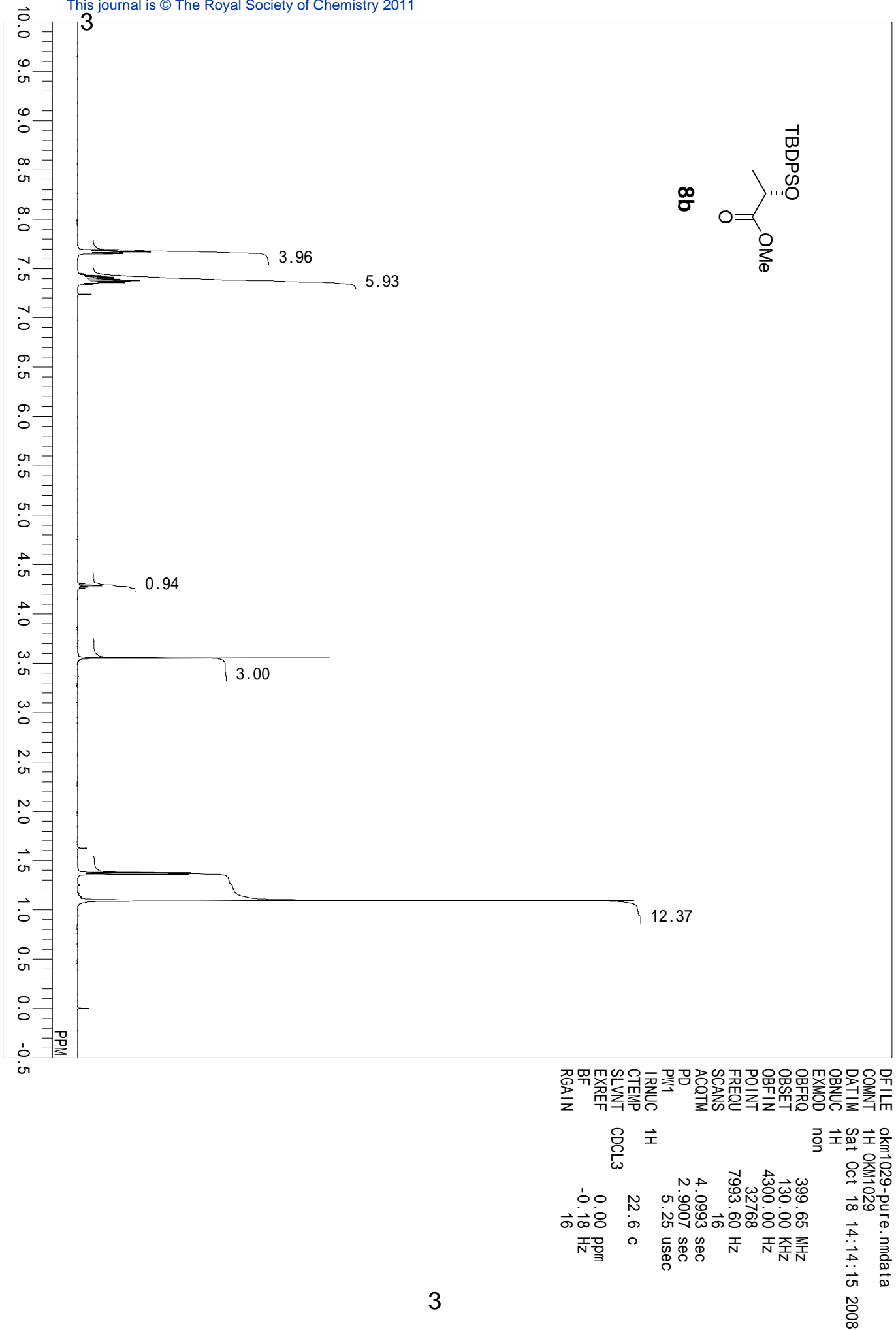
10

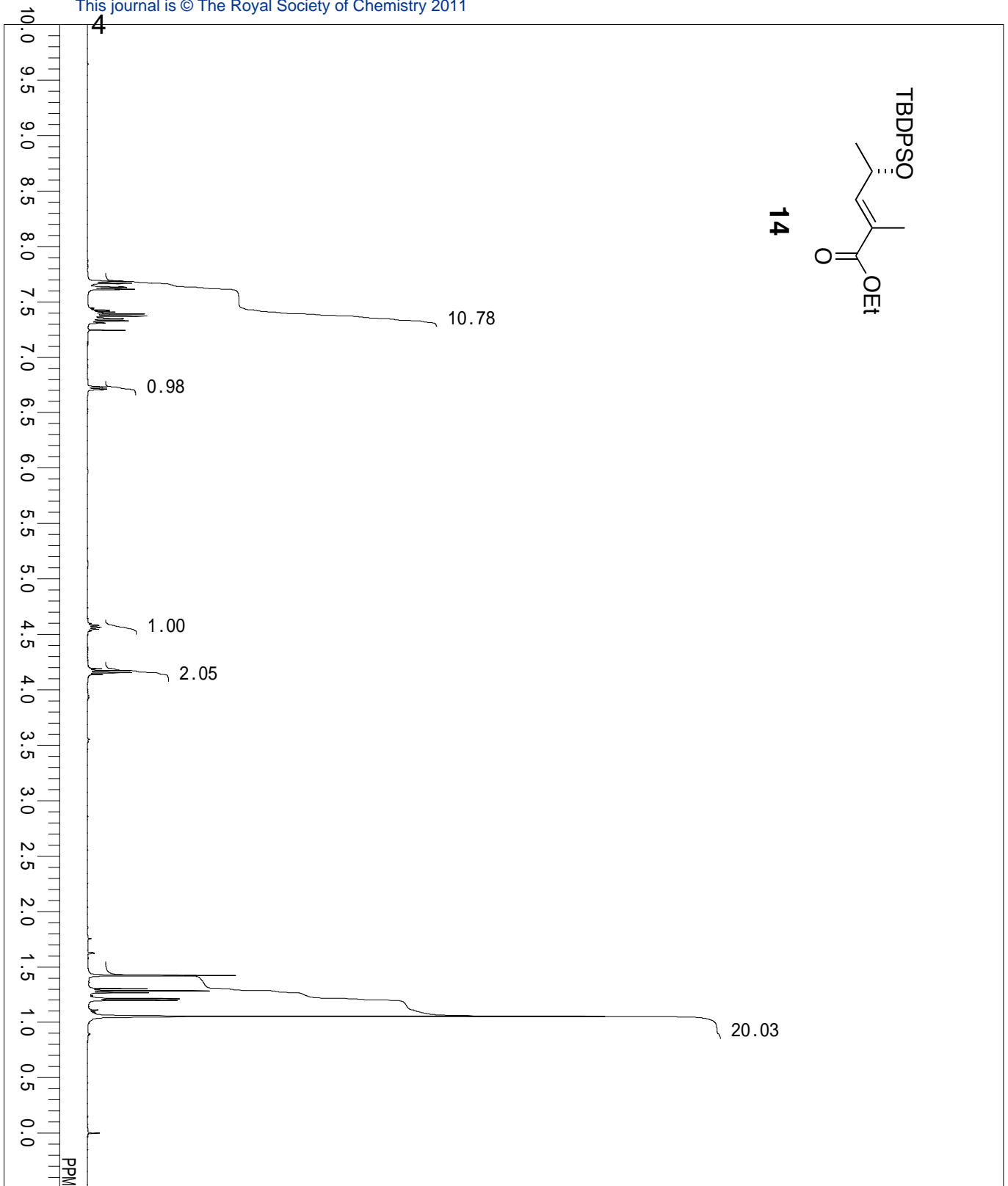


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OBSET	0.00	KHz
OBFIN	134300.00	Hz
POINT	8192	
FREQÜ	7993.60	Hz
SCANS	8	
ACQTM	1.0248	sec
PD	5.9752	sec
PWL	5.00	usec
IRNUC	1H	
CTEMP	22.7	C
SLVNT	CDCL3	
EXREF	0.00	ppm
BF	0.10	Hz
RGAIN	14	

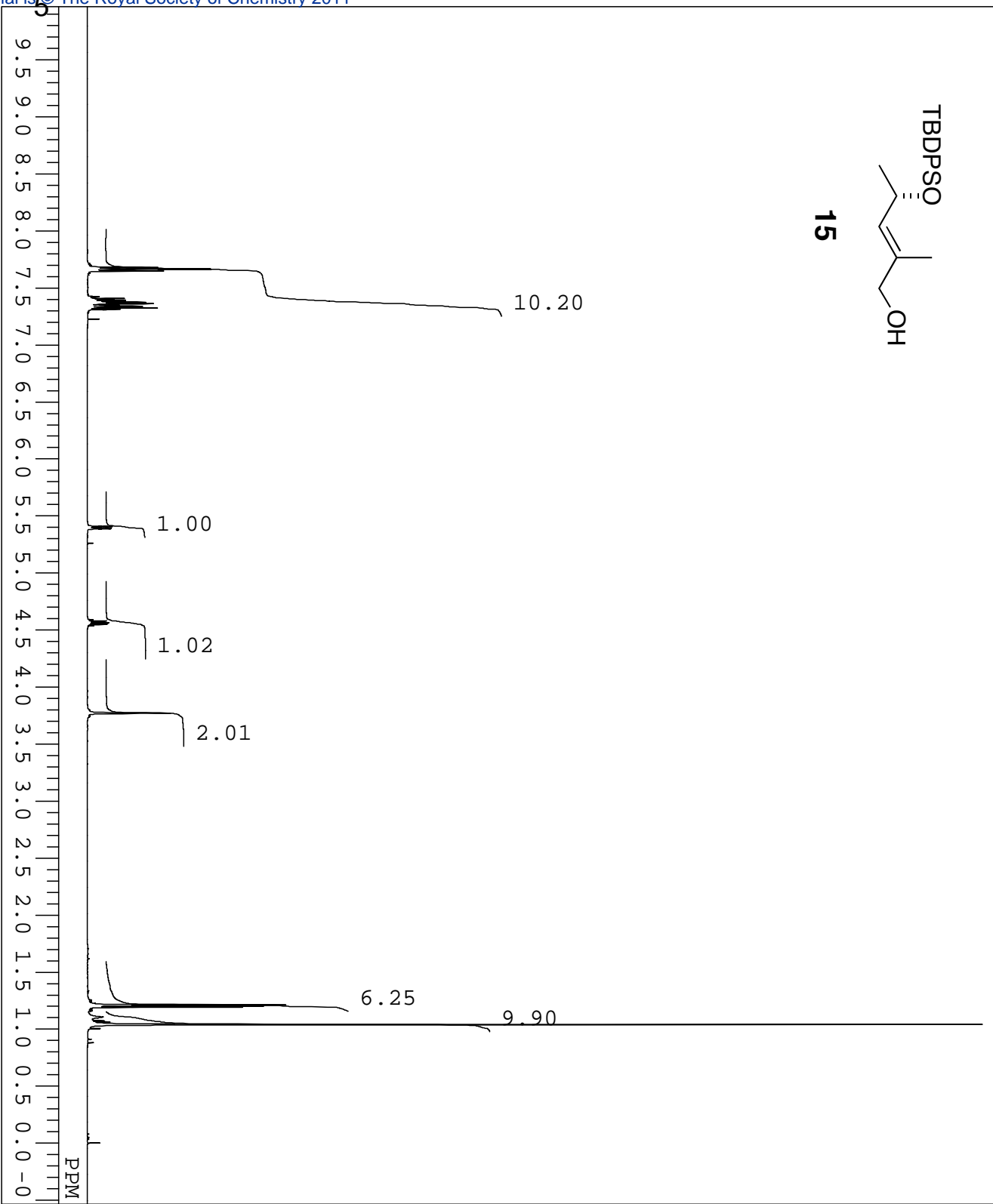
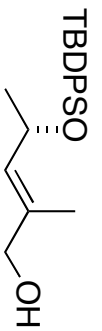


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 OBFIN 134300.00 Hz  
 POINT 8192  
 FREQU 7993.60 Hz  
 SCANS 4  
 ACQTM 1.0248 sec  
 PD 5.9752 sec  
 PW1 5.00 usec  
 IRNUC 1H  
 CTEMP 24.1 C  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF 0.10 Hz  
 RGAIN 13

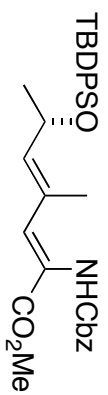




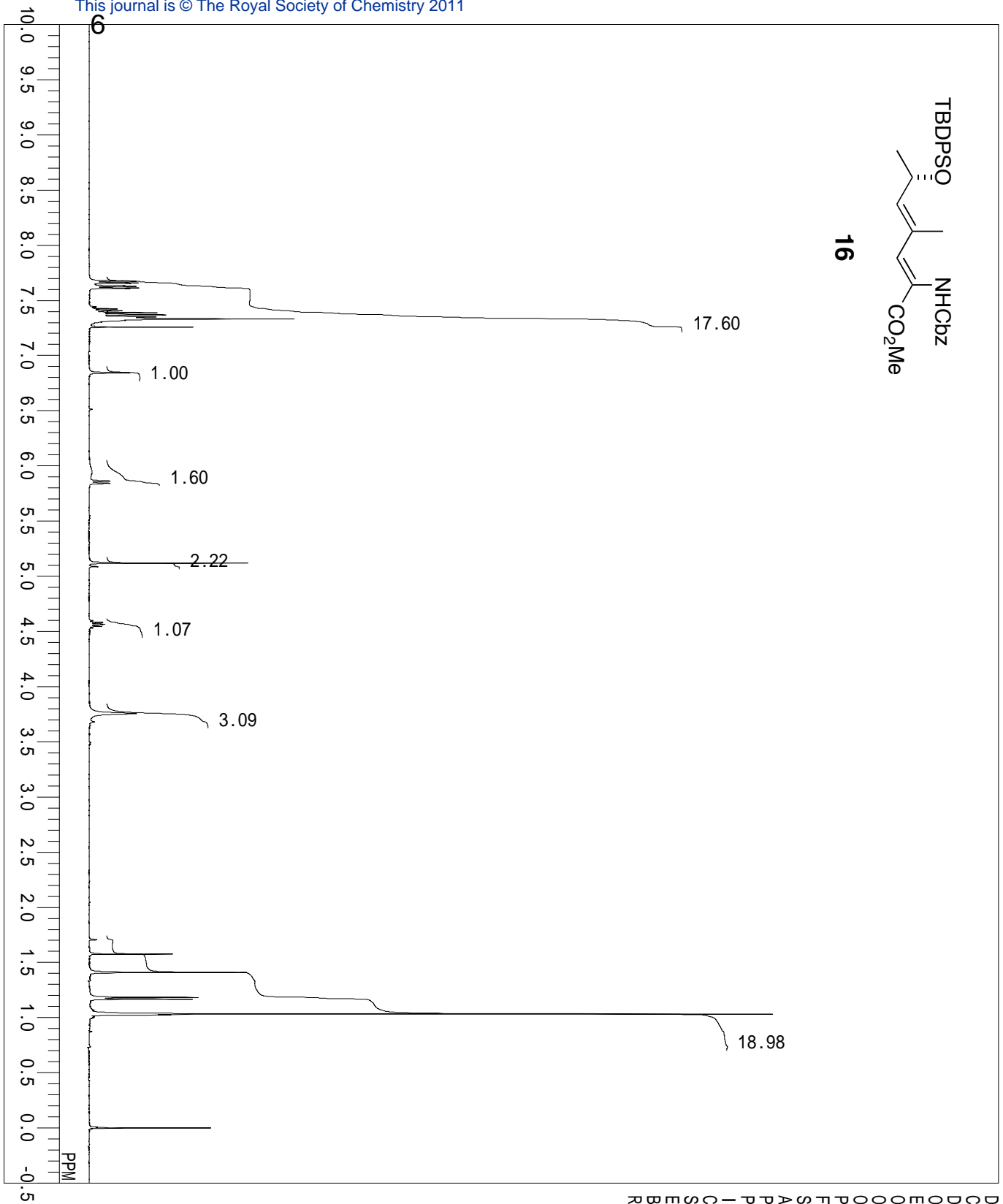
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EXMOD non  
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OBSET 130.00 KHz  
OBFIN 4300.00 Hz  
POINT 32768  
FREQ 7993.60 Hz  
SCANS 16  
ACQTM 4.0993 sec  
PD 2.9007 sec  
PW 5.25 usec  
IRNUC 1H  
CTEMP 23.4 C  
SLVNT CDCL3  
EXREF 0.00 ppm  
BF -0.18 Hz  
RGAIN 16



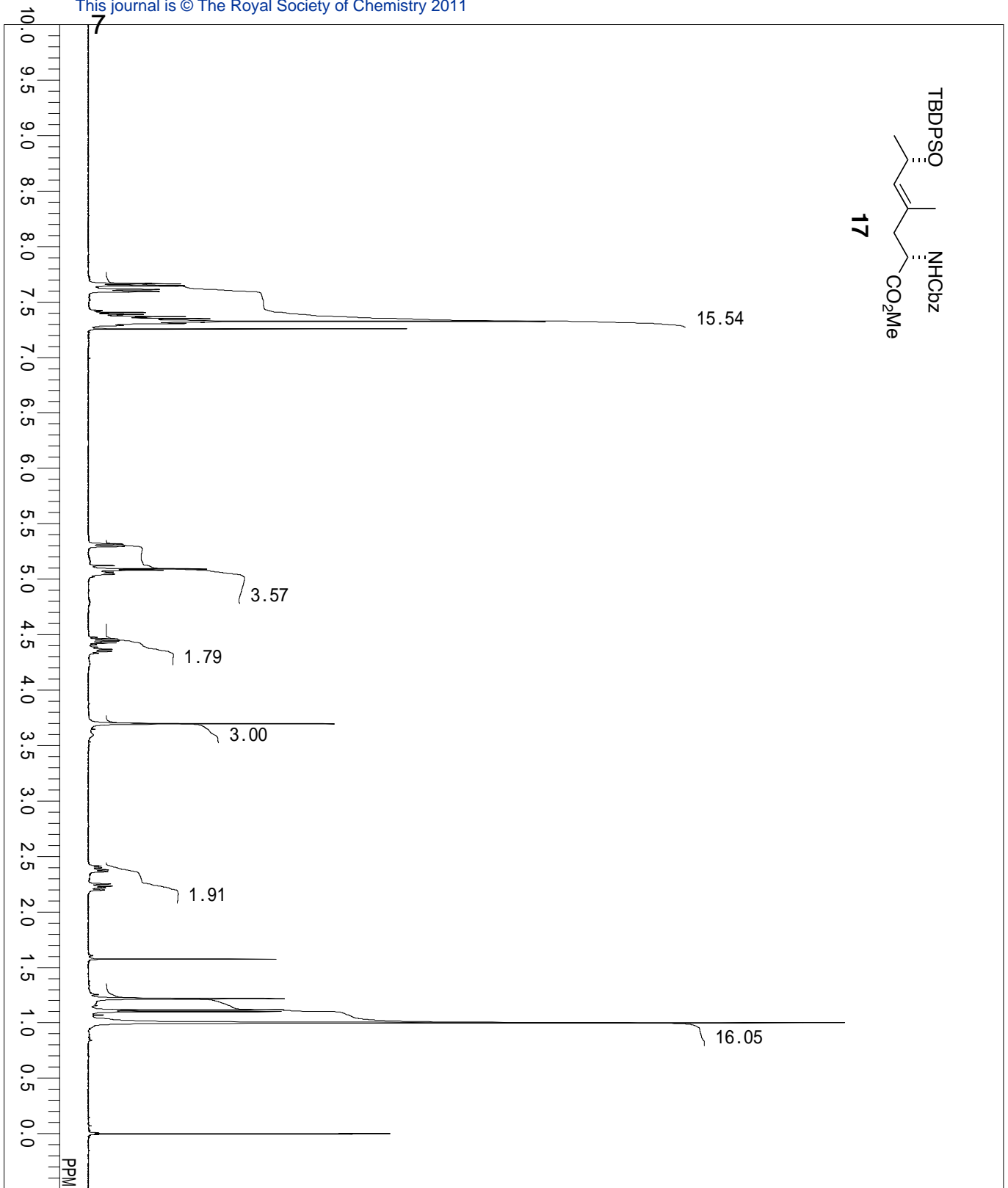
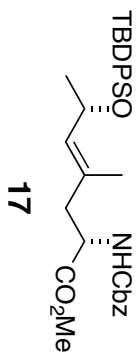
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DATIM 2010-09-17 21:39:25  
OBNUC 1H  
EXMOD proton.jxp  
OBFRO 500.16 MHz  
OBSET 2.41 KHz  
OBFIN 6.01 Hz  
POINT 16400  
FREQU 9384.38 Hz  
SCANS 8  
ACQTM 1.7459 sec  
PD 5.0000 sec  
PWL 4.68 usec  
IRNUC 1H  
CTEMP 22.6 c  
SLVNT CDCL3  
EXREF 0.00 ppm  
BF 0.10 Hz  
RGAIN 30



**16**

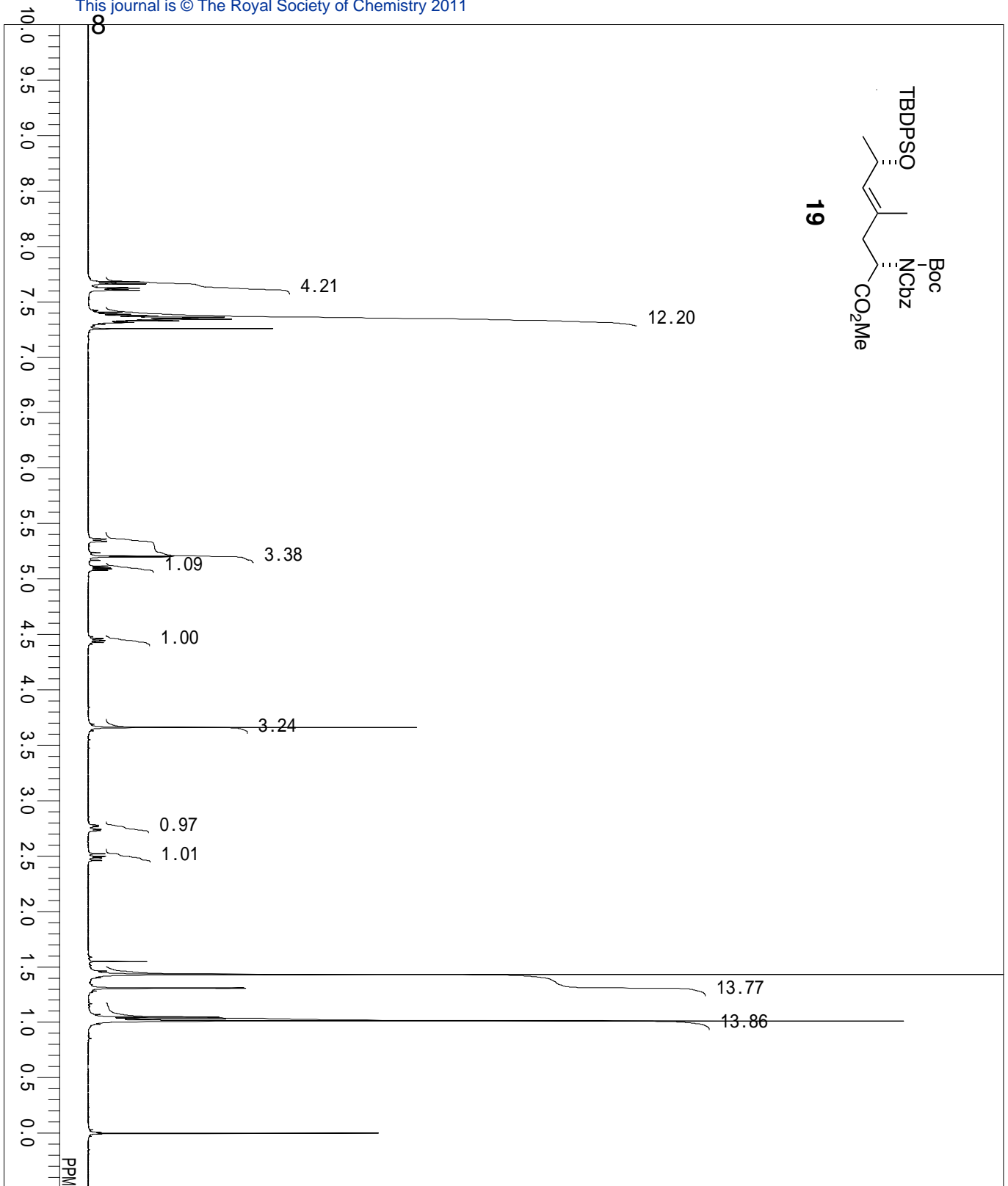


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 EXIMOD non  
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 OBFIN 4300.00 HZ  
 POINT 32768  
 FREQU 7993.60 HZ  
 SCANS 4  
 ACQTM 4.0993 sec  
 PD 2.9007 sec  
 PUL1 5.25 usec  
 IRNUC 1H  
 CTEMP 22.7 C  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF -0.18 HZ  
 RGA IN 22

