

