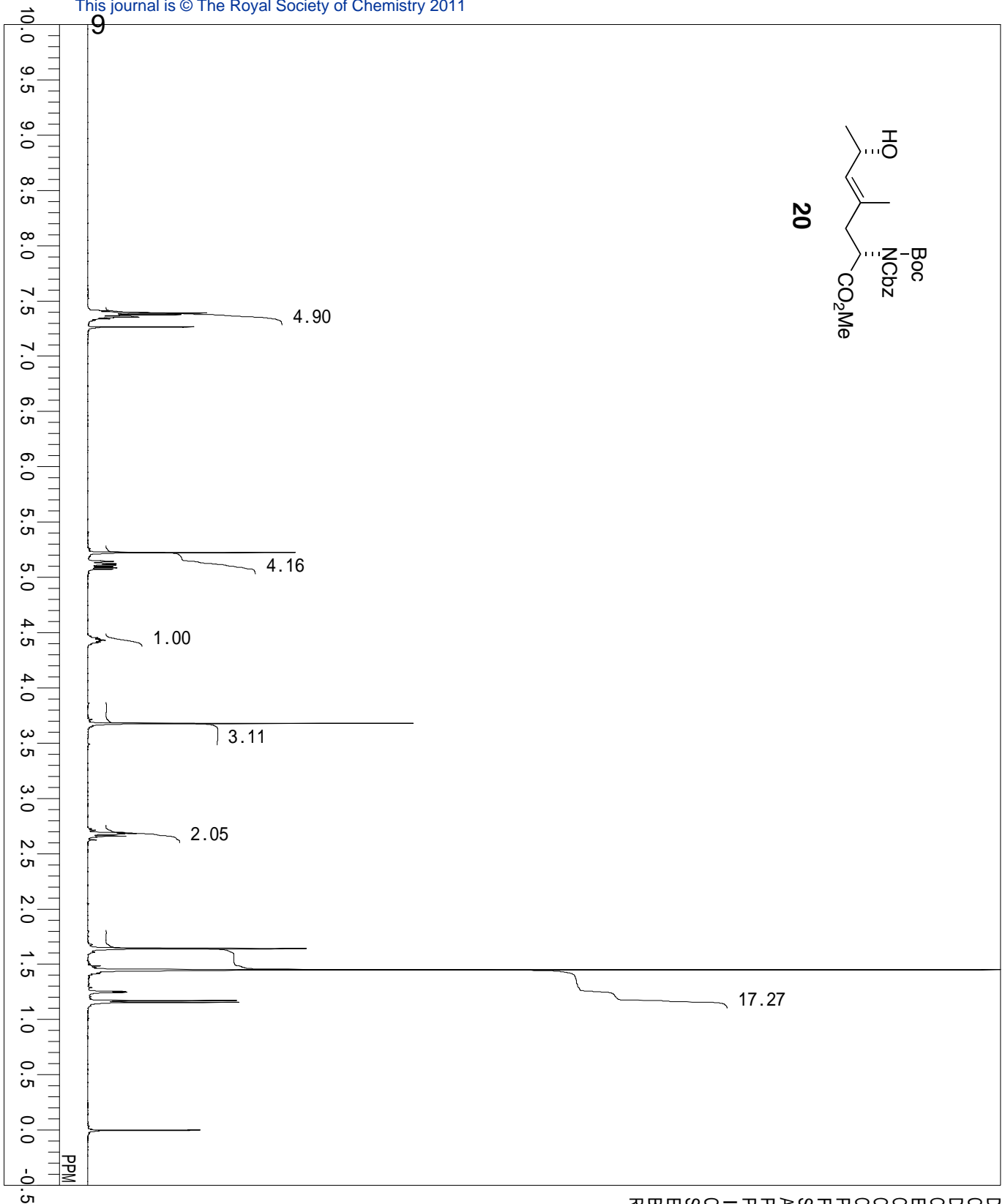
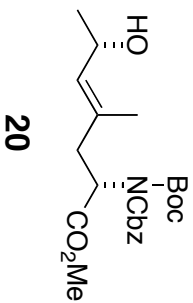


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 EXMOD non  
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 OBFIN 4300.00 Hz  
 POINT 32768  
 FREQU 7993.60 Hz  
 SCANS 4  
 ACQTM 4.0993 sec  
 PD 2.9007 sec  
 P1/1 5.25 usec  
 IRNUC 1H  
 CTEMP 21.9 C  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF -0.18 Hz  
 RGA IN 22

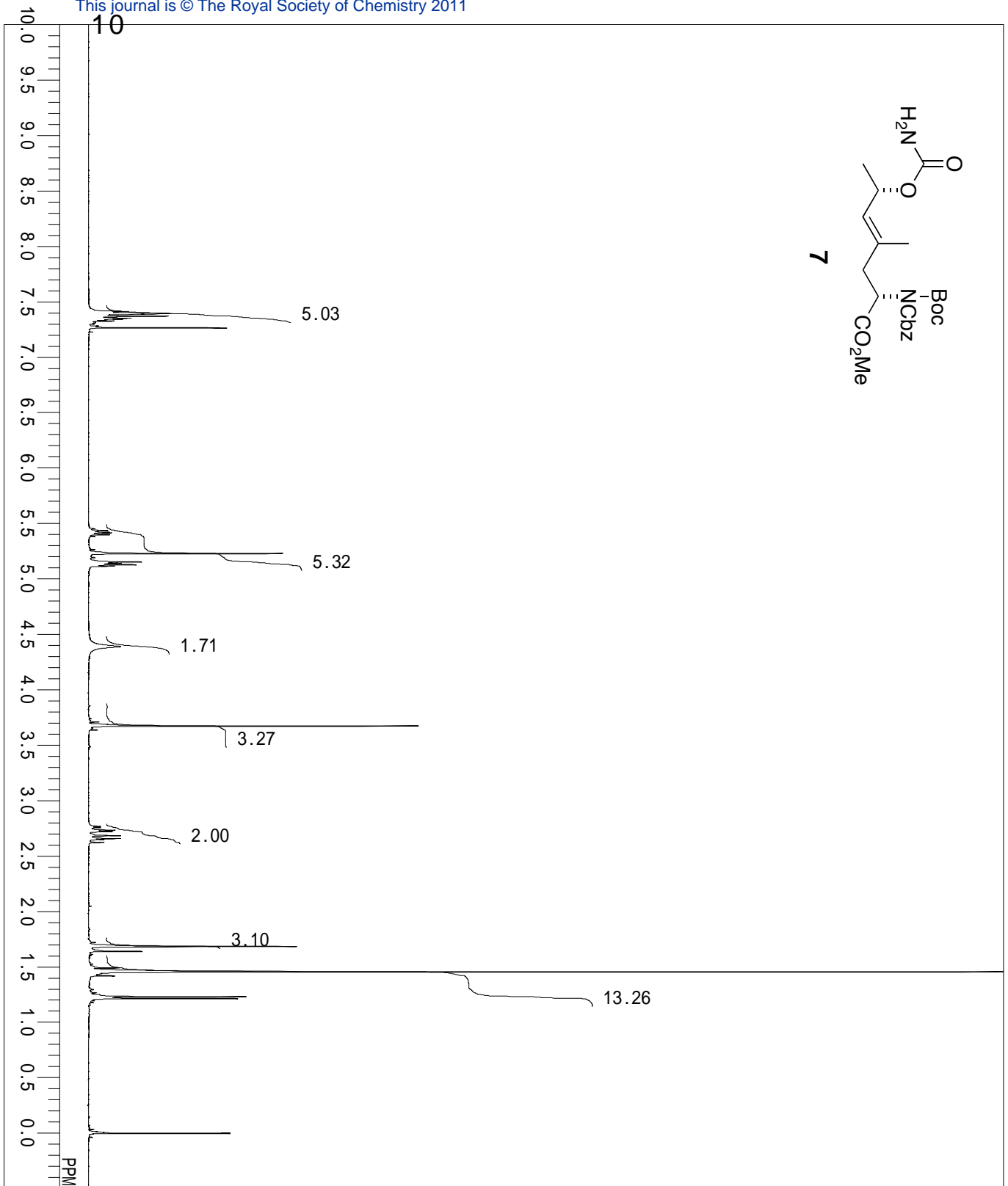




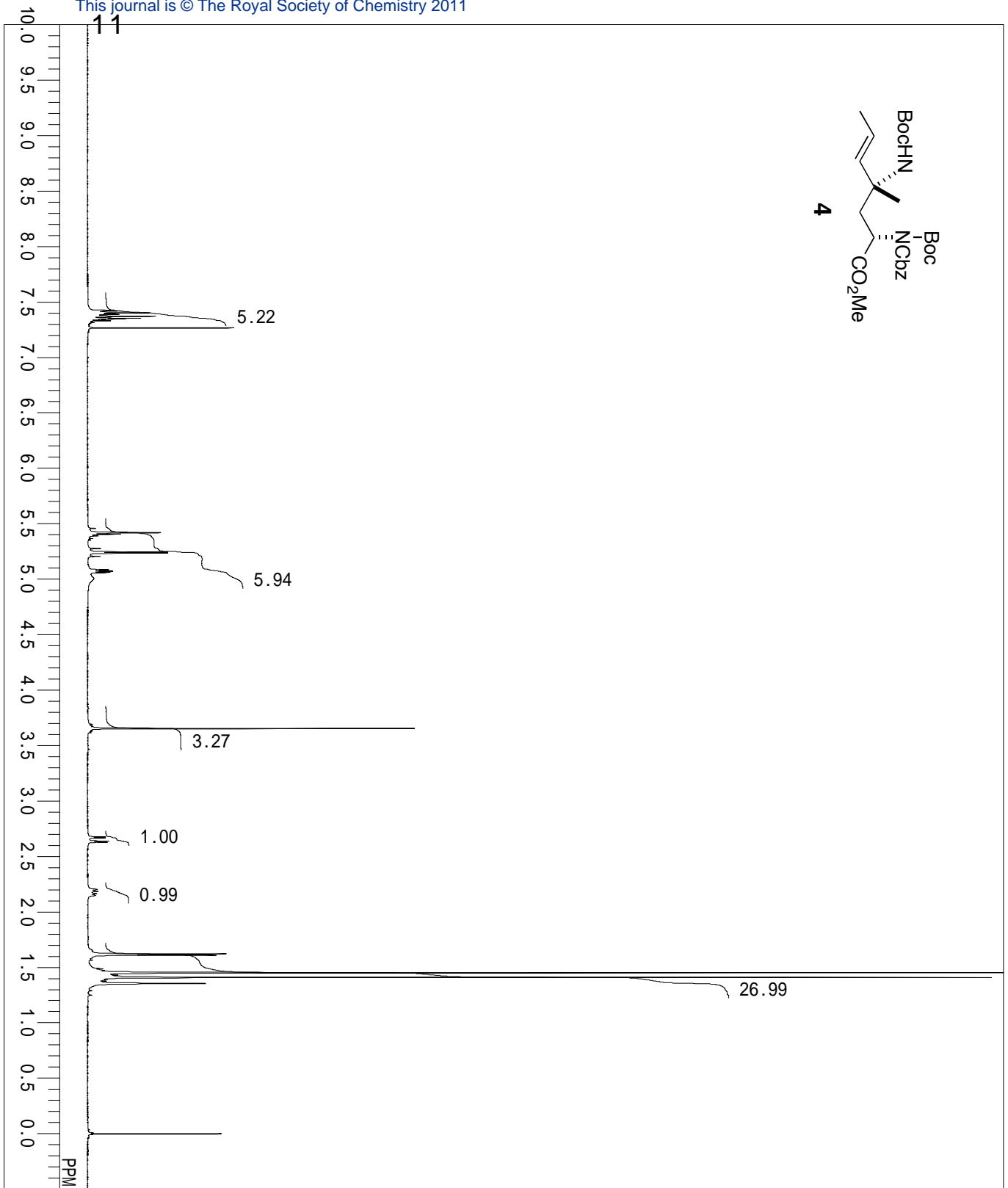
DF1LE okm4109.nmdata  
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 DATIM Fri Dec 19 13:43:31 2008  
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 EXMOD non  
 OBRQ 399.65 MHz  
 OBSET 130.00 KHz  
 OBFIN 4300.00 Hz  
 POINT 32768  
 FREQU 7993.60 Hz  
 SCANS 4  
 ACQTM 4.0993 sec  
 PD 2.9007 sec  
 PVI 7.00 usec  
 IRNUC 1H  
 CTEMP 23.1 C  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF -0.18 Hz  
 RGA IN 22



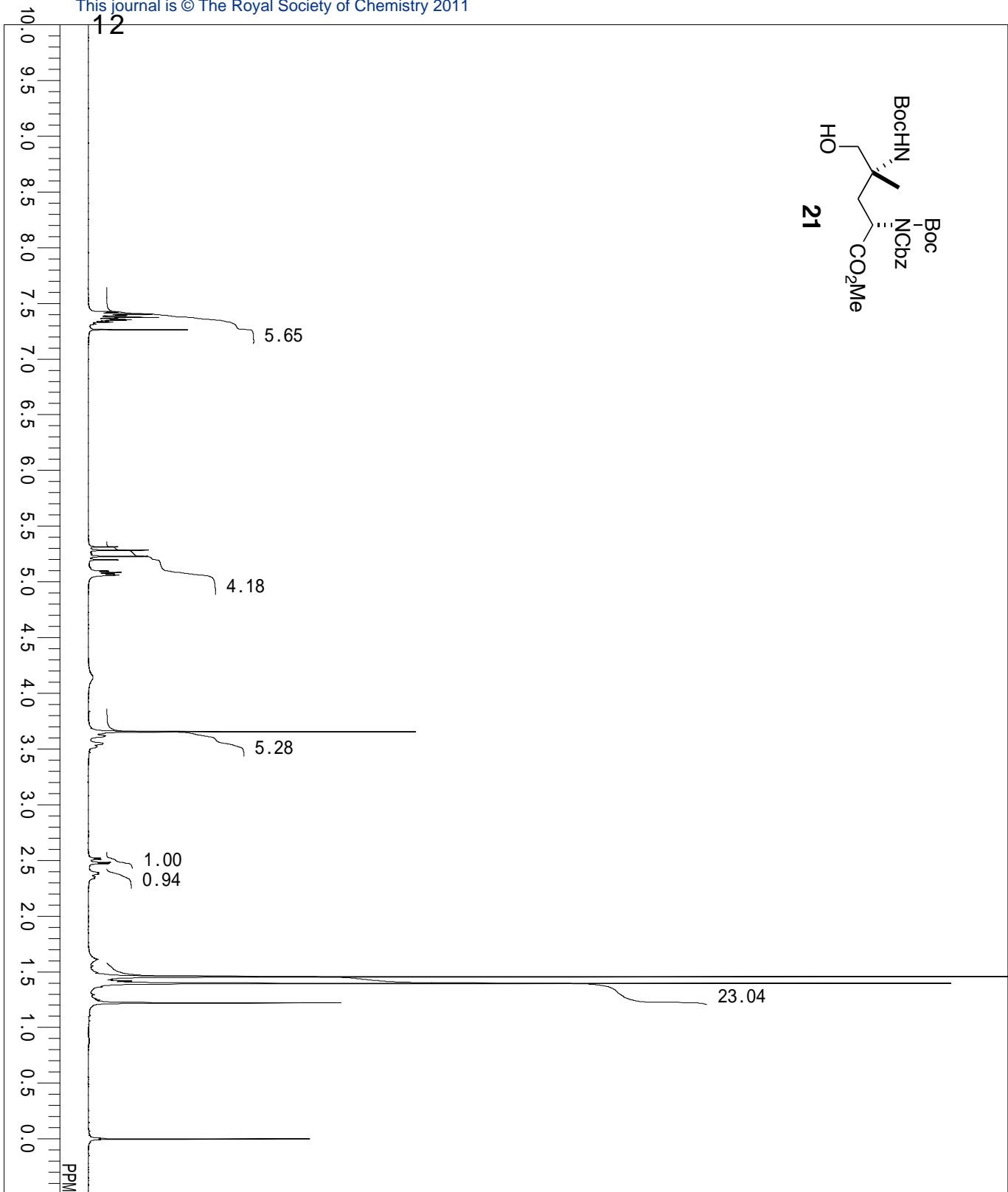
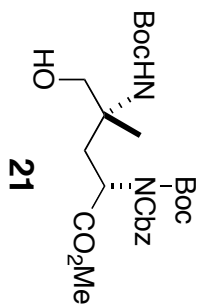
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 EXIMOD non  
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 OBSET 130.00 KHz  
 OBFIN 4300.00 Hz  
 POINT 32768  
 FREQU 7993.60 Hz  
 SCANS 4  
 ACQTM 4.0993 sec  
 PD 2.9007 sec  
 PM1 7.00 usec  
 IRNUC 1H  
 CTEMP 20.3 C  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF -0.18 Hz  
 RGA IN 21



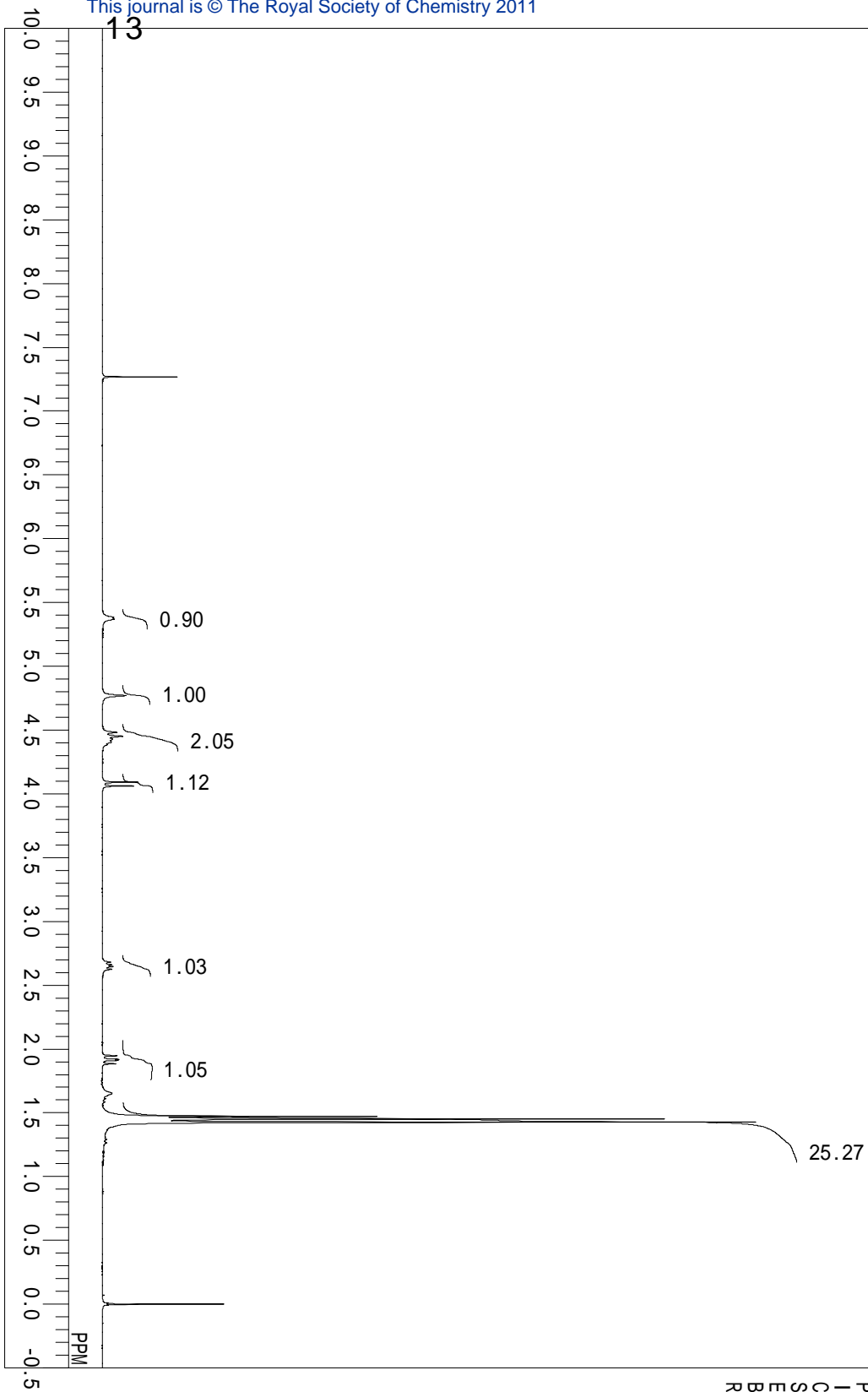
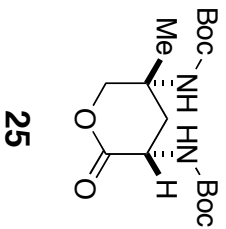
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 EXMOD non  
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 OBFIN 4300.00 HZ  
 POINT 32768  
 FREQU 7993.60 HZ  
 SCANS 4  
 ACQTM 4.0993 sec  
 PD 2.9007 sec  
 PUL1 7.00 usec  
 IRNUC 1H  
 CTEMP 19.7 C  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF -0.18 HZ  
 RGA IN 22



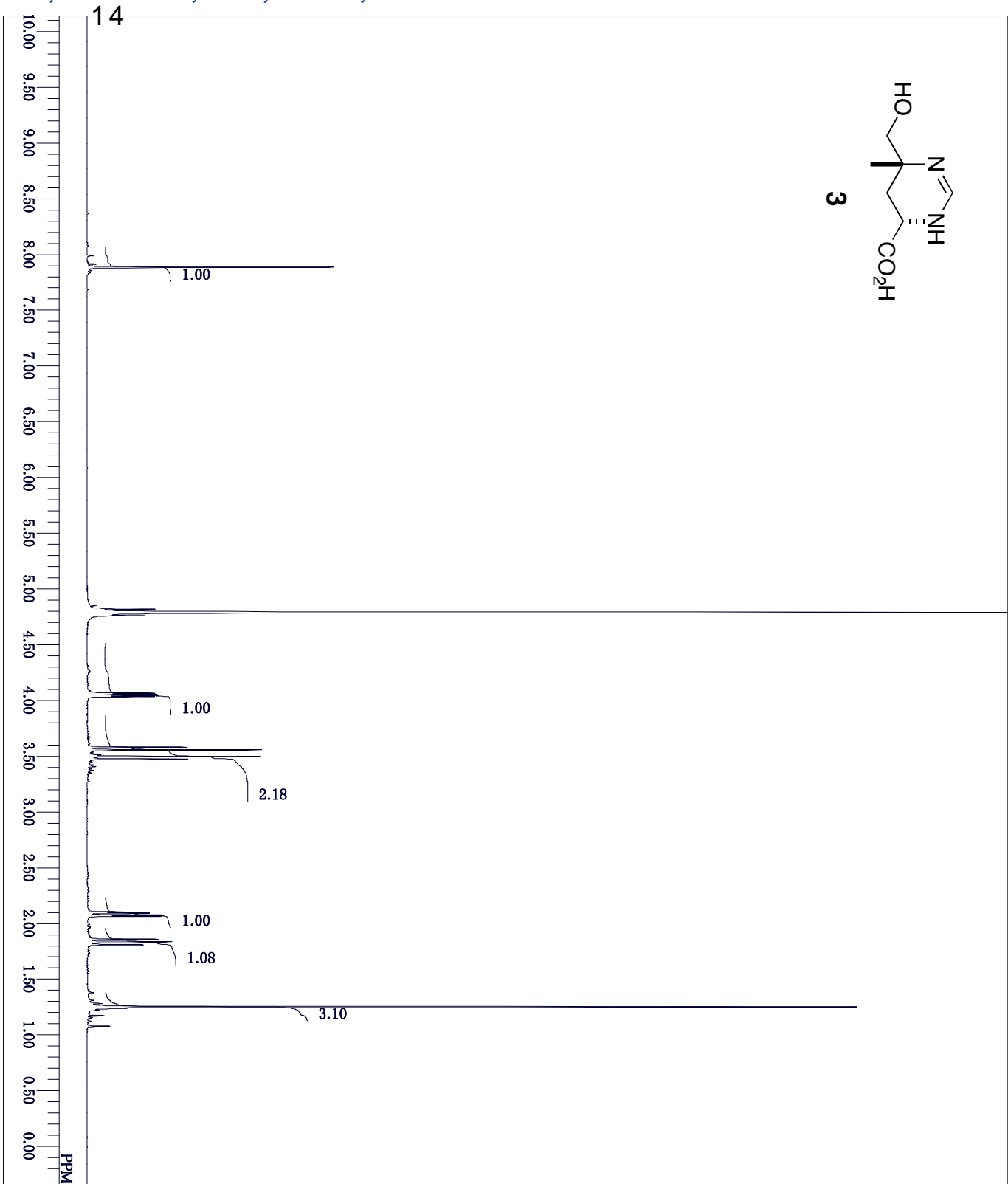
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 EXIMOD non  
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 OBFIN 4300.00 Hz  
 POINT 32768  
 FREQU 7993.60 Hz  
 SCANS 32  
 ACQTM 4.0993 sec  
 PD 2.9007 sec  
 P1/1 7.00 usec  
 IRNUC 1H  
 CTEMP 16.9 C  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF -0.18 Hz  
 RGA IN 19



DF FILE okm4137.nmdata  
 COMNT 1H OKM4137  
 DATIM Sun Mar 1 00:54:22 2009  
 OBNUC 1H  
 EXIMOD non  
 OBFRO 399.65 MHz  
 OBSET 130.00 KHz  
 OBFIN 4300.00 Hz  
 POINT 32768  
 FREQU 7993.60 Hz  
 SCANS 4  
 ACQTM 4.0993 sec  
 PD 2.9007 sec  
 PVI 7.00 usec  
 IRNUC 1H  
 CTEMP 22.2 C  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF -0.18 Hz  
 RGA IN 22

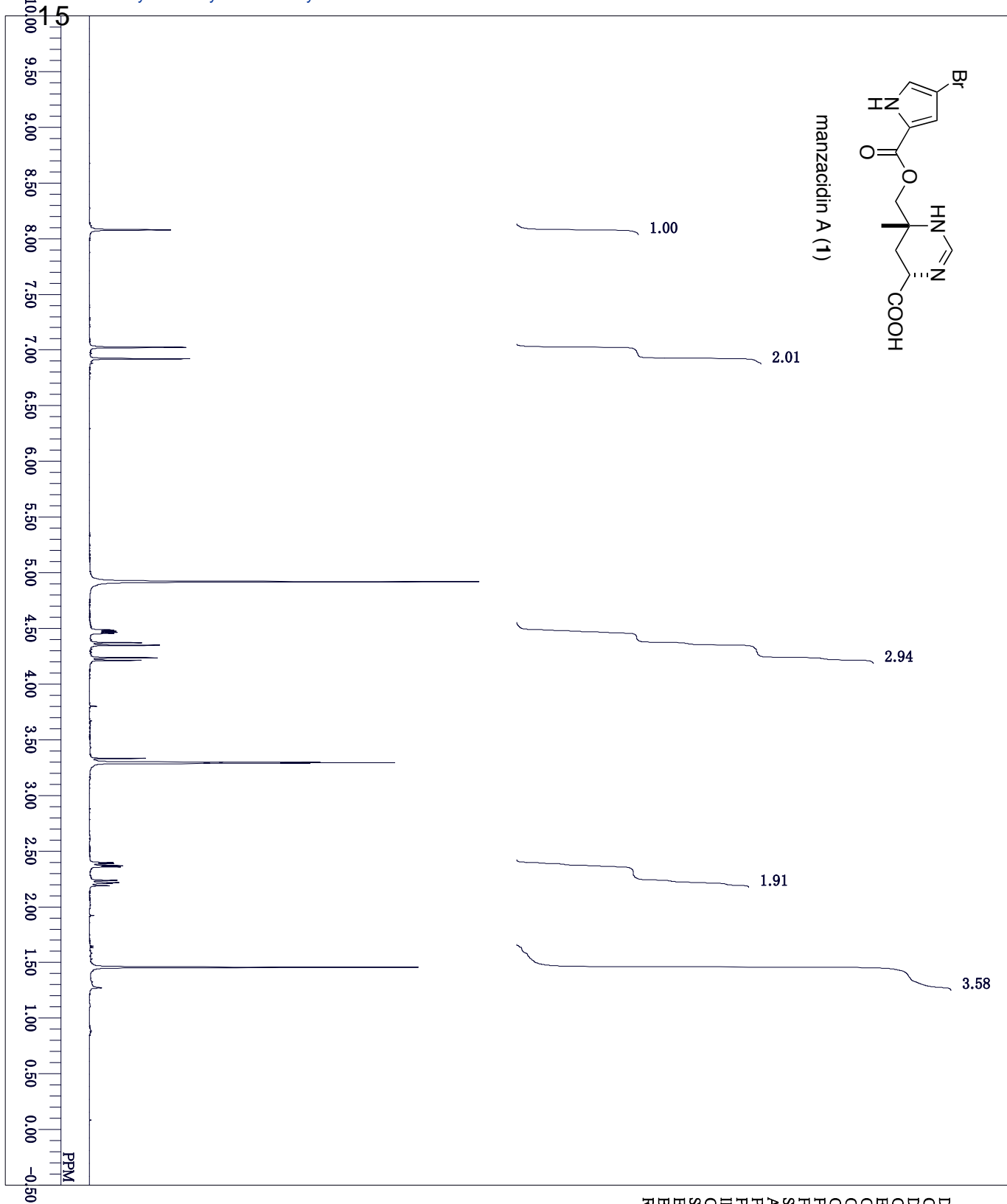


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 EXIMOD non  
 OBFRO 399.65 MHz  
 OBSET 130.00 KHZ  
 OBFIN 4300.00 HZ  
 POINT 32768  
 FREQU 7993.60 HZ  
 SCANS 4  
 ACQTM 4.0993 sec  
 PD 2.9007 sec  
 PVI 7.00 usec  
 IRNUC 1H  
 CTEMP 21.2 C  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF -0.18 HZ  
 RGA IN 20



DPFILE man 1061-pure-proton-1-1.jdt  
COMNT single-pulse  
DATIM 2011-02-23 17:13:51  
OBNUC 1H  
EXMOC proton.jxp  
OBFRO 500.16 MHz  
OBSFT 2.41 KHz  
OBRIN 6.01 Hz  
POINT 16400  
FREQU 9384.38 Hz  
SCANS 32  
ACQTM 1.7459 sec  
PD 5.0000 sec  
PWI 4.68 usec  
IRNUC 16.6 c  
CTEMP  
SLVNT  
EXREF  
BF  
RGAIN

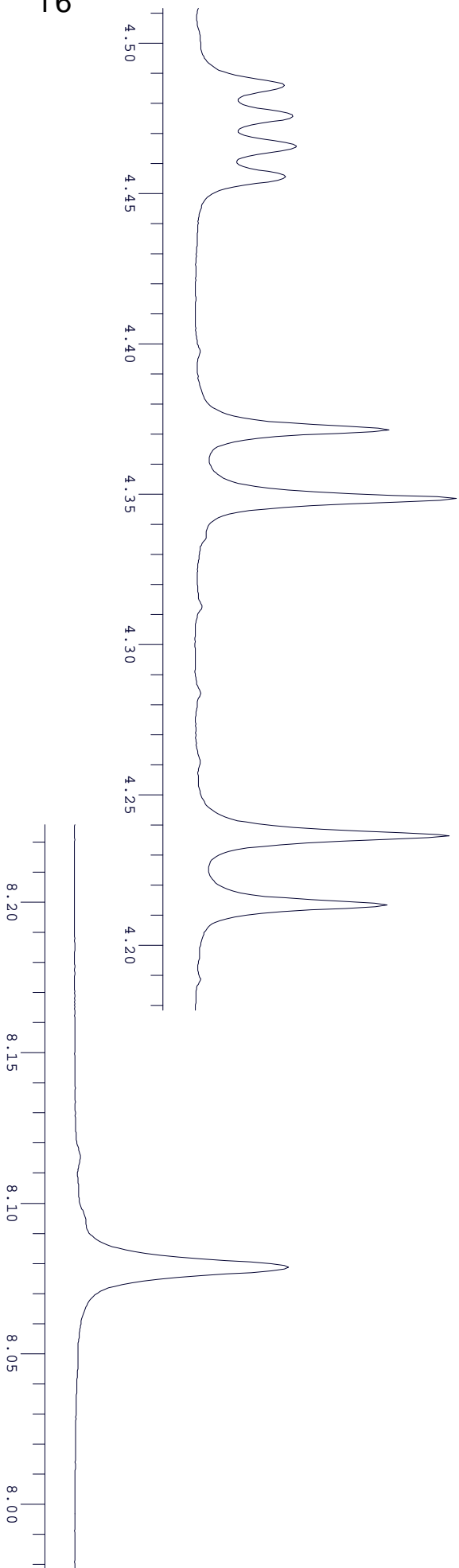
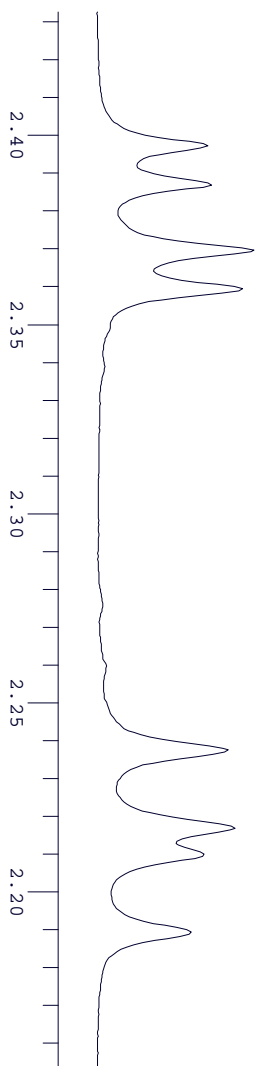
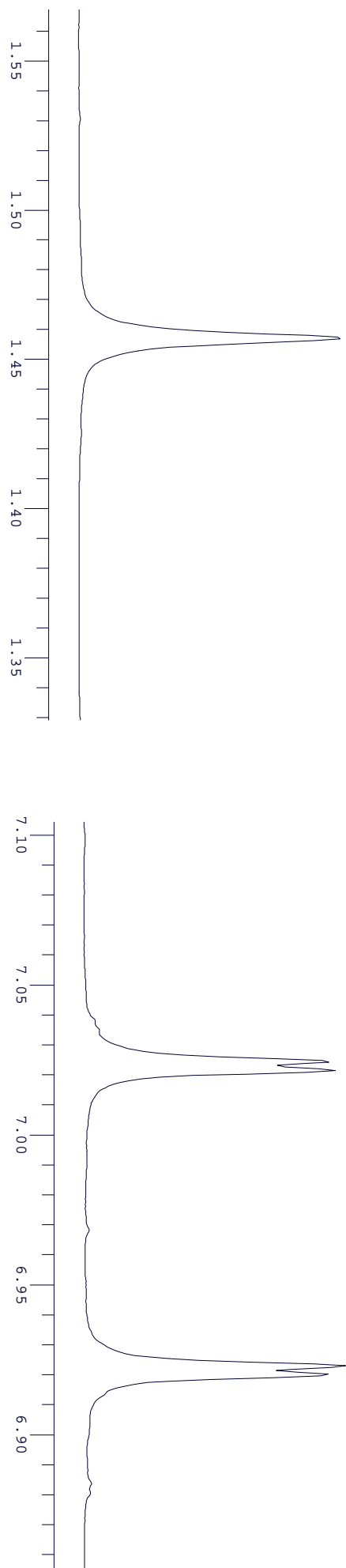
D2O 4.79 ppm  
0.12 Hz  
46



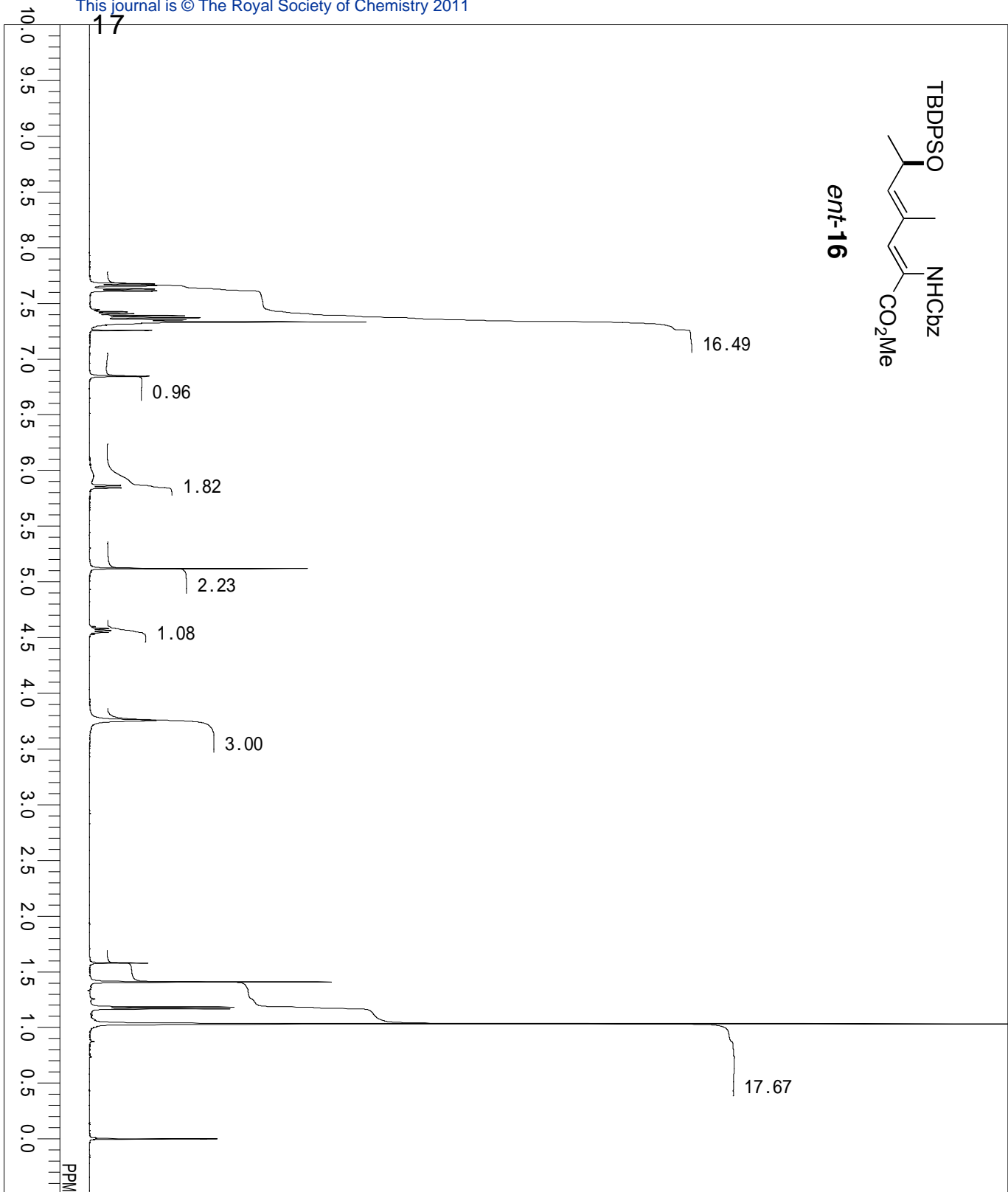
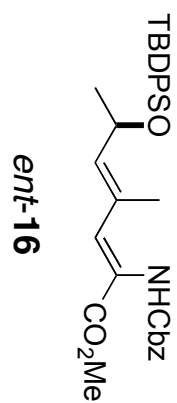
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 EXMVD proton.jxp  
 OBFRO 500.16 MHz  
 OBSET 2.41 KHz  
 OBRIN 6.01 Hz  
 POINT 26224  
 FREQU 7507.51 Hz  
 SCANS 8  
 ACQTM 3.4918 sec  
 PD 5.0000 sec  
 PW1 4.68 usec  
 IRNUC 1H  
 CTEMP 18.1 c  
 SLVNT CD3OD  
 EXREF 12.50 ppm  
 BF 0.12 Hz  
 RGAIN 50



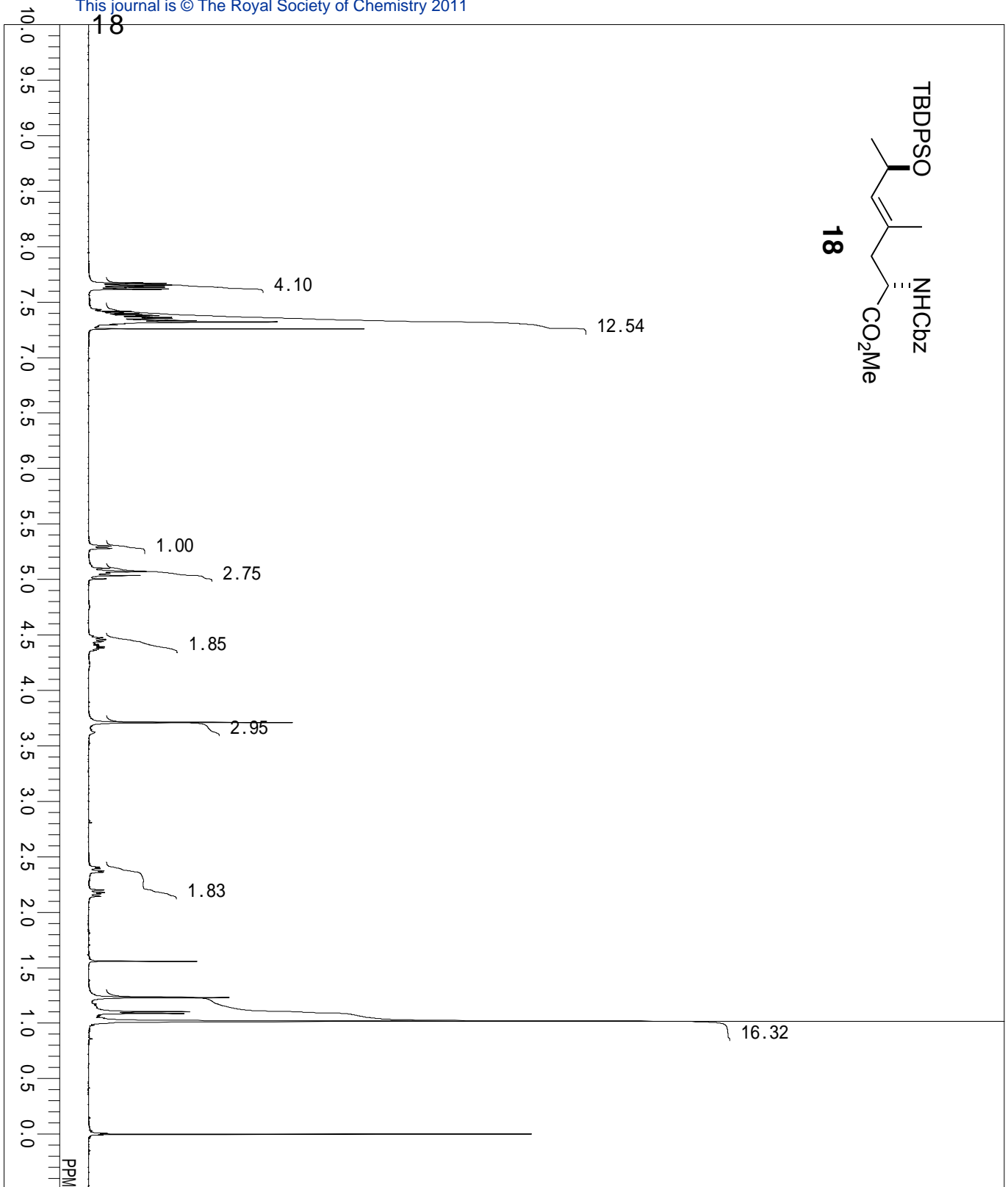
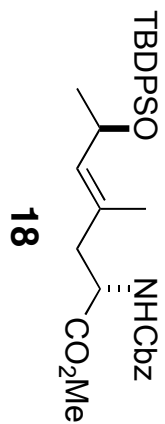
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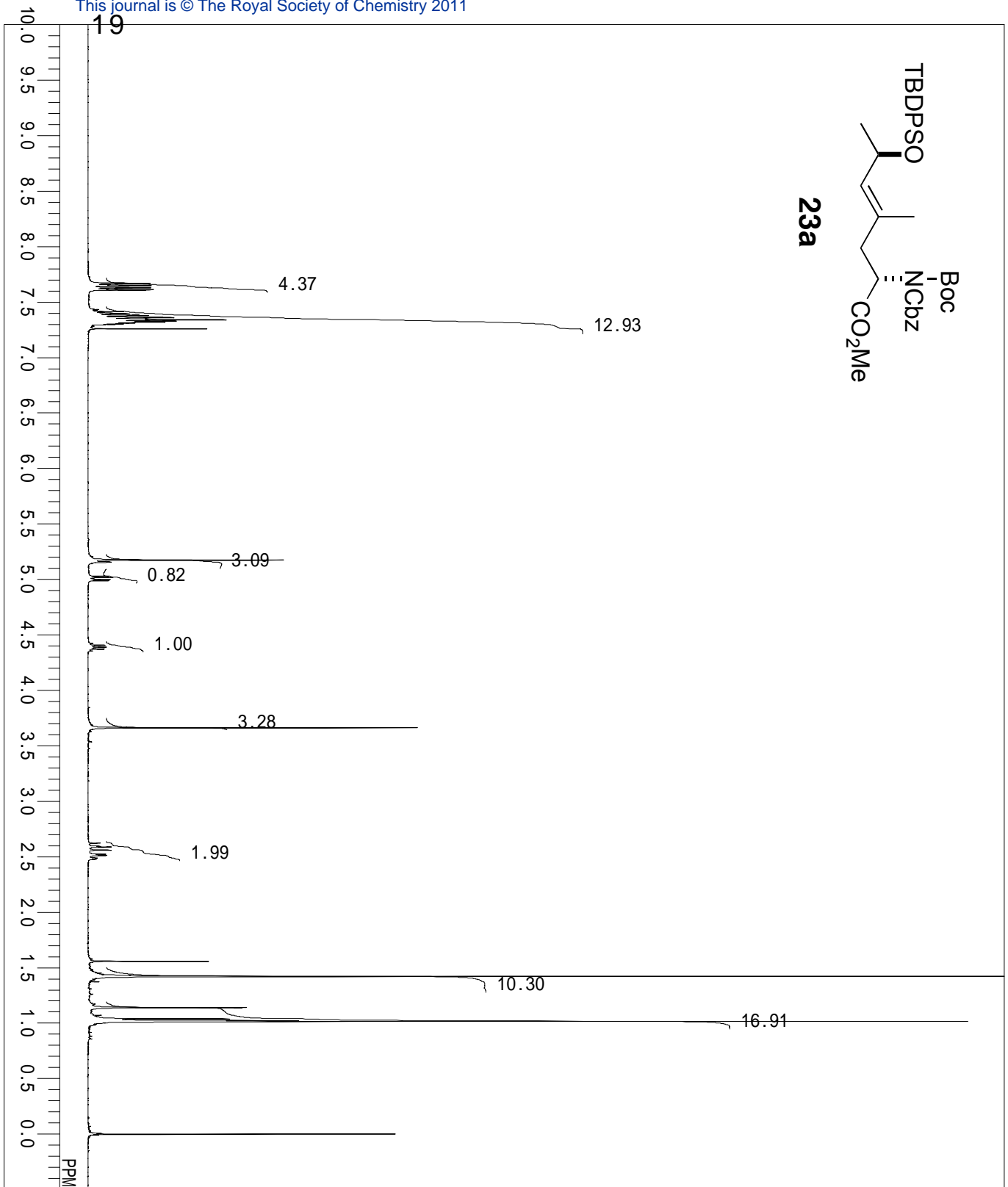
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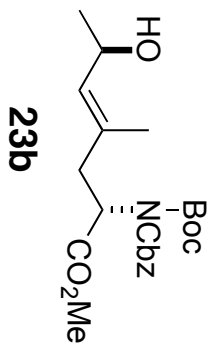
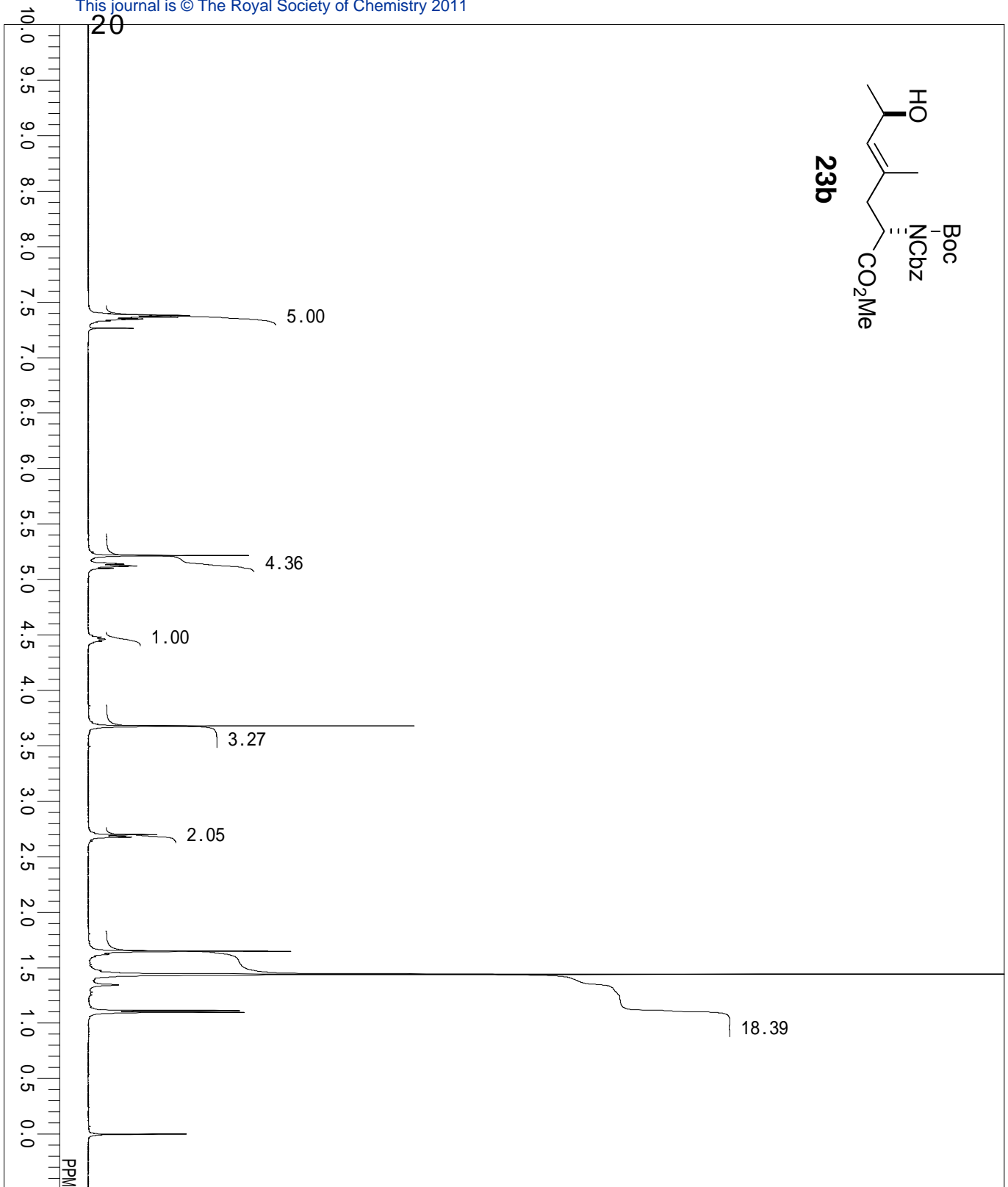
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 EXIMOD non  
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 OBSET 130.00 KHZ  
 OBFIN 4300.00 HZ  
 POINT 32768  
 FREQU 7993.60 HZ  
 SCANS 4  
 ACQTM 4.0993 sec  
 PD 2.9007 sec  
 P1/1 7.00 usec  
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 CTEMP 21.5 C  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF -0.18 HZ  
 RGA IN 20



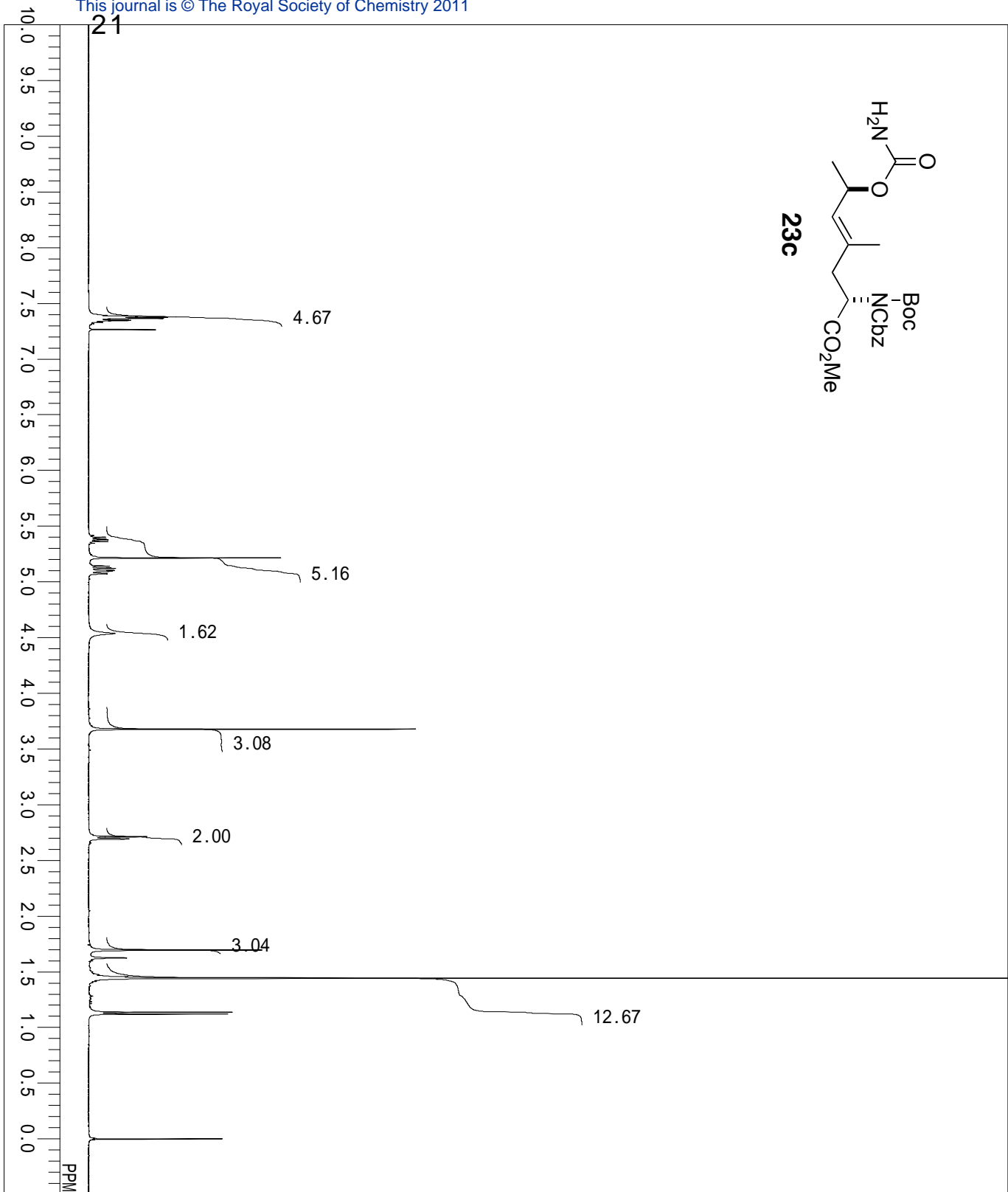
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 EXIMOD non  
 OBFRO 399.65 MHz  
 OBSET 130.00 KHz  
 OBFIN 4300.00 Hz  
 POINT 32768  
 FREQU 7993.60 Hz  
 SCANS 4  
 ACQTM 4.0993 sec  
 PD 2.9007 sec  
 PUL1 7.00 usec  
 IRNUC 1H  
 CTEMP 21.5 C  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF -0.18 Hz  
 RGA IN 22



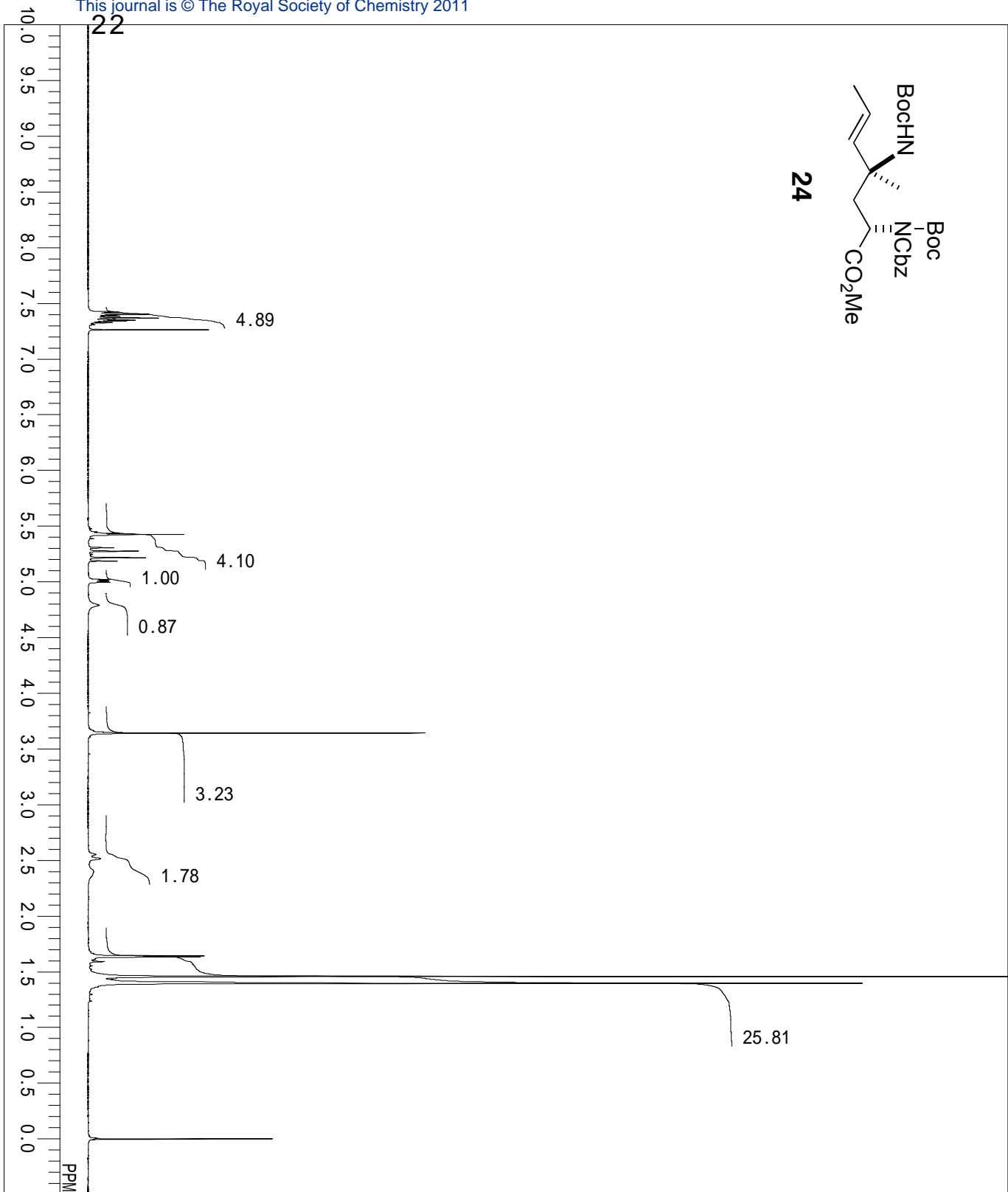
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 OBNUC 1H  
 EXIMOD non  
 OBFREQ 399.65 MHz  
 OBSET 130.00 KHz  
 OBFINT 4300.00 Hz  
 POINT 32768  
 FREQU 7993.60 Hz  
 SCANS 4  
 ACQTM 4.0993 sec  
 PD 2.9007 sec  
 P1 7.00 usec  
 IRNUC 1H  
 CTEMP 22.6 C  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF -0.18 Hz  
 RGA IN 22



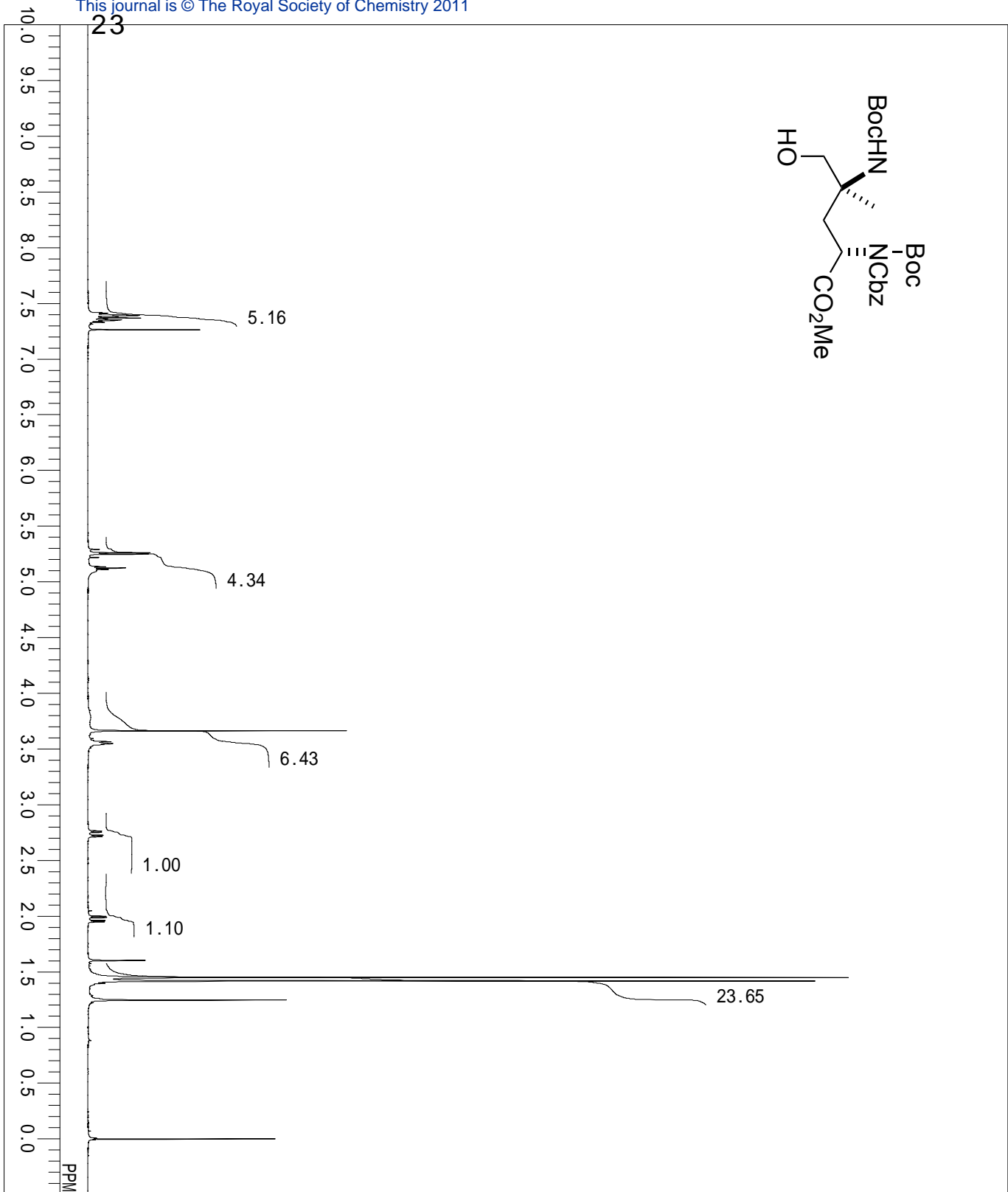
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 EXIMOD non  
 OBFRO 399.65 MHz  
 OBSET 130.00 KHz  
 OBFIN 4300.00 Hz  
 POINT 32768  
 FREQU 7993.60 Hz  
 SCANS 4  
 ACQTM 4.0993 sec  
 PD 2.9007 sec  
 PUL1 7.00 usec  
 IRNUC 1H  
 CTEMP 21.5 C  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF -0.18 Hz  
 RGA IN 20



DF FILE okm4141.nmdata  
 COMMENT 1H OKM4141  
 DATIM Thu Mar 5 15:37:58 2009  
 OBNUC 1H  
 EXIMOD non  
 OBFRO 399.65 MHz  
 OBSET 130.00 KHZ  
 OBFIN 4300.00 HZ  
 POINT 32768  
 FREQU 7993.60 HZ  
 SCANS 4  
 ACQTM 4.0993 sec  
 PD 2.9007 sec  
 PVI 7.00 usec  
 IRNUC 1H  
 CTEMP 21.6 C  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF -0.18 HZ  
 RGA IN 22

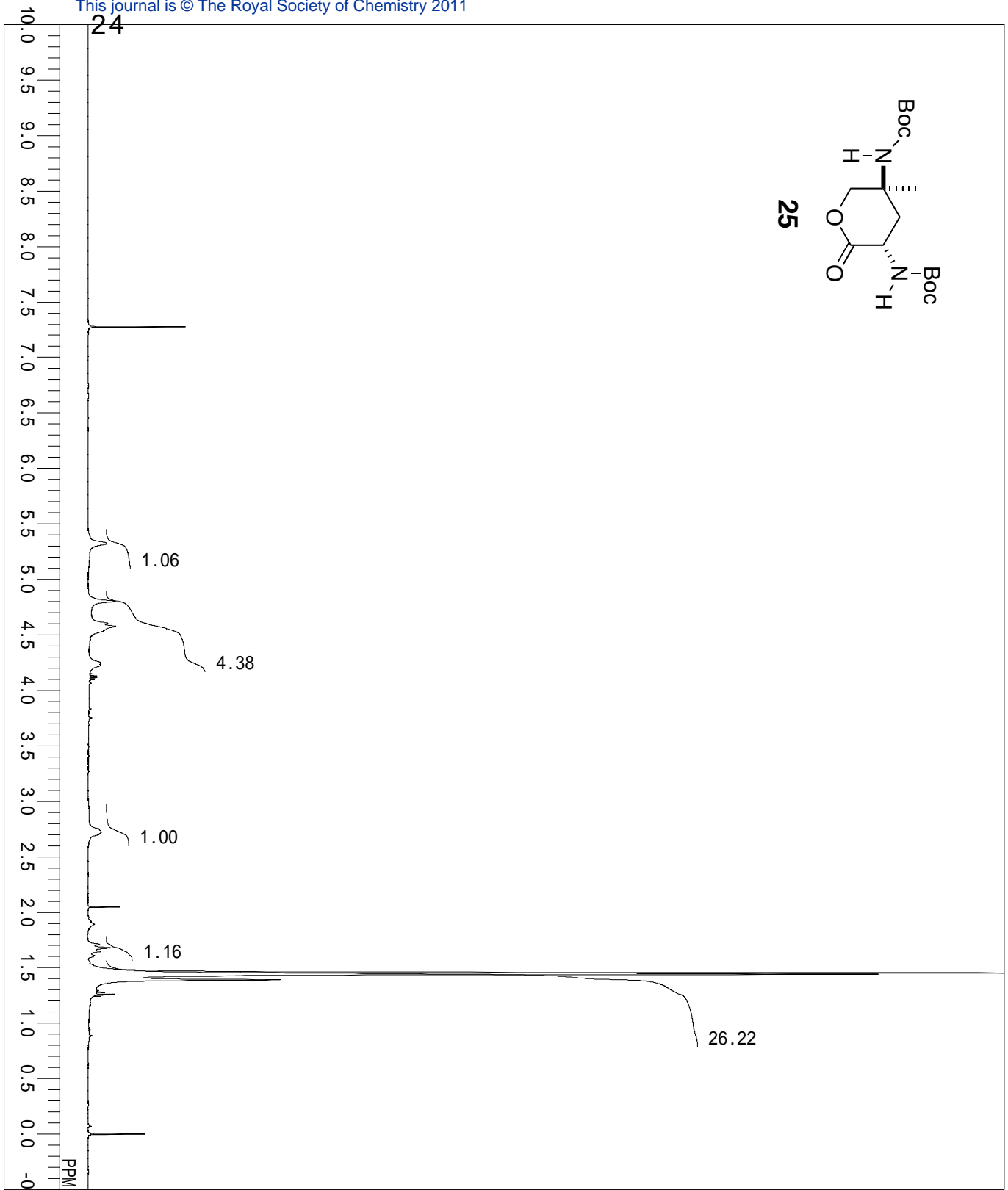
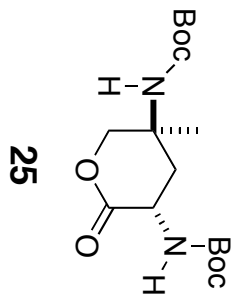


DF FILE okm4143.nmdata  
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 EXIMOD non  
 OBFRO 399.65 MHz  
 OBSET 130.00 KHz  
 OBFIN 4300.00 Hz  
 POINT 32768  
 FREQU 7993.60 Hz  
 SCANS 32  
 ACQTM 4.0993 sec  
 PD 2.9007 sec  
 PVI 7.00 usec  
 IRNUC 1H  
 CTEMP 23.6 C  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF -0.18 Hz  
 RGA IN 20

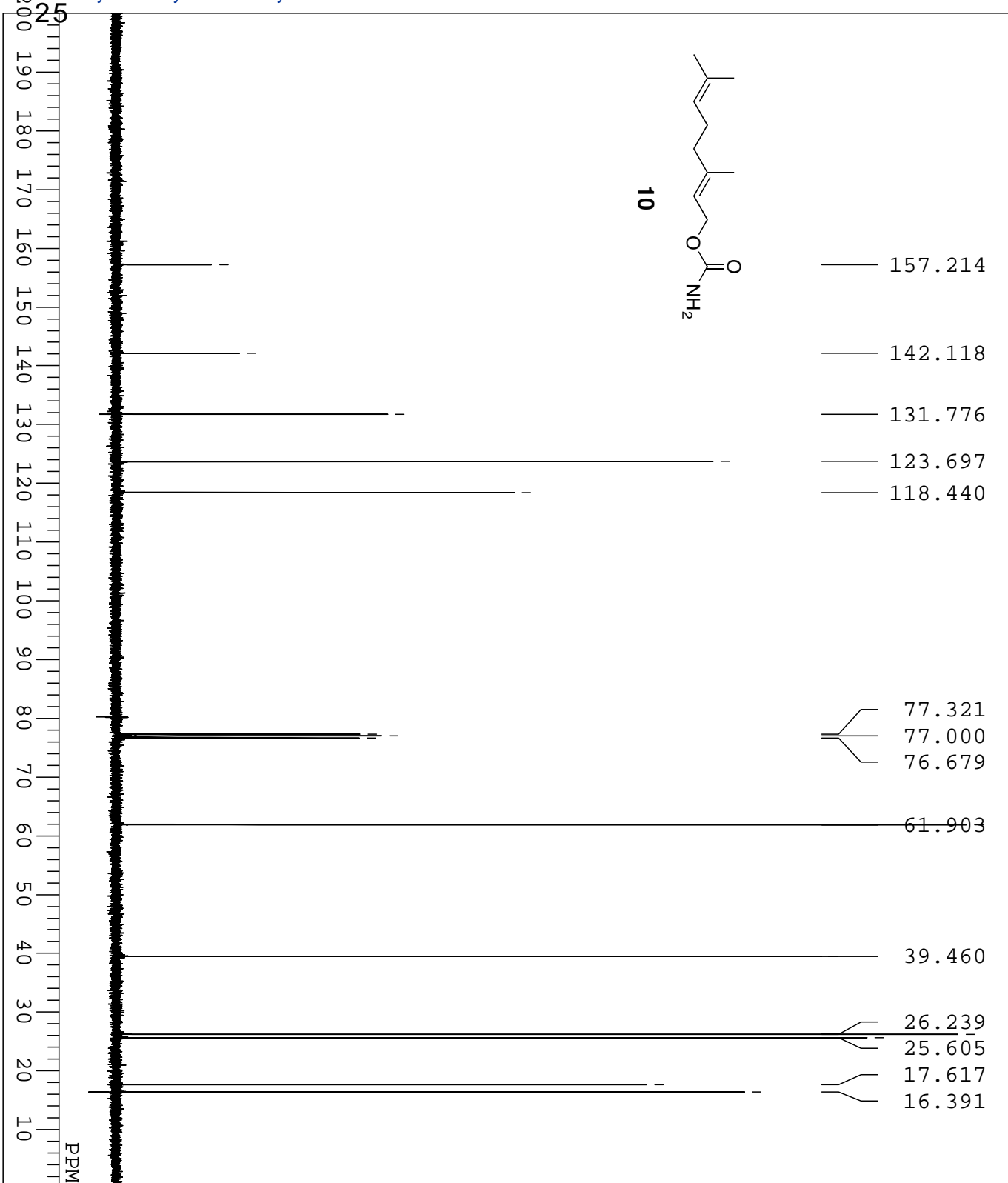


DF FILE okm4146.nmdata  
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 EXIMOD non  
 OBFRO 399.65 MHz  
 OBSET 130.00 KHz  
 OBFIN 4300.00 Hz  
 POINT 32768  
 FREQU 7993.60 Hz  
 SCANS 16  
 ACQTM 4.0993 sec  
 PD 2.9007 sec  
 PUL1 7.00 usec  
 IRNUC 1H  
 CTEMP 21.5 C  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF -0.18 Hz  
 RGA IN 22

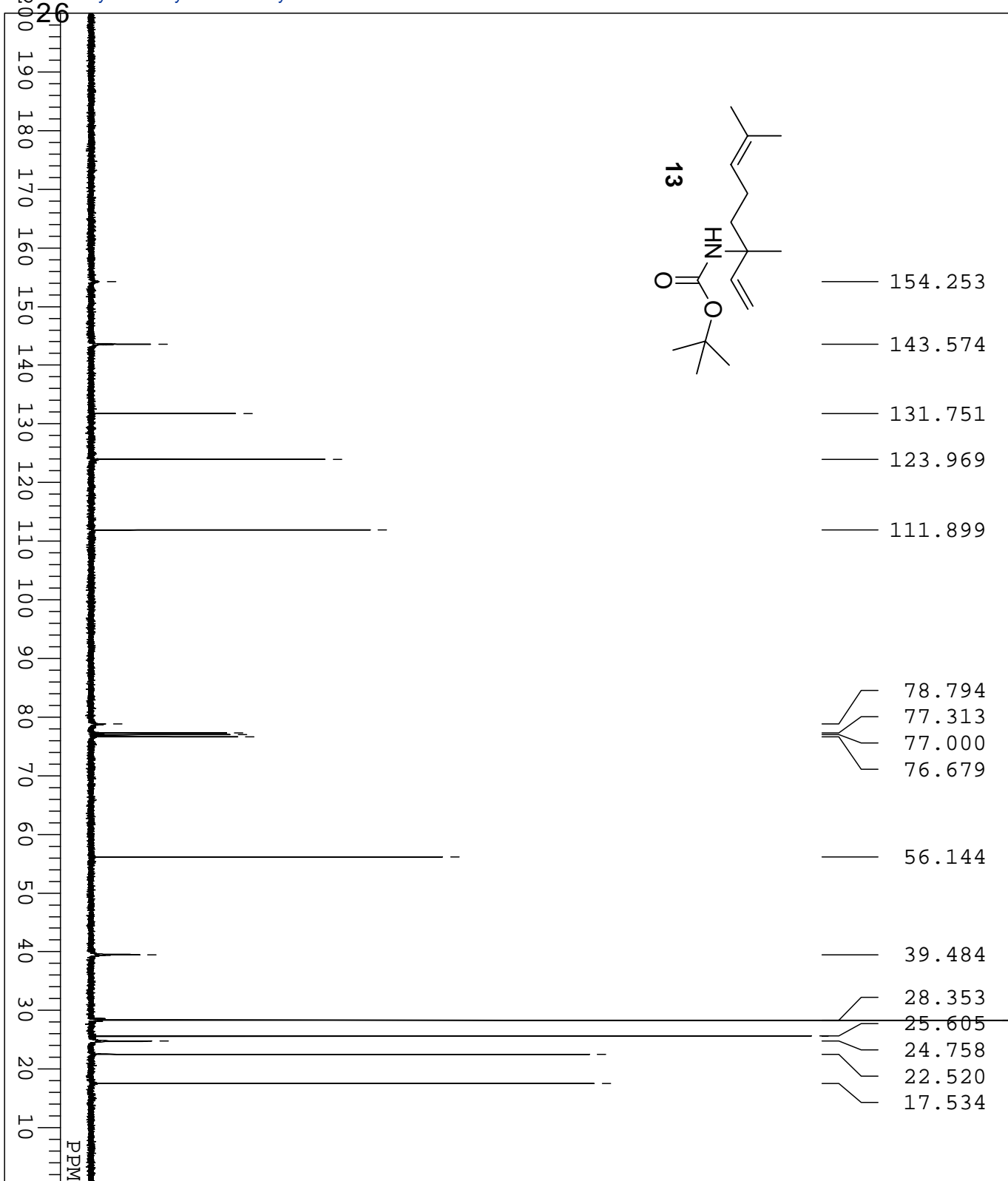




DF FILE okm4153.nmdata  
 COMNT 1H OKM4153  
 DATIM Fri Mar 20 00:19:49 2009  
 OBNUC 1H  
 EXIMOD non  
 OBFRO 399.65 MHz  
 OBSET 130.00 KHZ  
 OBFIN 4300.00 HZ  
 POINT 32768  
 FREQU 7993.60 Hz  
 SCANS 4  
 ACQTM 4.0993 sec  
 PD 2.9007 sec  
 PVI 7.00 usec  
 IRNUC 1H  
 CTEMP 22.7 C  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF -0.18 Hz  
 RGA IN 17

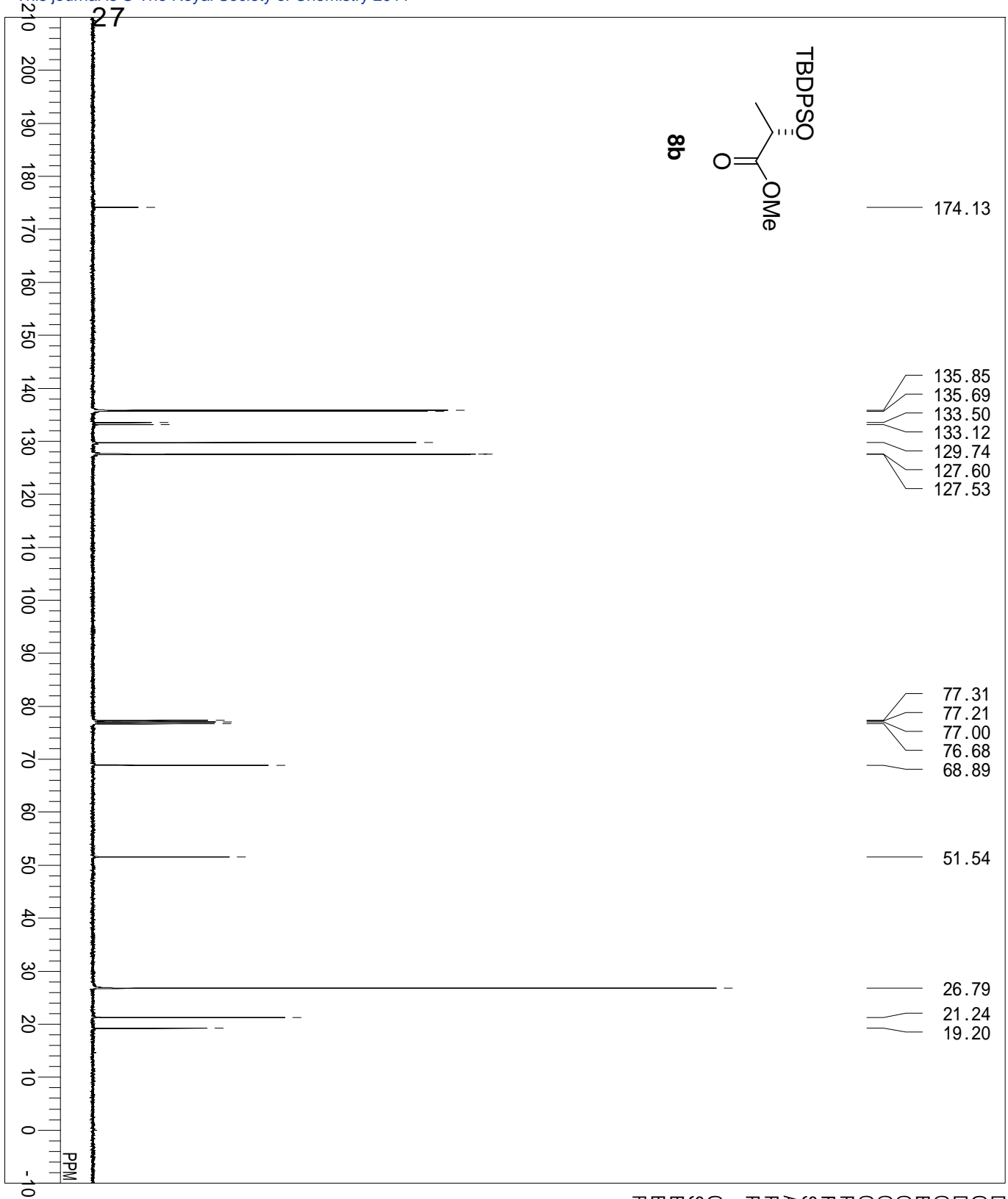


DFILE mtd cal-c.a1s  
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 DATIM Wed Sep 01 22:44:24 201  
 OBNUC 13C  
 EXMOD bcm  
 OBFREQ 100.40 MHz  
 OBSET 0.00 KHz  
 OBFIN 135500.00 Hz  
 POINT 32768  
 FREQU 27100.27 Hz  
 SCANS 360  
 ACQTM 1.2091 sec  
 PD 1.7909 sec  
 PW1 5.50 usec  
 IRNUC 1H  
 CTEMP 24.3 C  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 27

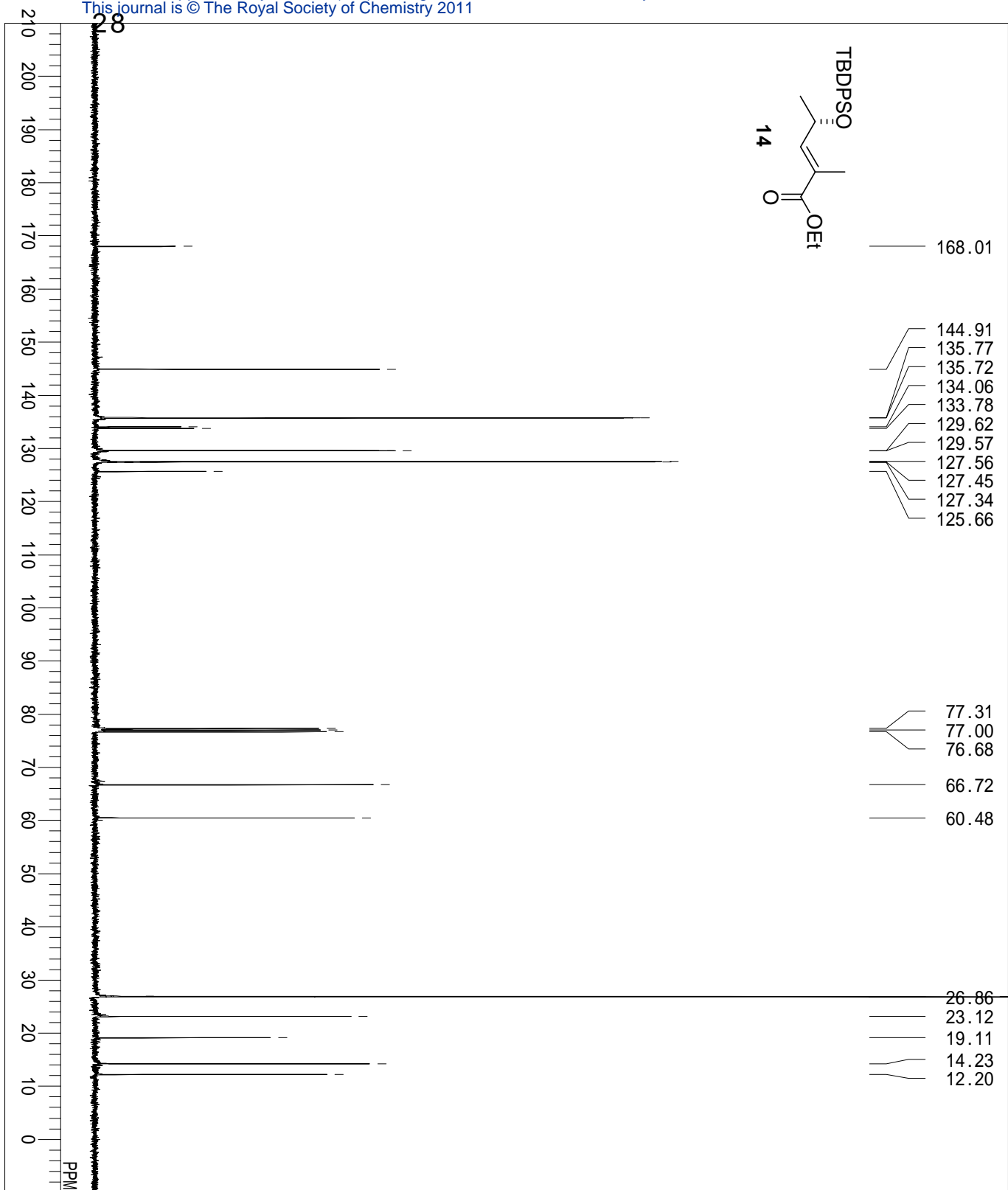


D:\FILE mtd Boc-C.a1s  
 COMNT Wed Sep 01 23:06:42 201  
 DATIM 13C  
 OBNUC bcm  
 EXMOD  
 OBFRO 100.40 MHz  
 OBSET 0.00 KHz  
 OBFIN 135500.00 Hz  
 POINT 32768  
 FREQU 27100.27 Hz  
 SCANS 360  
 ACQTM 1.2091 sec  
 PD 1.7909 sec  
 PW1 5.50 usec  
 IRNUC 1H  
 CTEMP 24.1 c  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 27

1H OKM1029-13C

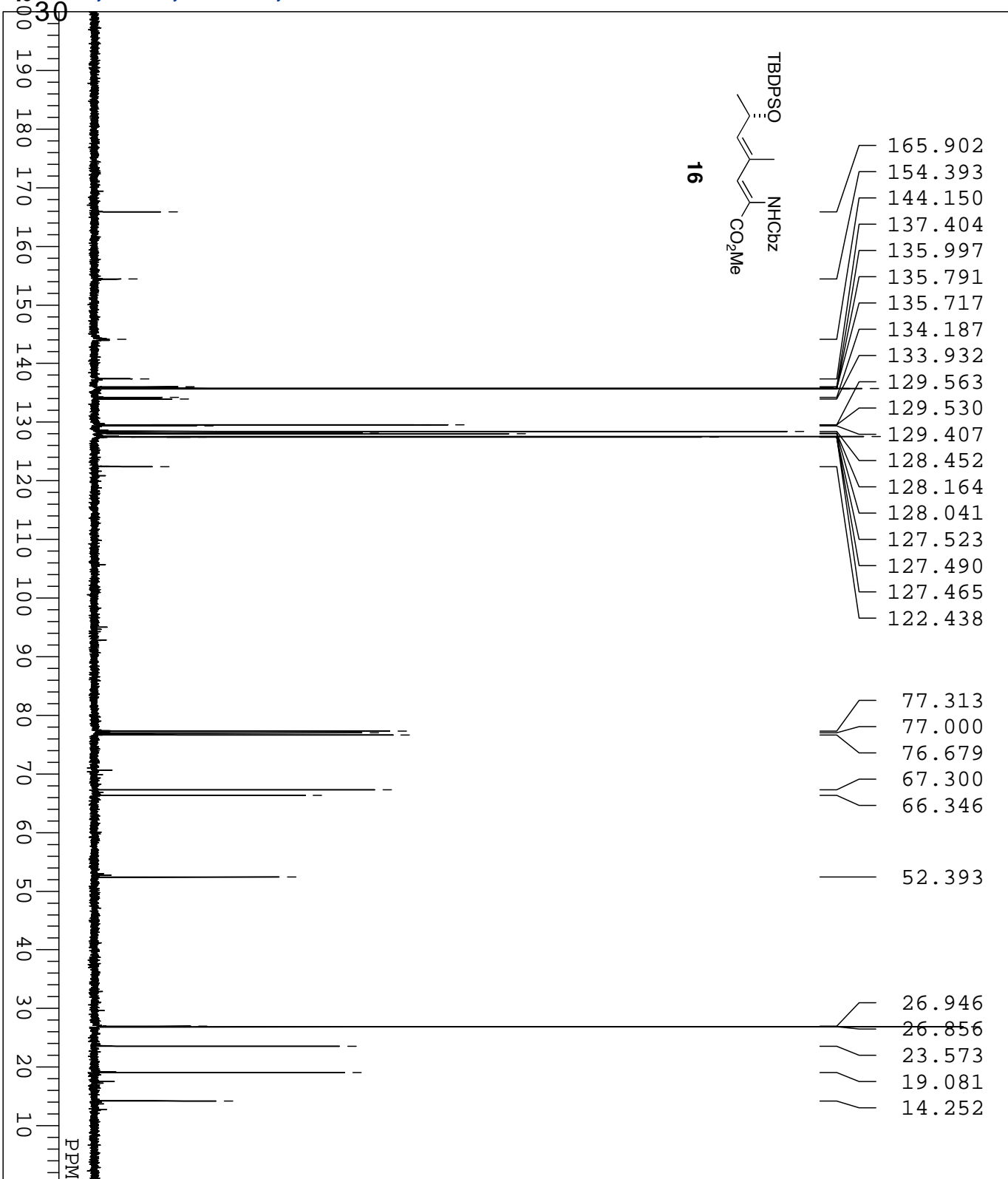


DF1LE okm1029-13c.nmdata  
 CONNT 1H OKM1029-13C  
 DATIM Sat Oct 18 14:37:19 2008  
 OBNUC 13C  
 EXMOD bcm  
 OBERQ 100.40 MHz  
 OBSET 130.00 KHz  
 POINT 5500.00 Hz  
 FREQU 32768  
 SCANS 27100.27 Hz  
 ACQTM 256  
 PD 1.2091 sec  
 PWR1 1.7909 sec  
 IRNUC 5.50 usec  
 CTEMP 24.6 C  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF -0.18 Hz  
 RGA IN 32

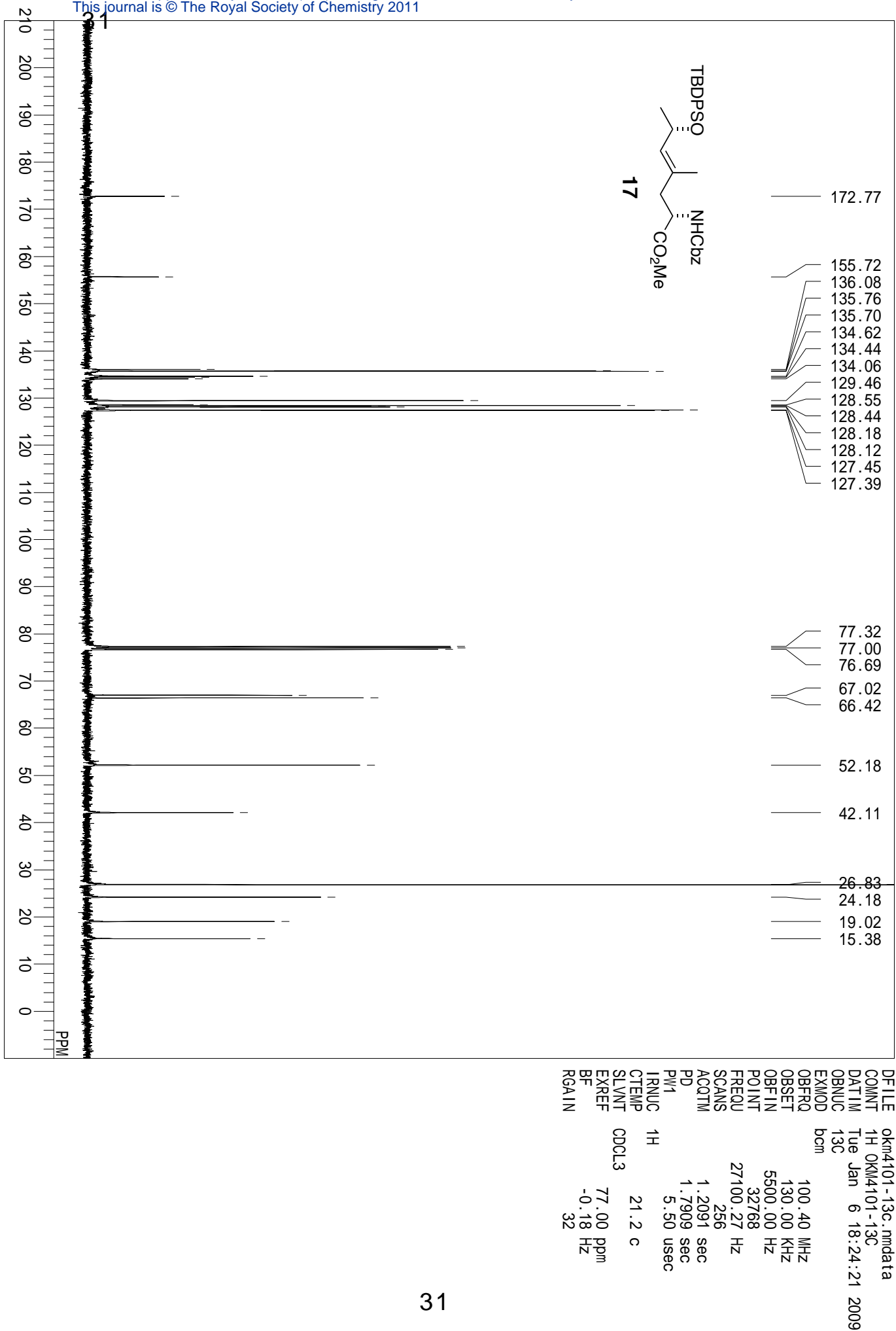


DFILIE okm3142-13C.mdata  
 COMNT 1H OKM3142-13C  
 DATIM Sat Oct 18 15:06:35 2008  
 OBNUC 13C  
 EXMOD bcm  
 OBFRO 100.40 MHz  
 OBSRT 130.00 KHZ  
 OBFIN 5500.00 HZ  
 POINT 32768  
 FREQU 27100.27 HZ  
 SCANS 256  
 ACQTM 1.2091 sec  
 PD 1.7909 sec  
 PWT 5.50 usec  
 IRNUC 1H  
 CTEMP 24.9 c  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF -0.18 HZ  
 RGA IN 32

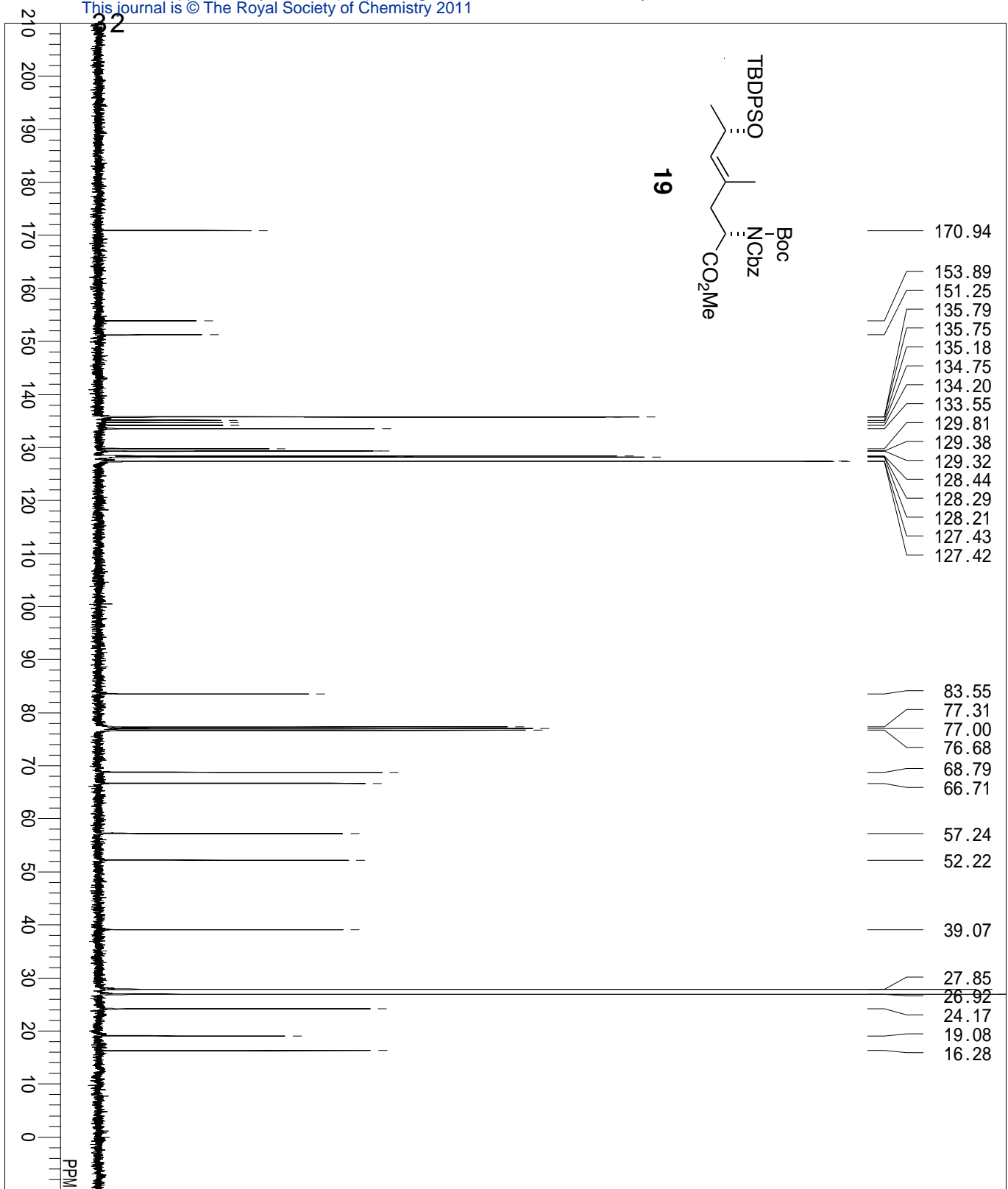




DFILE OKM-4c.a1s  
 COMNT  
 DATIM Fri Sep 17 11:26:48 201  
 OBNUC 13C  
 EXMOD bcm  
 OBFRO 100.40 MHz  
 OBSET 0.00 KHz  
 OBFIN 135500.00 Hz  
 POINT 32768  
 FREQU 27100.27 Hz  
 SCANS 802  
 ACQTM 1.2091 sec  
 PD 1.7909 sec  
 PWL 5.50 usec  
 IRNUC 1H  
 CTEMP 25.4 C  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF 0.10 Hz  
 RGAIN 27

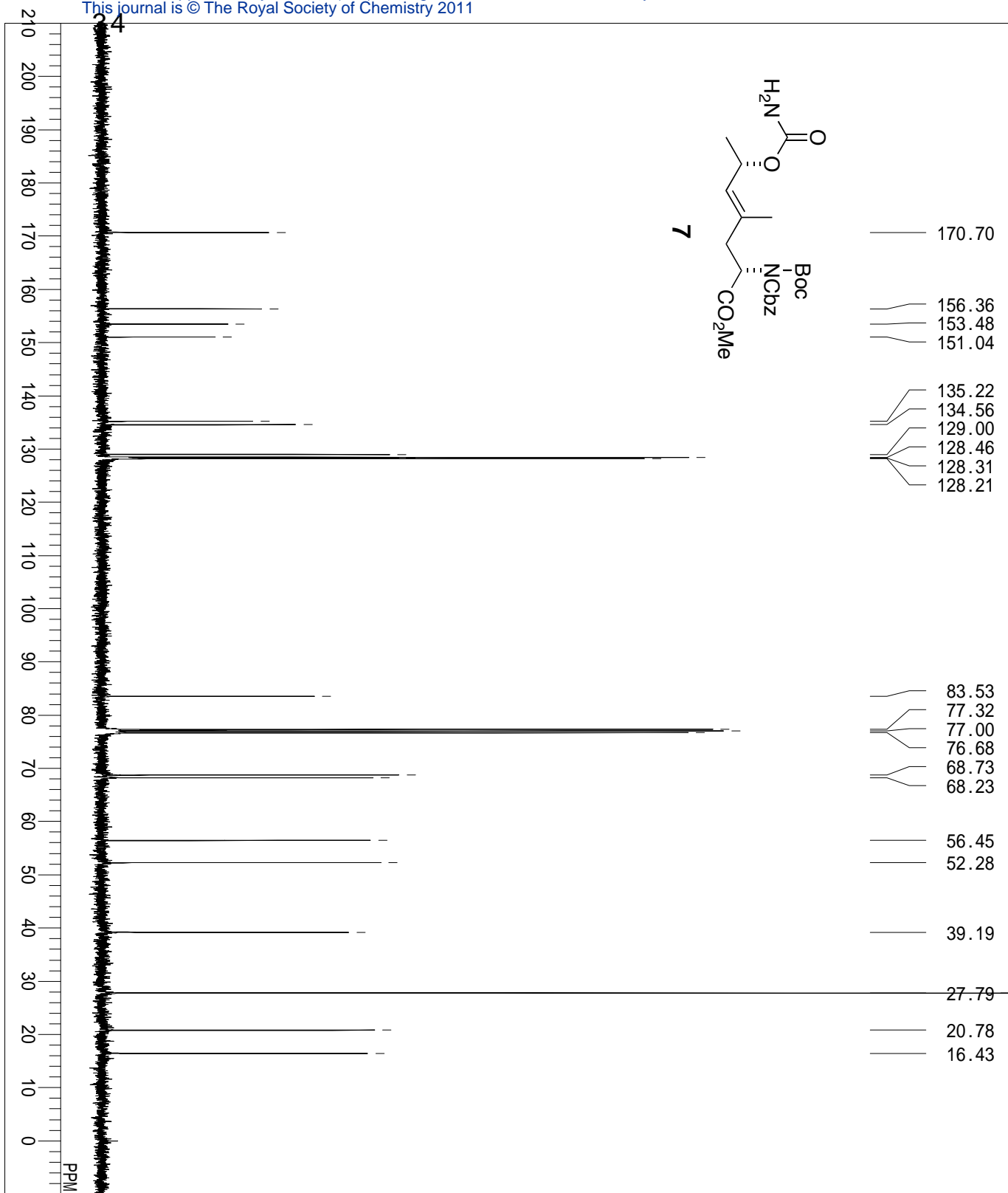




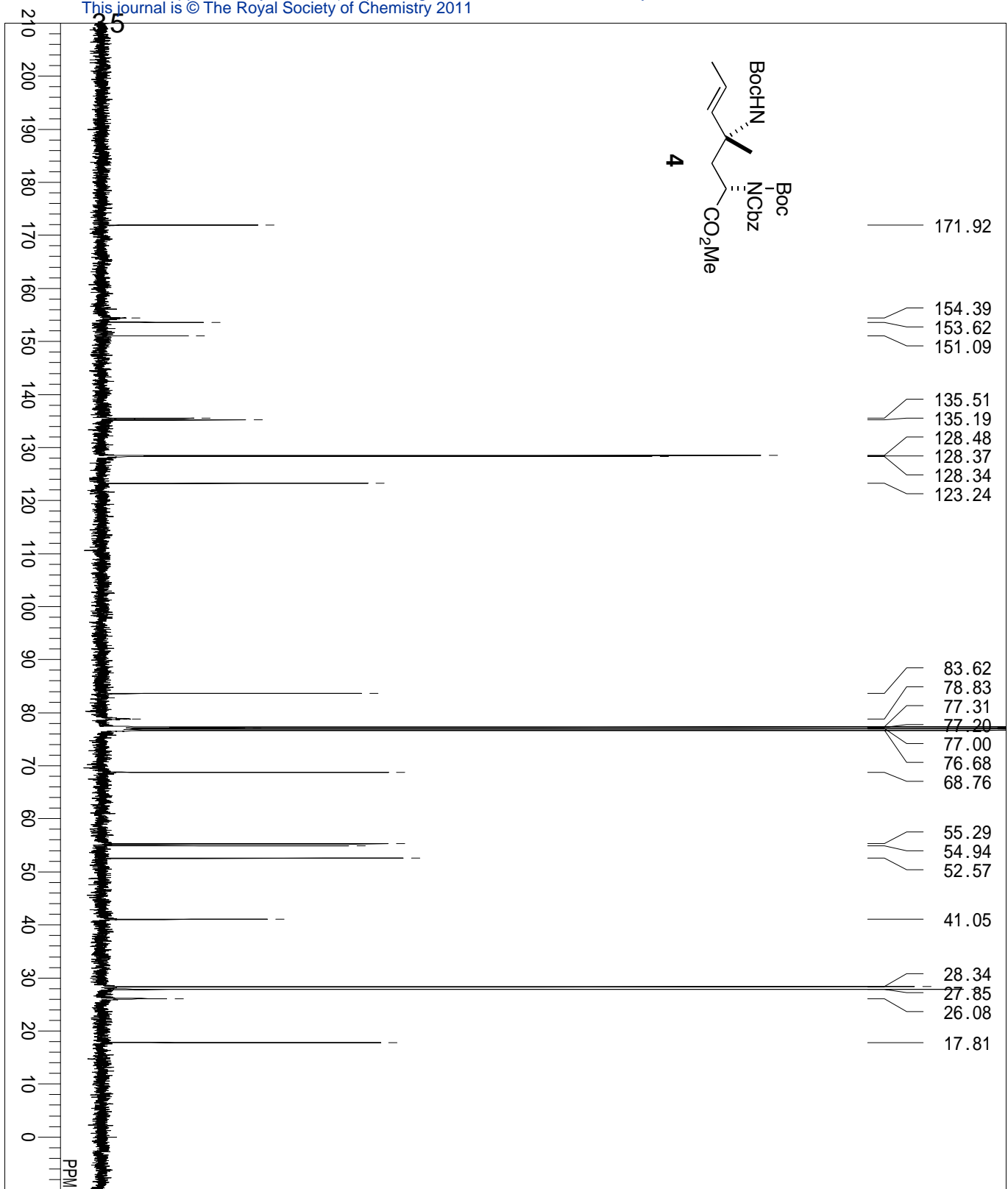


DFILF okm4109-13c.mdata  
 COMNT 1H OKM4109-13C  
 DATIM Fri Dec 19 14:03:13 2008  
 OBNUC 13C  
 EXMOD bcm  
 OBFRO 100.40 MHz  
 OBSRT 130.00 KHZ  
 OBFIN 5500.00 HZ  
 POINT 32768  
 FREQU 27100.27 HZ  
 SCANS 256  
 ACQTM 1.2091 sec  
 PD 1.7909 sec  
 PWT 5.50 usec  
 IRNUC 1H  
 CTEMP 23.9 c  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF -0.18 HZ  
 RGA IN 32

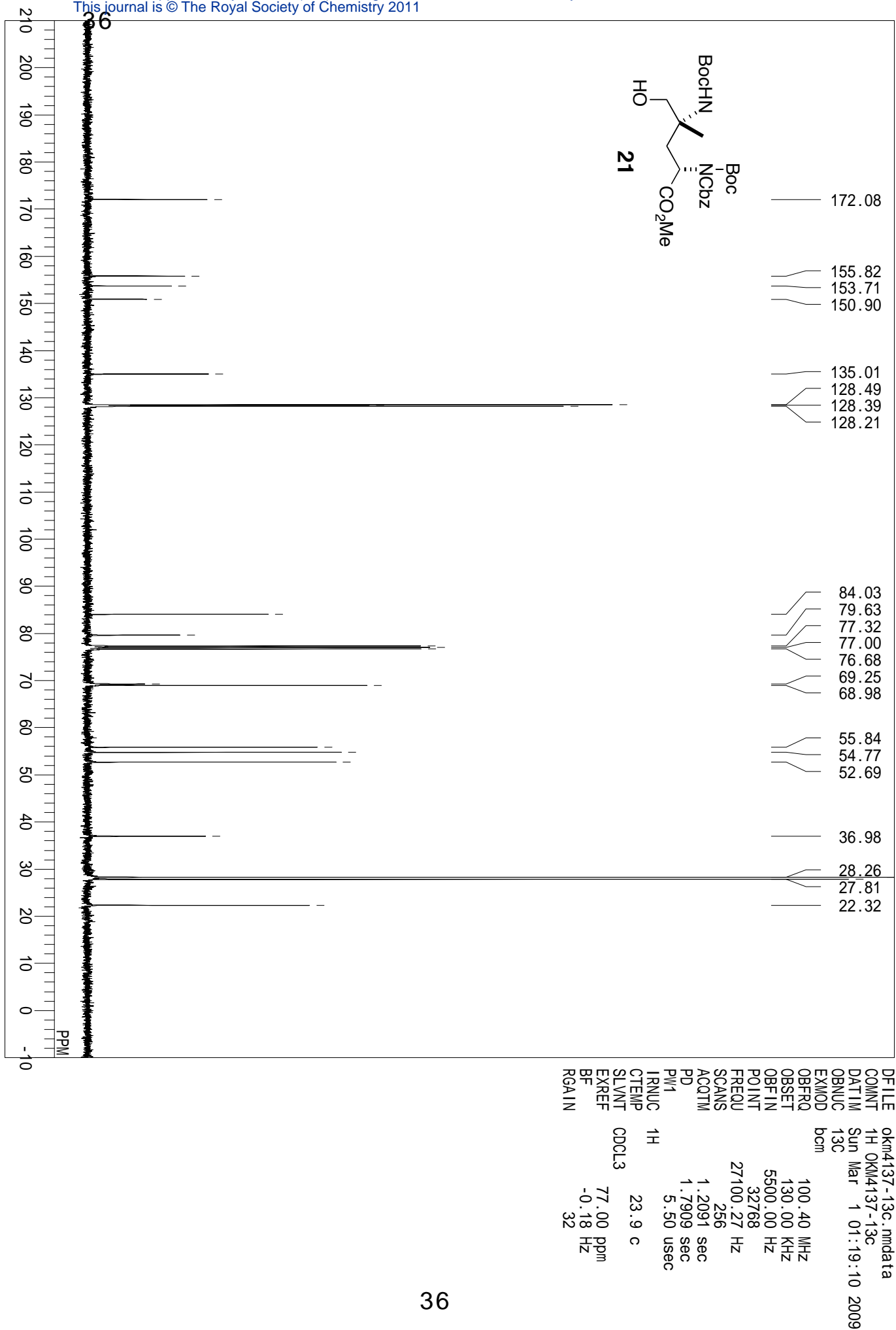


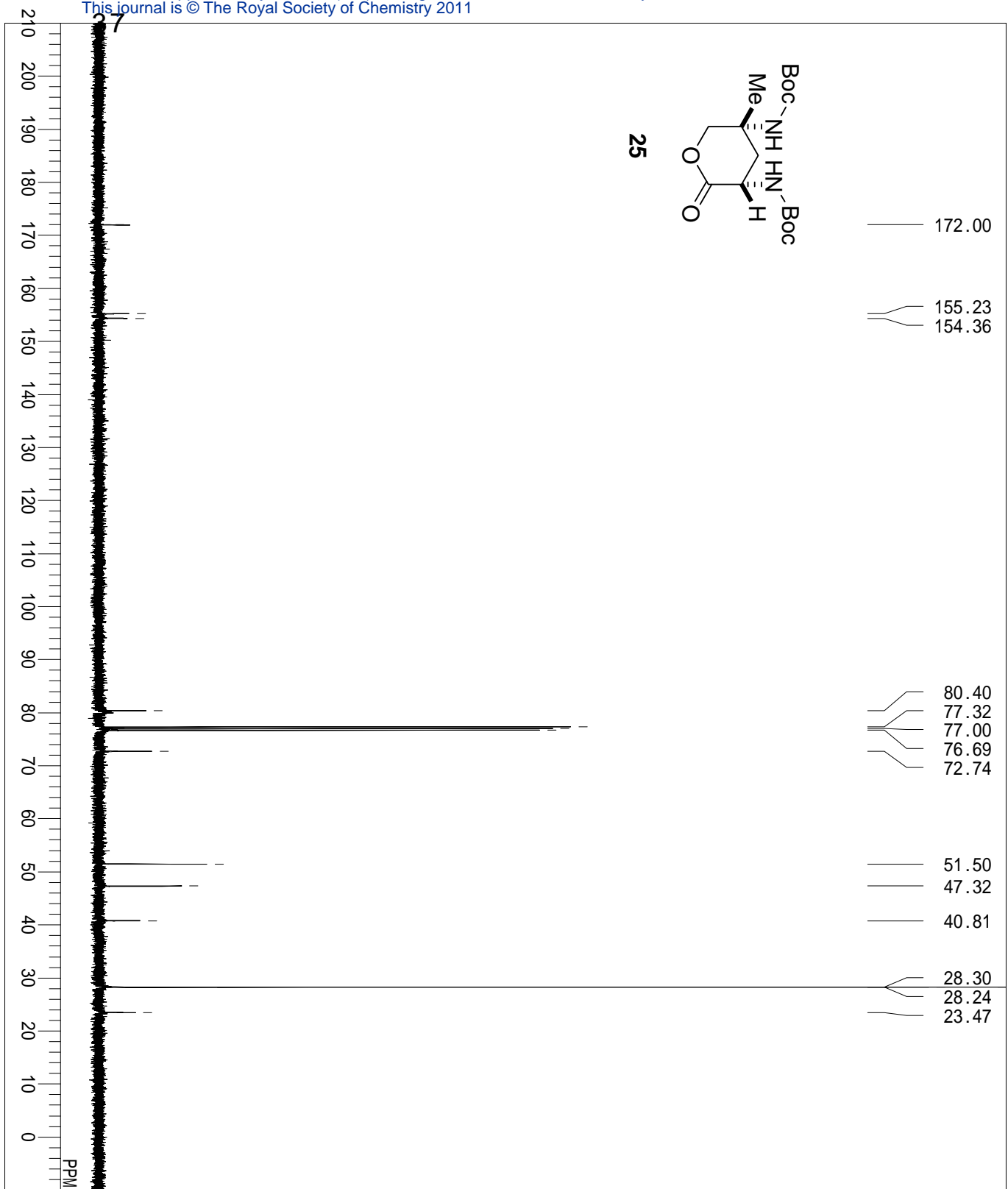


DFILF 0km4117-13c.mdata  
 COMNT 1H OKM4117-13C  
 DATIM Fri Jan 9 23:07:56 2009  
 OBNUC 13C  
 EXMOD bcm  
 OBFRO 100.40 MHz  
 OBSRT 130.00 KHZ  
 OBFIN 5500.00 HZ  
 POINT 32768  
 FREQU 27100.27 HZ  
 SCANS 256  
 ACQTM 1.2091 sec  
 PD 1.7909 sec  
 PWT 5.50 usec  
 IRNUC 1H  
 CTEMP 21.0 c  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF -0.18 HZ  
 RGA IN 33

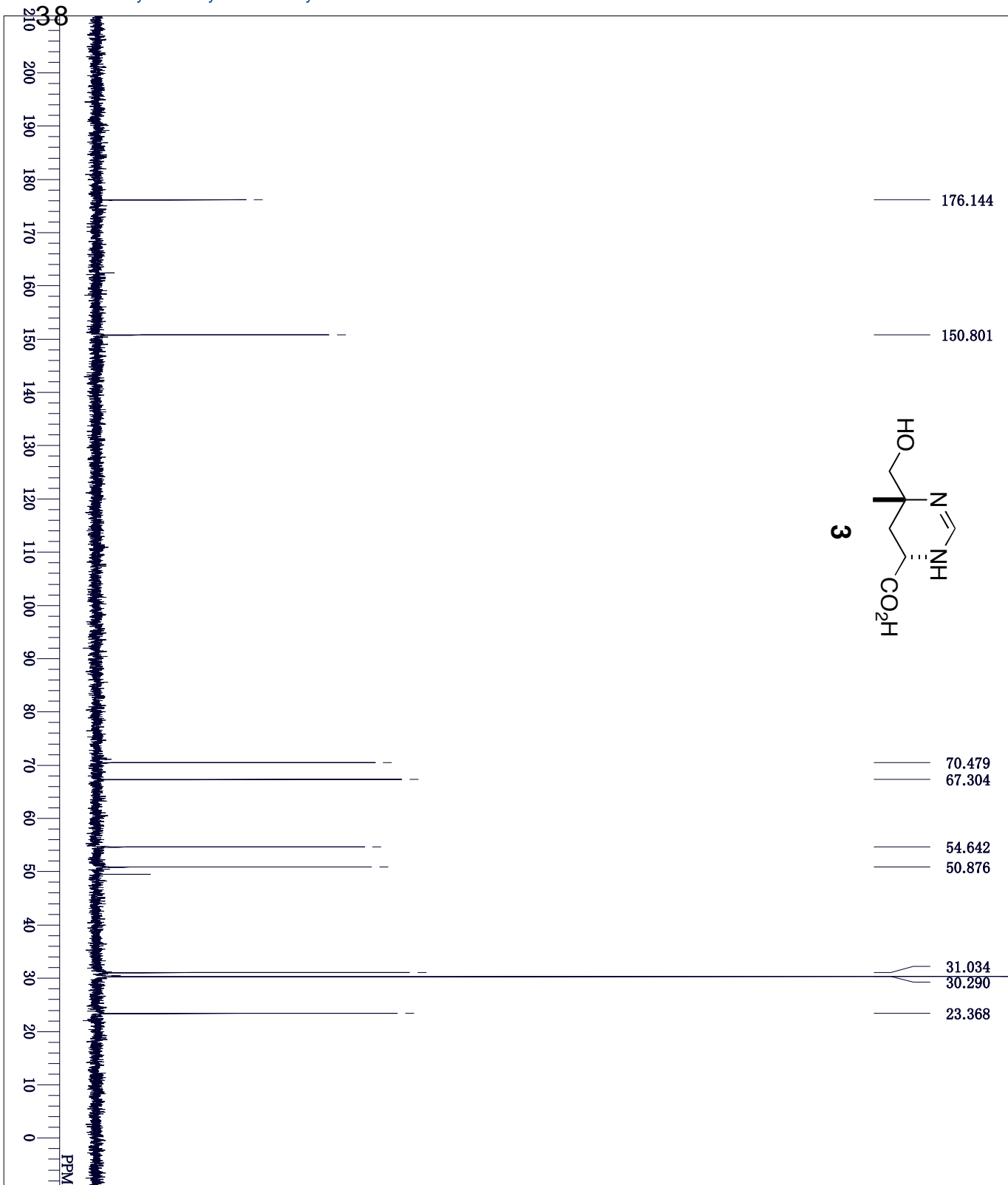


DFILIE okm4119-13c.mdata  
 COMNT 1H OKM4119-13C  
 DATIM Sat Jan 17 02:32:34 2009  
 OBNUC 13C  
 EXMOD bcm  
 OBFRO 100.40 MHz  
 OBSRT 130.00 KHZ  
 OBFIN 5500.00 HZ  
 POINT 32768  
 FREQU 27100.27 HZ  
 SCANS 512  
 ACQTM 1.2091 sec  
 PD 1.7909 sec  
 PWT 5.50 usec  
 IRNUC 1H  
 CTEMP 18.6 c  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF -0.18 Hz  
 RGA IN 32

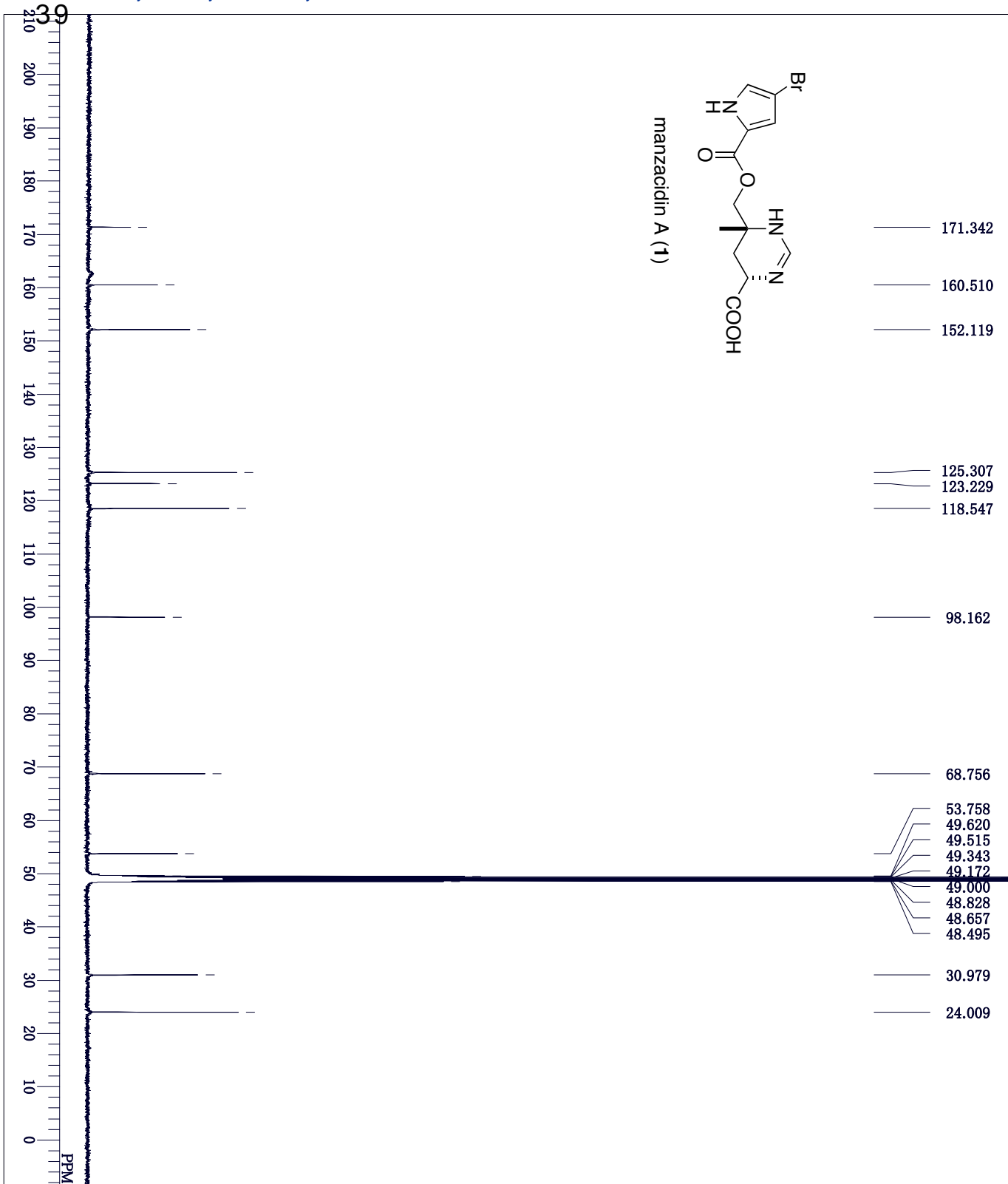




DFILIE okm4122-13c.nmdata  
 COMNT 1H OKM4122-13c  
 DATIM Sun Mar 15 00:12:51 2009  
 OBNUC 13C  
 EXMOD bcm  
 OBFREQ 100.40 MHz  
 OBSSET 130.00 KHZ  
 OBF IN 5500.00 HZ  
 POINT 32768  
 FREQU 27100.27 HZ  
 SCANS 512  
 ACQTM 1.2091 sec  
 PD 1.7909 sec  
 PWT 5.50 usec  
 IRNUC 1H  
 CTEMP 21.1 c  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF -0.18 HZ  
 RGA IN 32

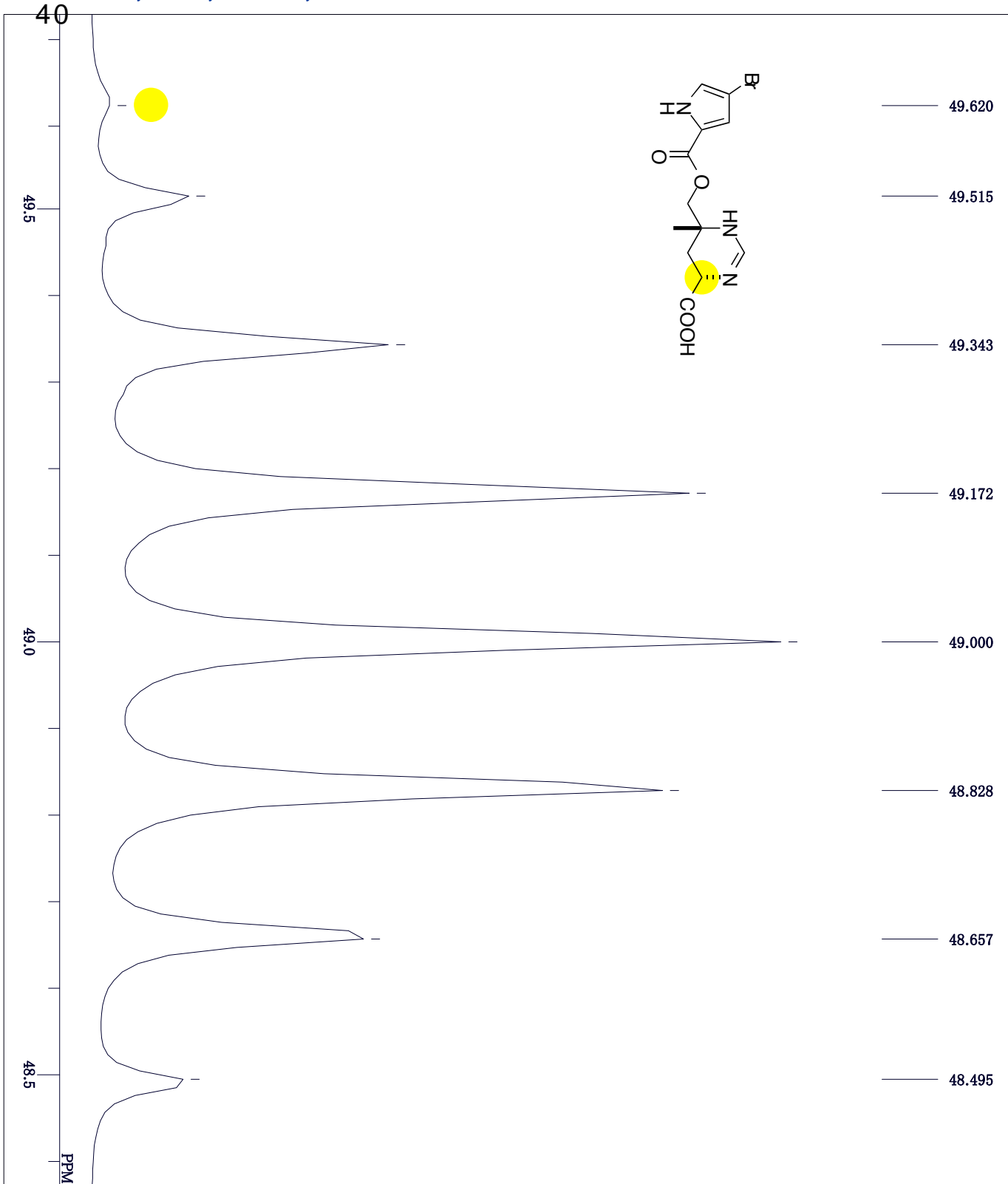


D:\FILE man 1061-2-Carbon-1-1.jif  
 COMINT single pulse decoupled gated NOE  
 DATIM 2011-03-02 16:11:10  
 13C  
 carbon.jxp  
 125.77 MHz  
 7.87 KHz  
 OBSET 4.21 Hz  
 OBRIN 32780  
 POINT 39308.18 Hz  
 FREQU 2048  
 SCANS 0.8336 sec  
 ACQTM 2.0000 sec  
 PD 2.72 usec  
 PW1  
 IRNUC  
 CTEMP 16.9 c  
 SLVNT  
 EXREF  
 BF  
 RGAIN  
 D2O 30.29 ppm  
 0.10 Hz  
 58



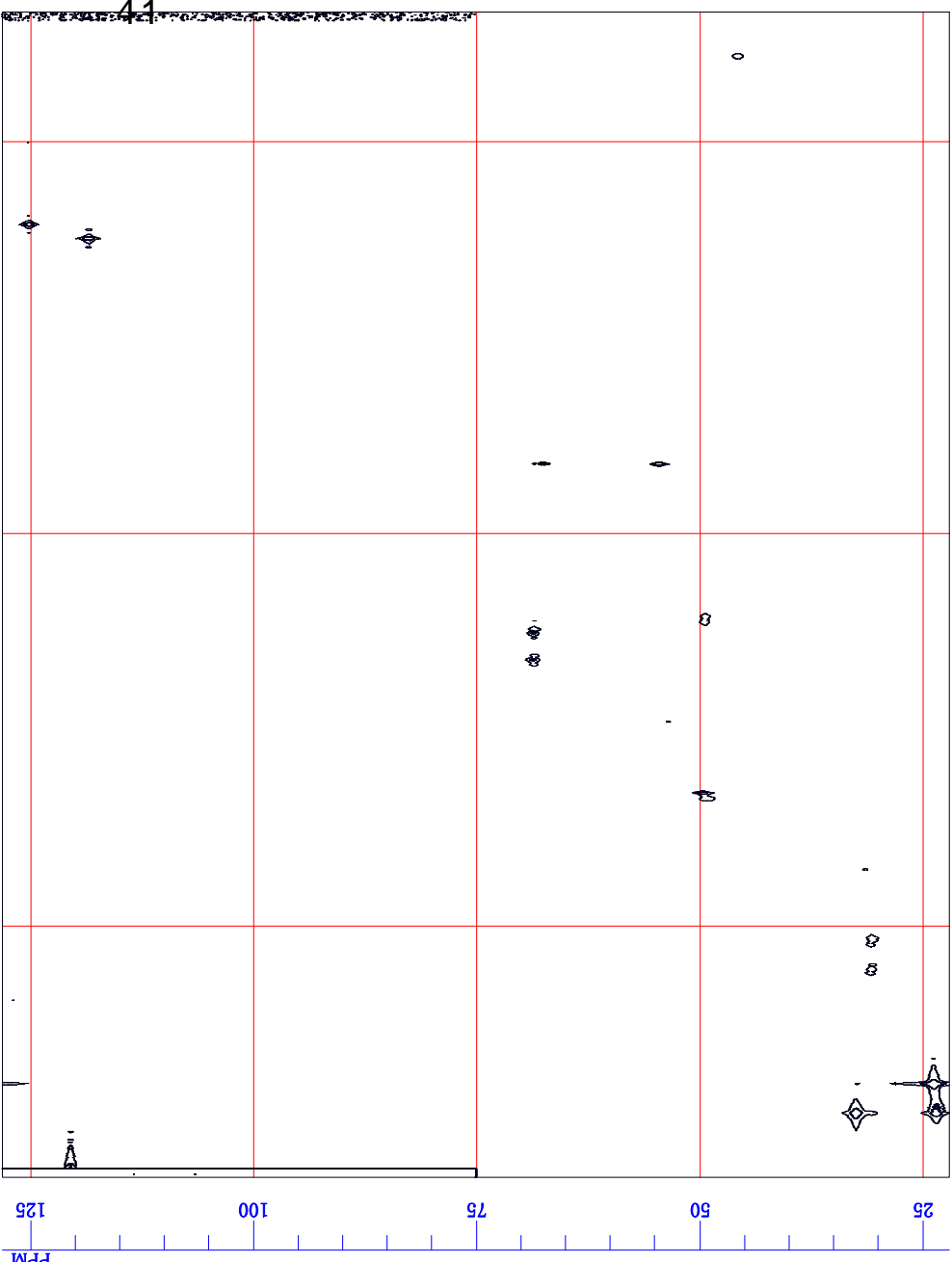
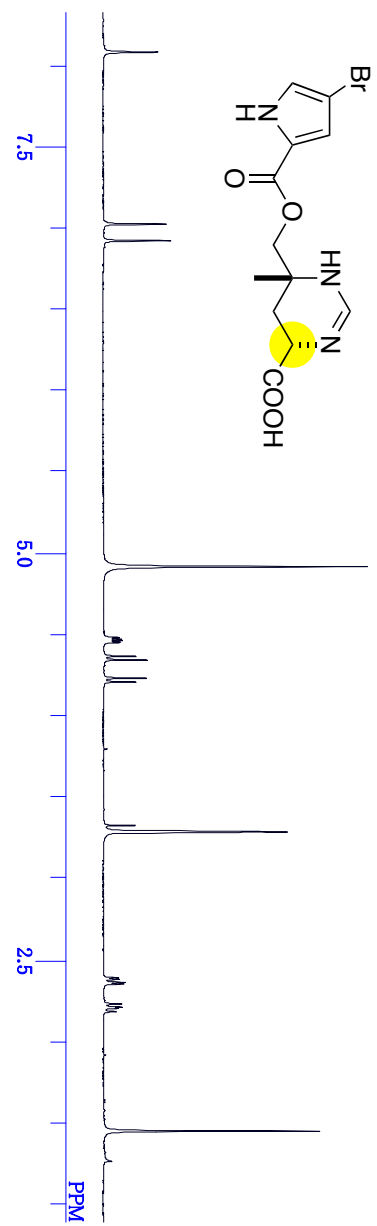
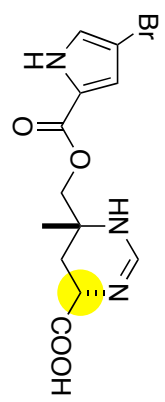
DFILE 1079\_Carbon-1-1.jdf  
 COMNT single pulse decoupled gated NOE  
 DATIM 2011-04-30 09:22:11  
 OBNUC 13C  
 EXMVD carbon.jxp  
 OBFRO 125.77 MHz  
 OBSET 7.87 KHz  
 OBRIN 4.21 Hz  
 POINT 32780  
 FREQU 39308.18 Hz  
 SCANS 4096  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 2.72 usec  
 IRNUC 1H  
 CTEMP 18.4 c  
 CD3OD 49.00 ppm  
 EXREF 0.10 Hz  
 RGAIN 50



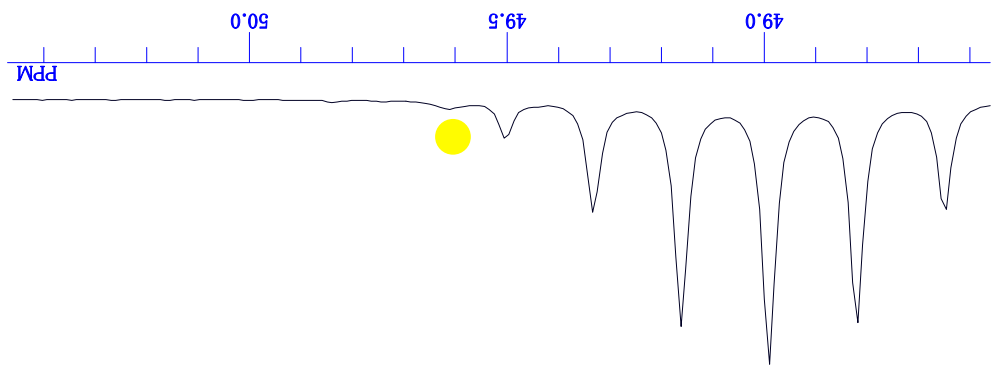
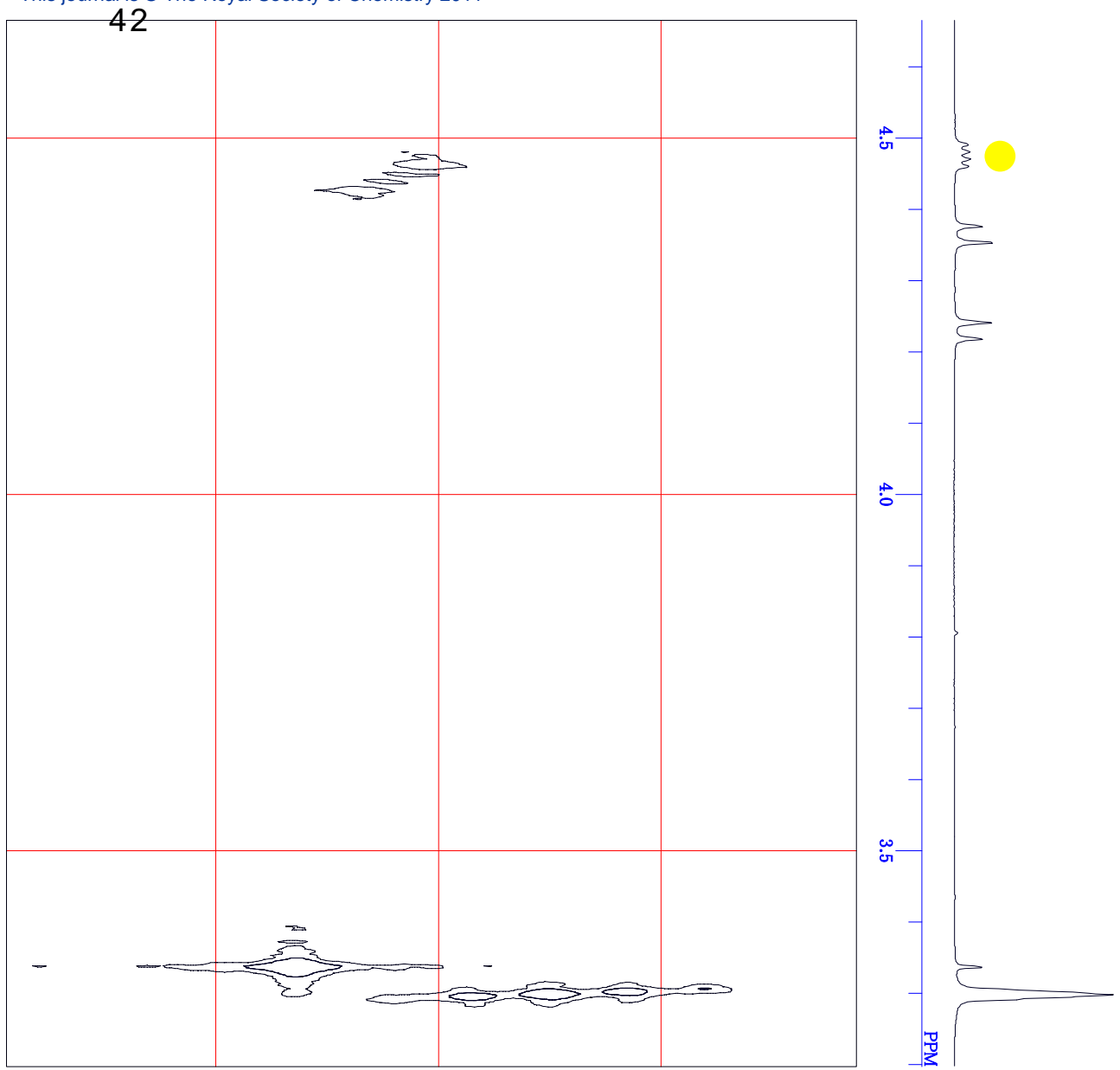


DFILE 1079\_Carbon-1-1.jif  
 COMNT single pulse decoupled gated NOE  
 DATIM 2011-04-30 09:22:11  
 OBNUC <sup>13</sup>C  
 EXMOD carbon.jcp  
 OBFREQ 125.77 MHz  
 OBSRT 7.87 KHz  
 OBRIN 4.21 Hz  
 POINT 32780  
 FREQU 39308.18 Hz  
 SCANS 4096  
 ACQTIM 0.8336 sec  
 PD 2.0000 sec  
 PW1 2.72 usec  
 IRNUC <sup>1</sup>H  
 CTEMP 18.4 c  
 SLVNT CD3OD  
 EXREF 49.00 ppm  
 BF 0.10 Hz  
 RGAIN 50

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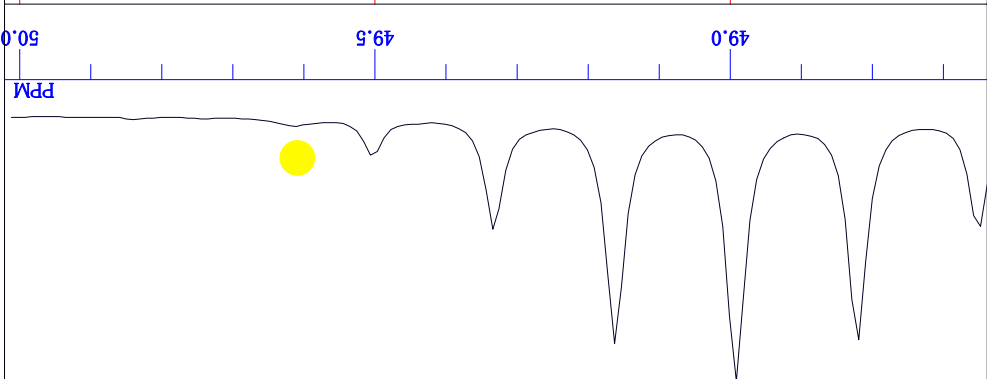
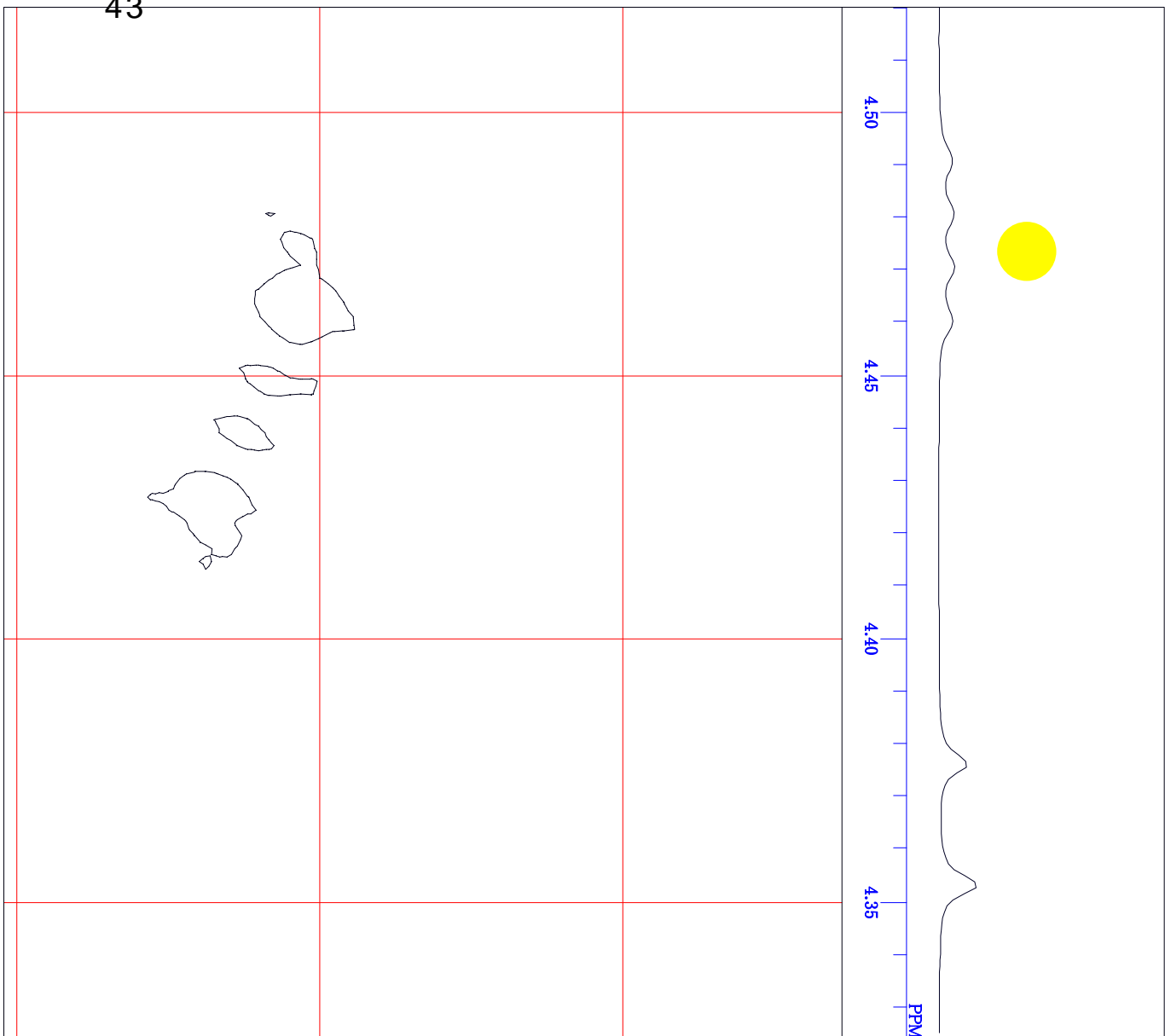
man1069ch\_HMQC-1-1.als  
 gradient enhanced HMQC with X  
 12-05-2011 00:09:16  
 hmqc.jxp  
 IH  
 500.16 MHz  
 2.21 KHz  
 8.73 Hz  
 1664  
 3711.95 Hz  
 512  
 256  
 13354.70 Hz  
 16  
 0.4414 sec  
 1.5000 sec  
 9.35 usec  
 0.00 usec  
 0.00 usec  
 0.00 usec  
 0.0000 msec  
 0.0000 msec  
 0.0000 msec  
 13C 18.4 c  
 CD3OD  
 12.51 ppm  
 EXPRF 49.00  
 CLEXR 50  
 RGAIN



hmgcman\_HMQC-1-1.als  
 gradient enhanced HMQC with X  
 13-05-2011 10:01:31  
 hmgc.jpg  
 IH  
 500.16 MHz  
 1.77 KHz  
 4.00 Hz  
 1040  
 1262.37 Hz  
 512  
 256  
 1120.57 Hz  
 4  
 SCANS  
 CLPNT  
 TODAY  
 CLFRQ  
 FREQU  
 POINT  
 OBFIN  
 OBSET  
 OBFRO  
 OBNUC  
 EXMOD  
 DATM  
 COMNT  
 FILE

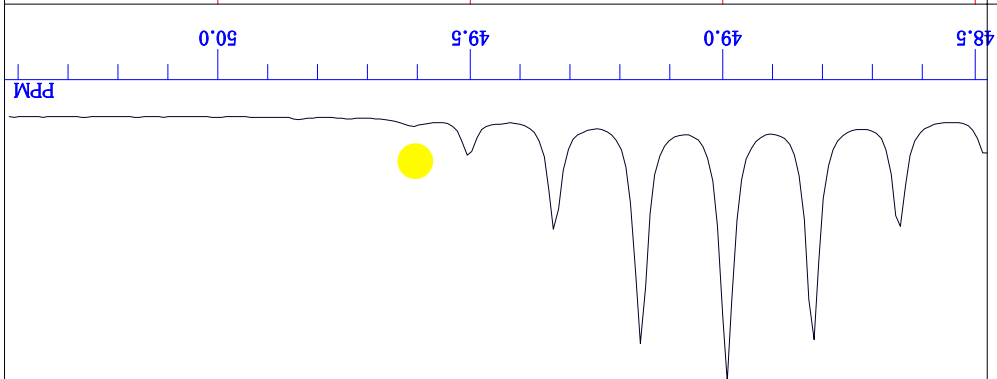
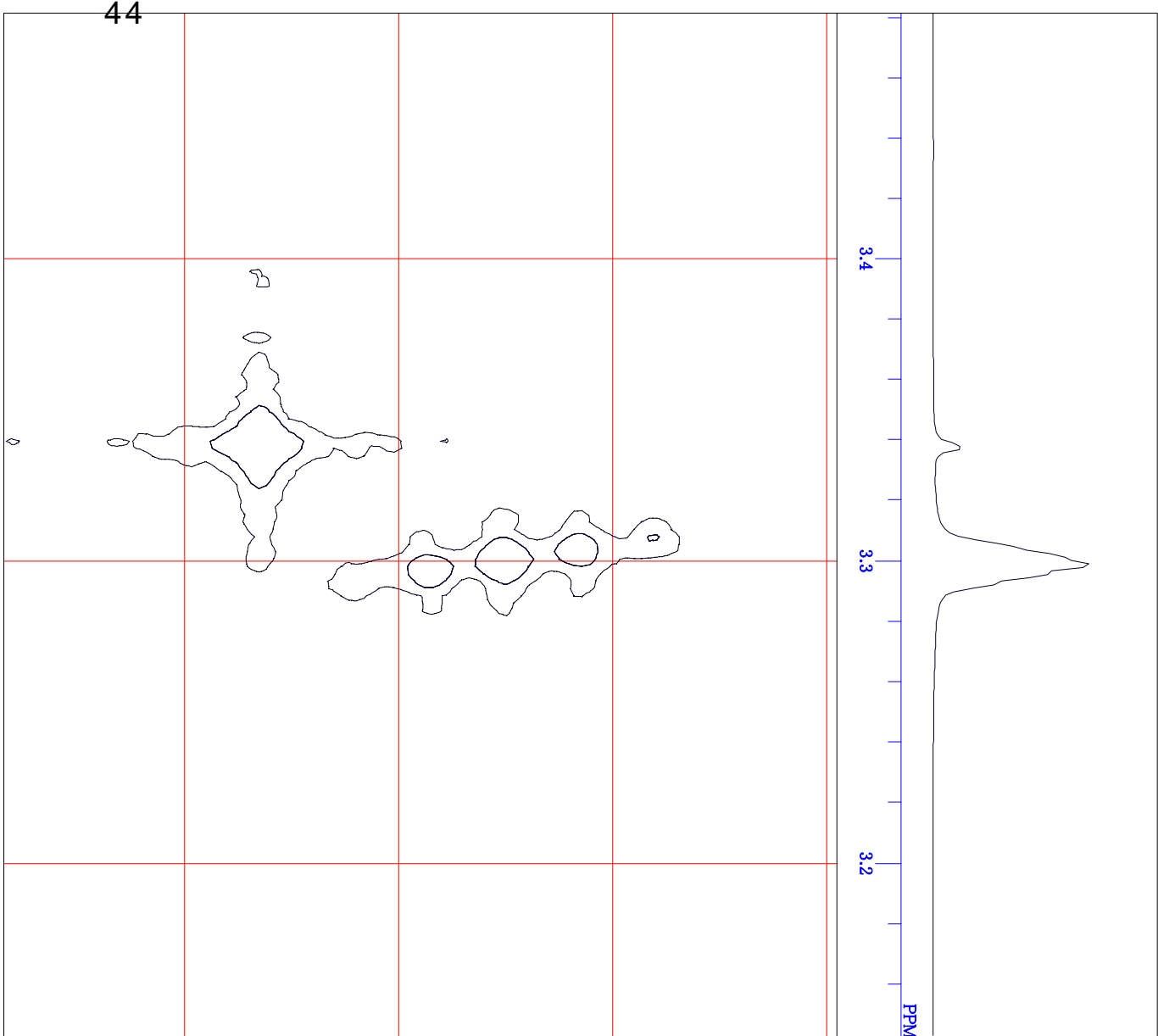
CD3OD  
 18.5 c  
 12.51 ppm  
 49.00  
 50  
 13C  
 0.0000 msec  
 0.0000 msec  
 0.0000 msec  
 0.00 usec  
 0.00 usec  
 9.35 usec  
 1.5000 sec  
 0.8112 sec  
 ACQTM  
 PD  
 PW1  
 PW2  
 PW3  
 P11  
 P12  
 P13  
 IRNUC  
 CTEMP  
 SLVNT  
 EXPRF  
 CLEXR  
 RGAIN

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FILE  
 COMNT  
 DATIM  
 EXMOD  
 OBNUC  
 OBFRQ  
 OBSFT  
 OBFIN  
 POINT  
 FREQU  
 CLPNT  
 TODAY  
 CLFRQ  
 SCANS  
 ACQTM  
 PD  
 PW1  
 PW2  
 PW3  
 P11  
 P12  
 P13  
 IRNUC  
 CTEMP  
 SLVNT  
 EXPRF  
 CLEXR  
 RGAIN

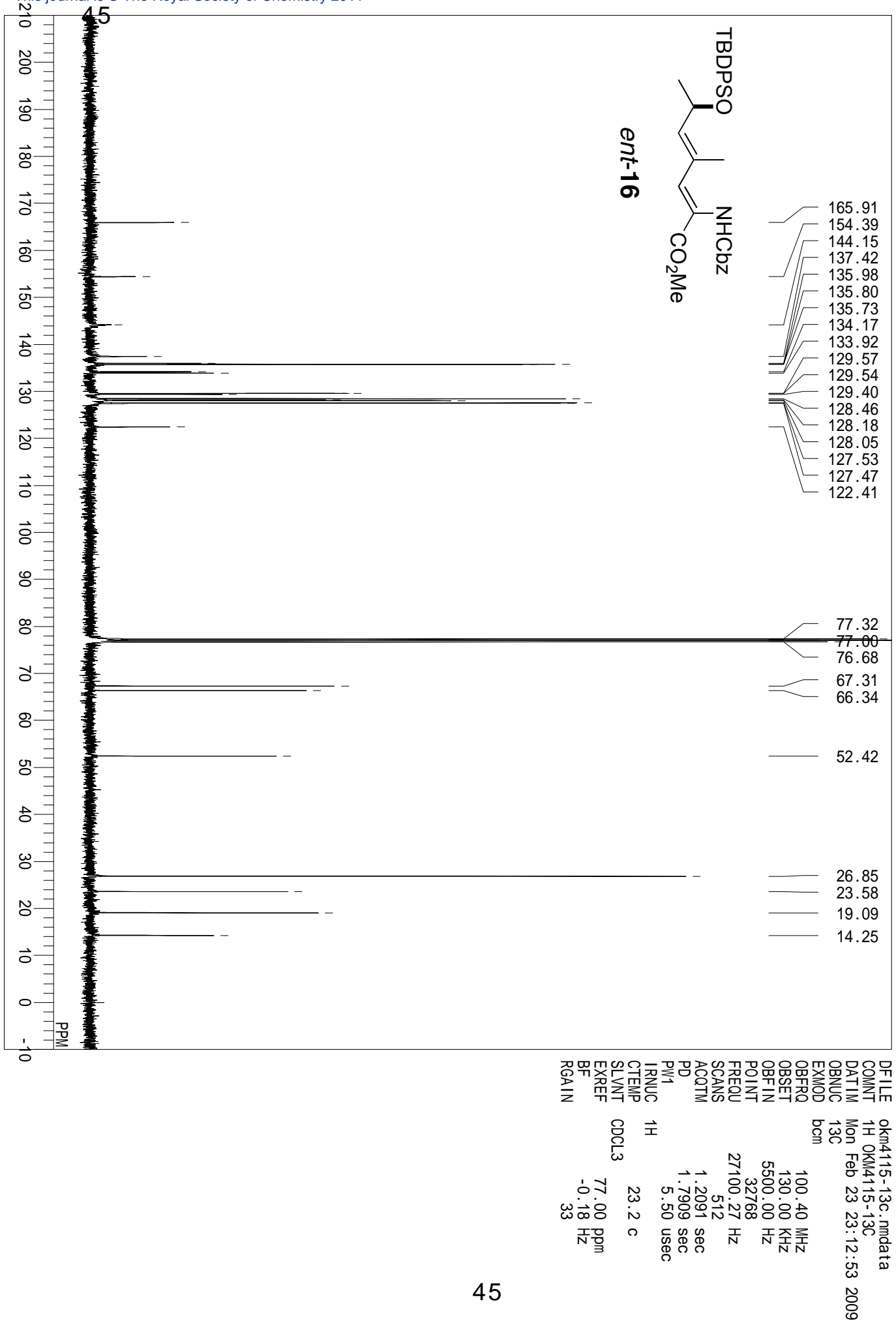
hmqcman\_HMQC-1-1.als  
 gradient enhanced HMQC with X  
 13-05-2011 10:01:31  
 hmqc.jpg  
 IH  
 500.16 MHz  
 1.77 KHz  
 4.00 Hz  
 1040  
 1262.37 Hz  
 512  
 256  
 1120.57 Hz  
 4  
 0.8112 sec  
 1.5000 sec  
 9.35 usec  
 0.00 usec  
 0.00 usec  
 0.0000 msec  
 0.0000 msec  
 0.0000 msec  
 13C 18.5 c  
 CD3OD  
 12.51 ppm  
 49.00  
 50

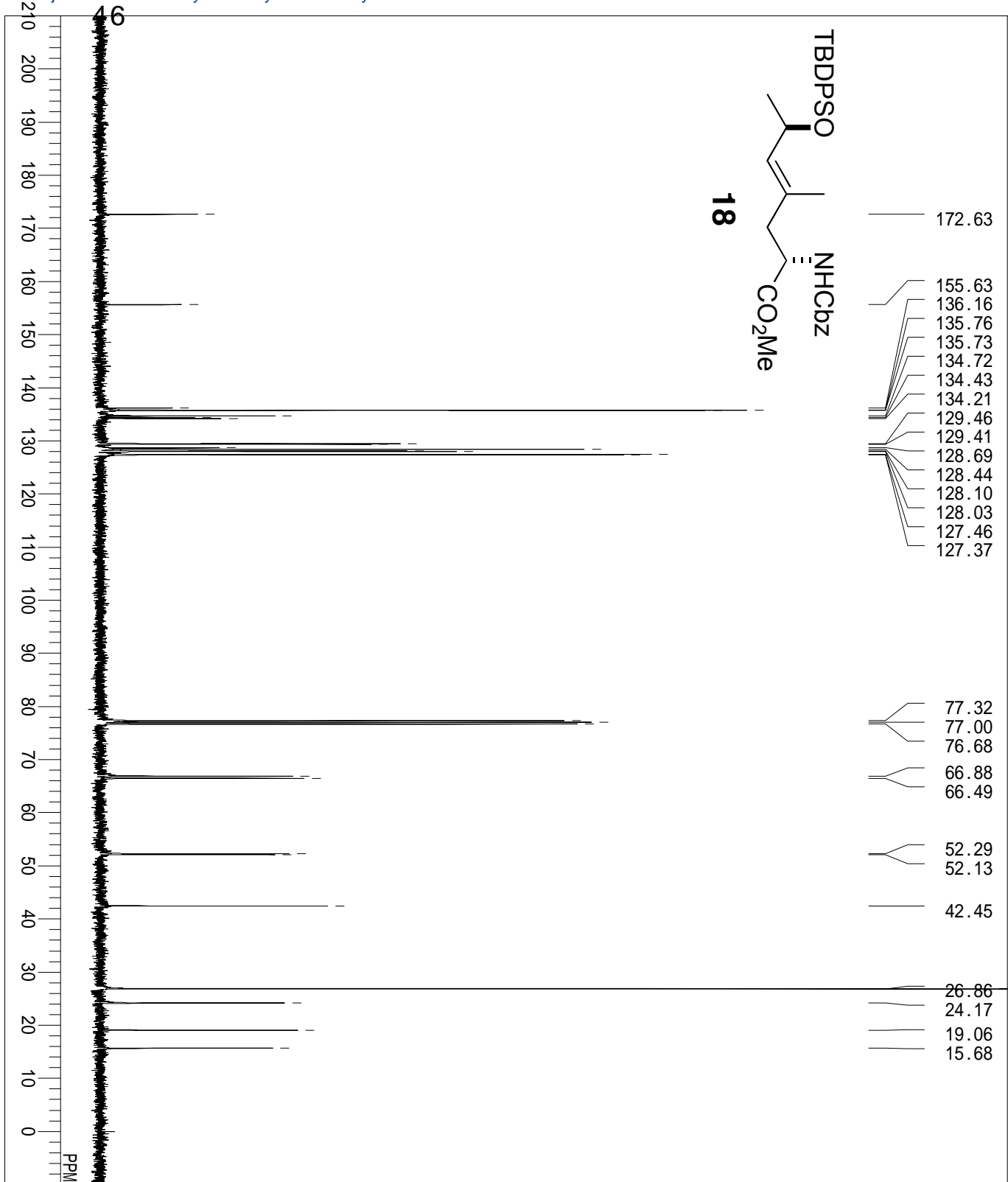


DPFILE  
 COMINT  
 DATIM  
 EXMOD  
 OBNUC  
 OBFREQ  
 OBSSET  
 OBFIN  
 POINT  
 FREQU  
 CLPNT  
 TODAT  
 CLFRQ  
 SCANS  
 ACQTM  
 PD  
 PW1  
 PW2  
 PW3  
 P11  
 P12  
 P13  
 IRNUC  
 CTEMP  
 SLVNT  
 EXPRF  
 CLEXR  
 RGAIN

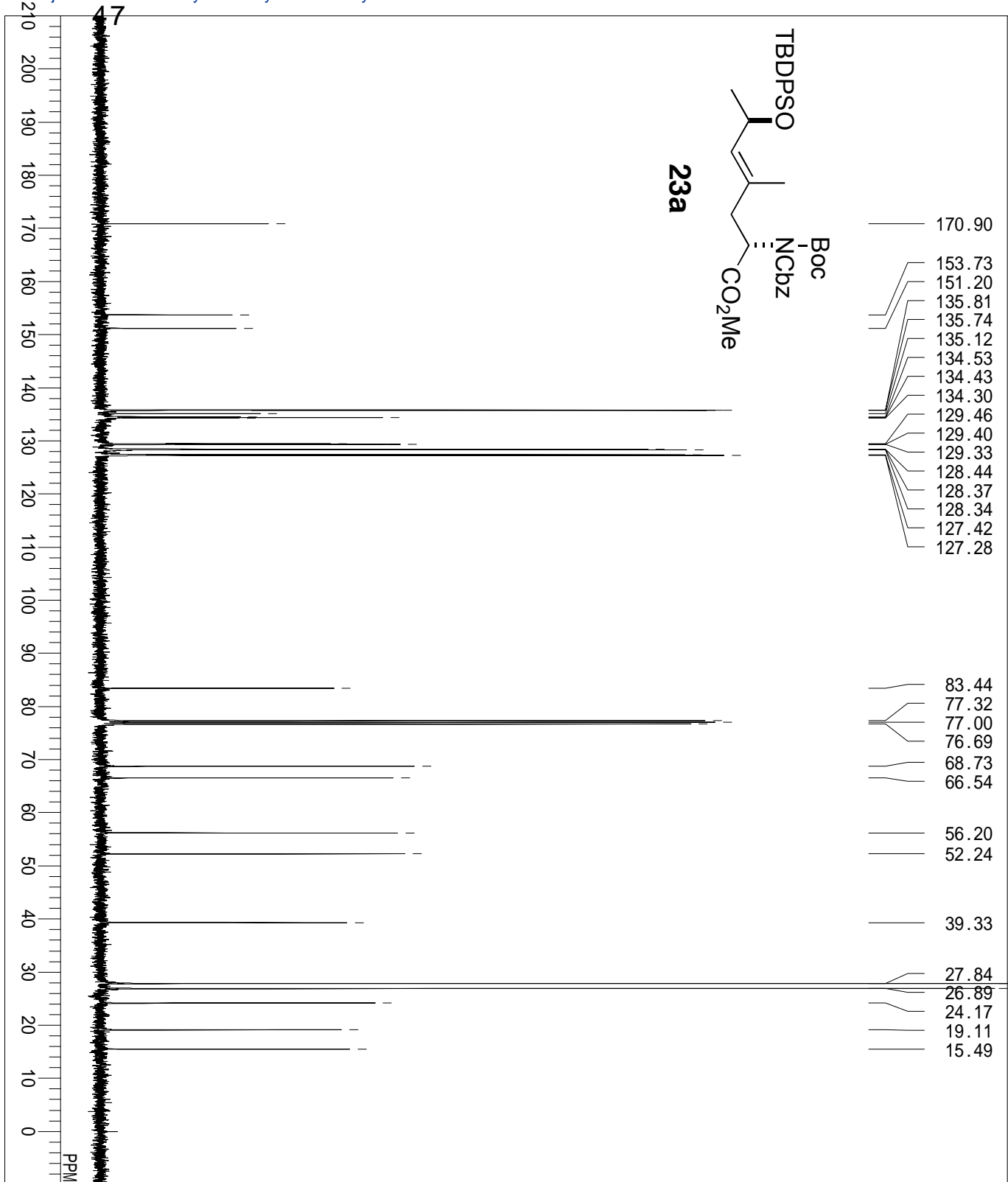
hmqcman\_HMQC-1-1.als  
 Gradient enhanced HMQC with X  
 13-05-2011 10:01:31  
 hmqc.jpg  
 IH  
 500.16 MHz  
 1.77 KHz  
 4.00 Hz  
 1040  
 1262.37 Hz  
 512  
 256  
 1120.57 Hz  
 4  
 0.8112 sec  
 1.5000 sec  
 9.35 usec  
 0.00 usec  
 0.00 usec  
 0.0000 msec  
 0.0000 msec  
 0.0000 msec  
 0.0000 msec  
 13C 18.5 c  
 CD3OD  
 12.51 ppm  
 49.00  
 50

1H OKM4115-13C



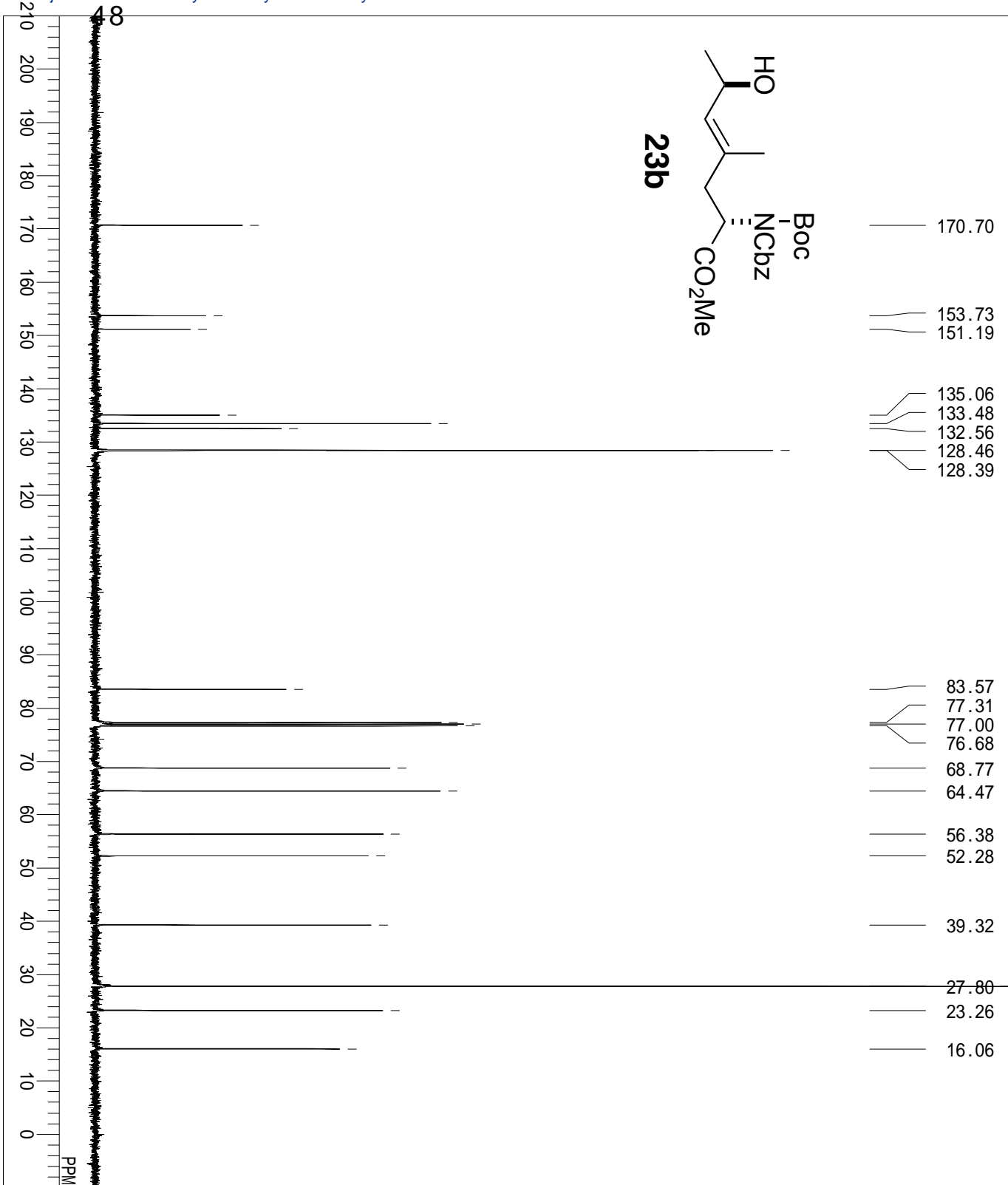


DFILF 0km4144-13c.nmdata  
 COUNT 1H 0km4144-13c  
 DATIM Mon Mar 9 22:49:40 2009  
 OBNUC 13C  
 EXMOD bcm  
 OBERQ 100.40 MHZ  
 OBSSET 130.00 KHZ  
 OBFIN 5500.00 HZ  
 POINT 32768  
 FREQU 27100.27 HZ  
 SCANS 256  
 ACQTM 1.2091 sec  
 PD 1.7909 sec  
 PWR1 5.50 usec  
 IRNUC 1H  
 CTEMP 22.3 C  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF -0.18 HZ  
 RGA IN 32

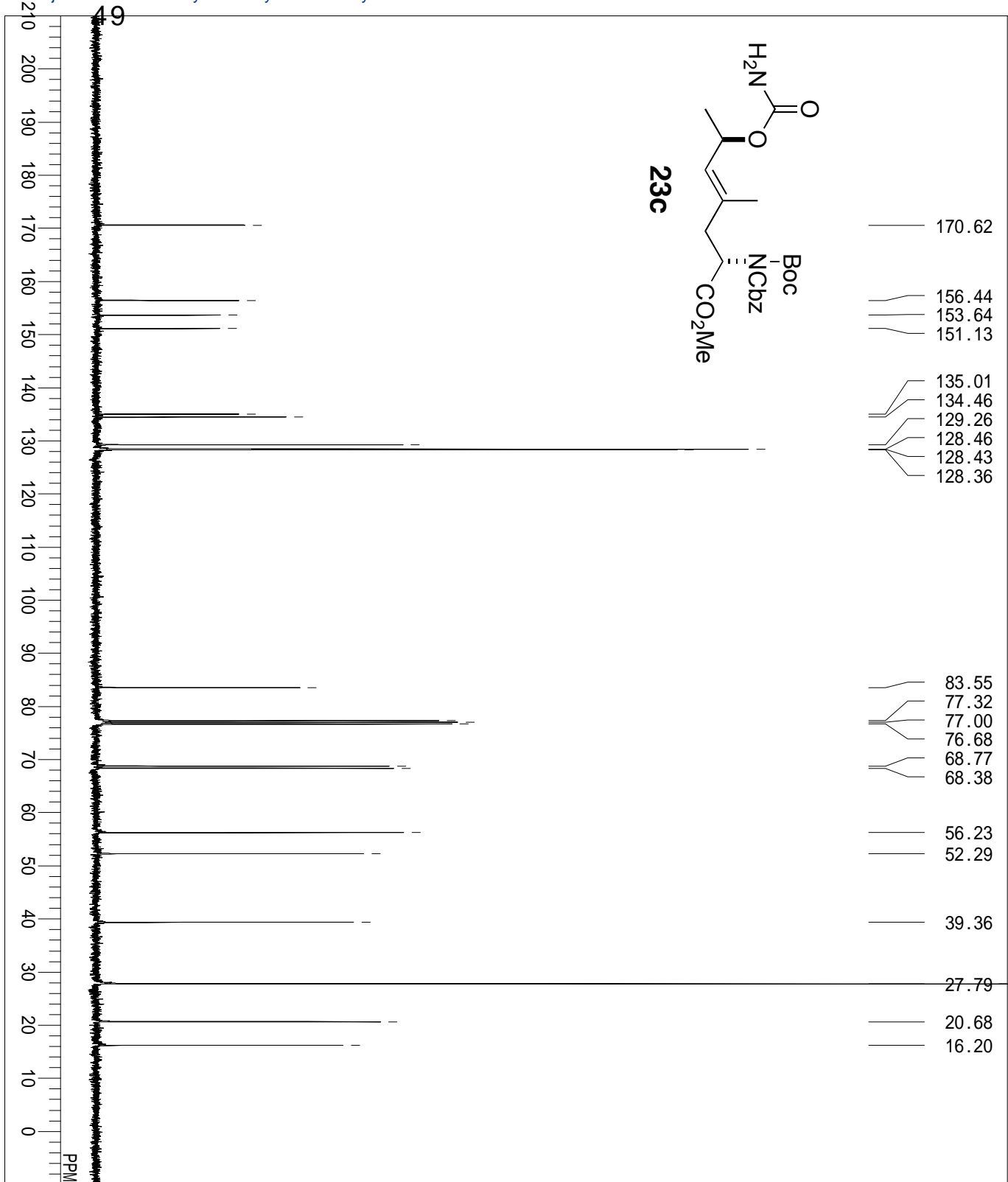


DFILF 0km4135-13c.nmdata  
 COUNT 1H 0KM4135-13C  
 DATIM Fri Feb 27 21:43:50 2009  
 OBNUC 13C  
 EXMOD bcm  
 OBERQ 100.40 MHZ  
 OBSSET 130.00 KHZ  
 OBFIN 5500.00 HZ  
 POINT 32768  
 FREQU 27100.27 HZ  
 SCANS 256  
 ACQTM 1.2091 sec  
 PD 1.7909 sec  
 PUL1 5.50 usec  
 IRNUC 1H  
 CTEMP 24.1 C  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF -0.18 HZ  
 RGA IN 33

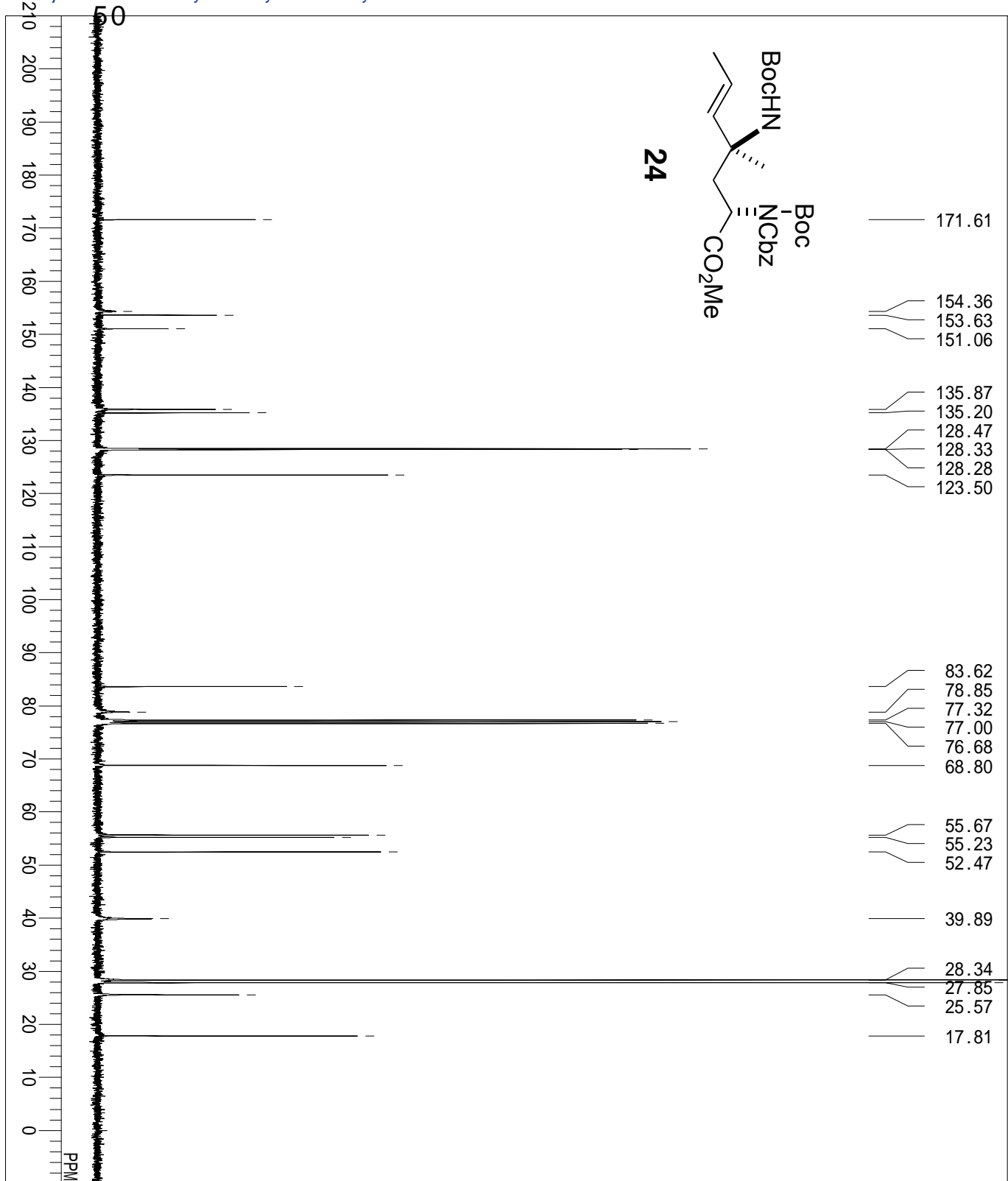




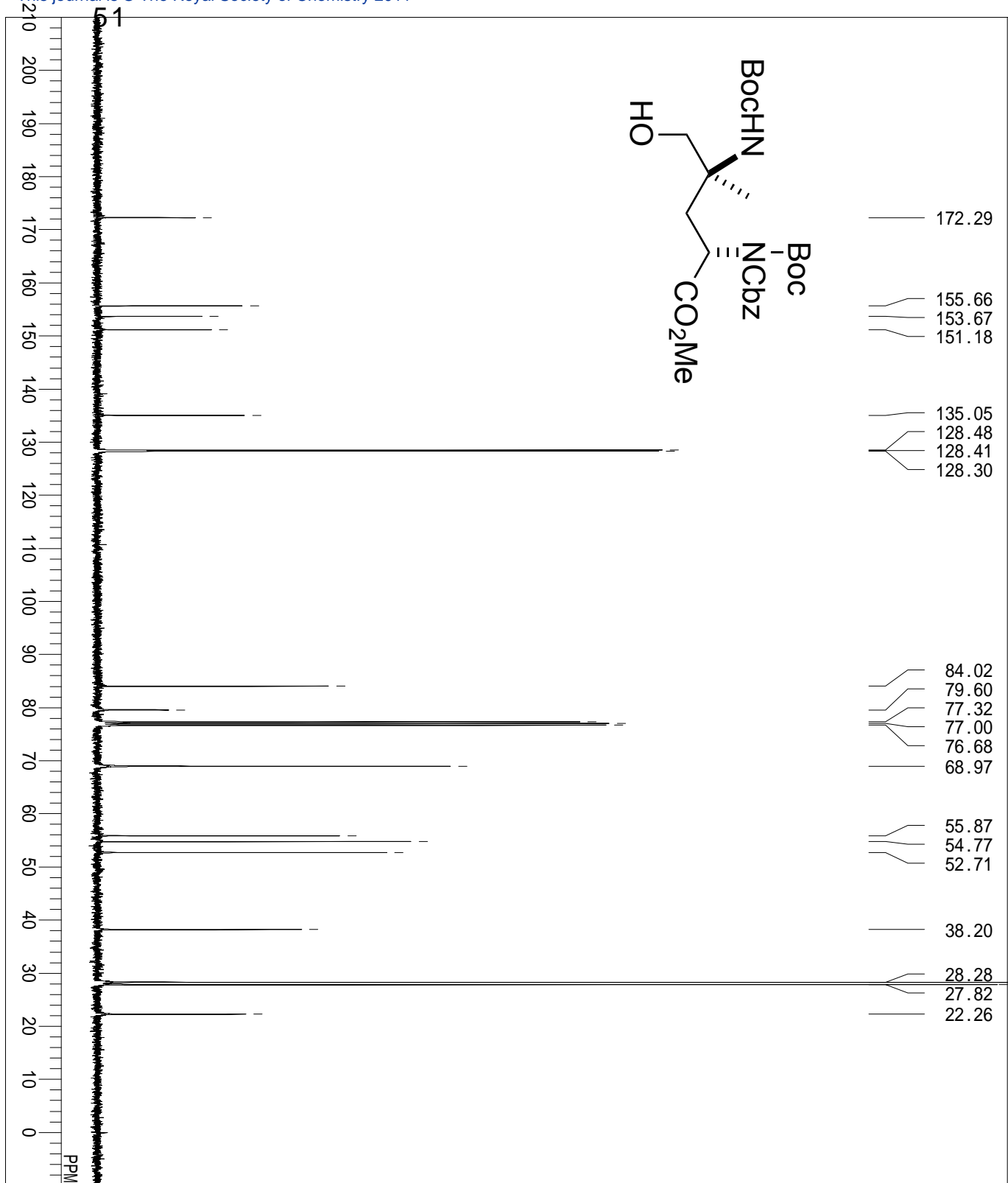
DFILF 0km4138-13c.nmdata  
 COUNT 1H OKM4138-13c  
 DATIM Tue Mar 3 00:37:48 2009  
 OBNUC 13C  
 EXMOD bcm  
 OBERQ 100.40 MHZ  
 OBSET 130.00 KHZ  
 OBFIN 5500.00 HZ  
 POINT 32768  
 FREQU 27100.27 HZ  
 SCANS 256  
 ACQTM 1.2091 sec  
 PD 1.7909 sec  
 PUL1 5.50 usec  
 IRNUC 1H  
 CTEMP 23.2 C  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF -0.18 HZ  
 RGA IN 32



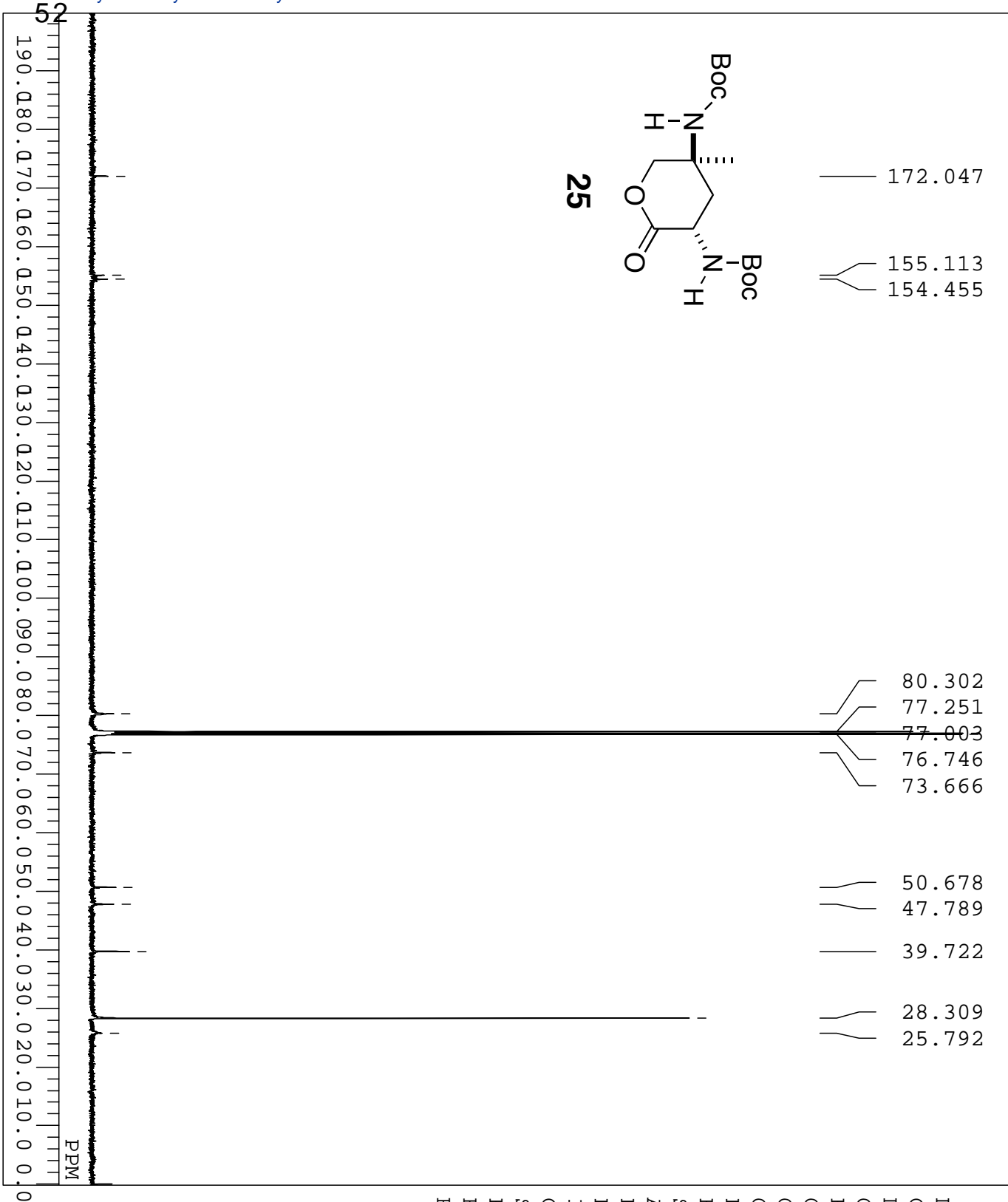
DFILF 0km4141-13c.nmdata  
 COMNT OKM4141-13C  
 DATIM Thu Mar 5 17:00:55 2009  
 OBNUC 13C  
 EXMOD bcm  
 OBFREQ 100.40 MHz  
 OBSET 130.00 KHz  
 OBFIN 5500.00 Hz  
 POINT 32768  
 FREQU 27100.27 Hz  
 SCANS 256  
 ACQTM 1.2091 sec  
 PD 1.7909 sec  
 PUL1 5.50 usec  
 IRNUC 1H  
 CTEMP 23.6 C  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF -0.18 Hz  
 RGA IN 32



DFILF OKM4143-13C.nmdata  
 COUNT 1H OKM4143-13C  
 DATIM Sat Mar 7 20:43:27 2009  
 OBNUC 13C  
 EXMOD bcm  
 OBERQ 100.40 MHz  
 OBSSET 130.00 KHz  
 OBFIN 5500.00 Hz  
 POINT 32768  
 FREQU 27100.27 Hz  
 SCANS 512  
 ACQTM 1.2091 sec  
 PD 1.7909 sec  
 PUL1 5.50 usec  
 IRNUC 1H  
 CTEMP 24.8 C  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF -0.18 Hz  
 RGA IN 32



DF11E Okm4146-13c.nmdata  
 COUNT 1H Okm4146-13c  
 DATIM Wed Mar 11 20:00:40 2009  
 OBNUC 13C  
 EXMOD bcm  
 OBERQ 100.40 MHz  
 OBSSET 130.00 KHz  
 OBFIN 5500.00 Hz  
 POINT 32768  
 FREQU 27100.27 Hz  
 SCANS 512  
 ACQTM 1.2091 sec  
 PD 1.7909 sec  
 PUL1 5.50 usec  
 IRNUC 1H  
 CTEMP 23.1 C  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF -0.18 Hz  
 RGA IN 32



DFILE man 1013 CDCl3\_Carbon-1  
 COMNT single pulse decoupled  
 DATIM 2010-12-01 17:27:42  
 OBNUC 13C  
 EXMOD carbon.jxp  
 OBFRO 125.77 MHz  
 OBSET 7.87 KHz  
 OBFIN 4.21 Hz  
 POINT 32780  
 FREQU 39308.18 Hz  
 SCANS 1024  
 ACQTM 0.8336 sec  
 PD 2.0000 sec  
 PW1 2.72 usec  
 IRNUC 1H  
 CTEMP 23.7 c  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF 0.10 Hz  
 RGAIN 60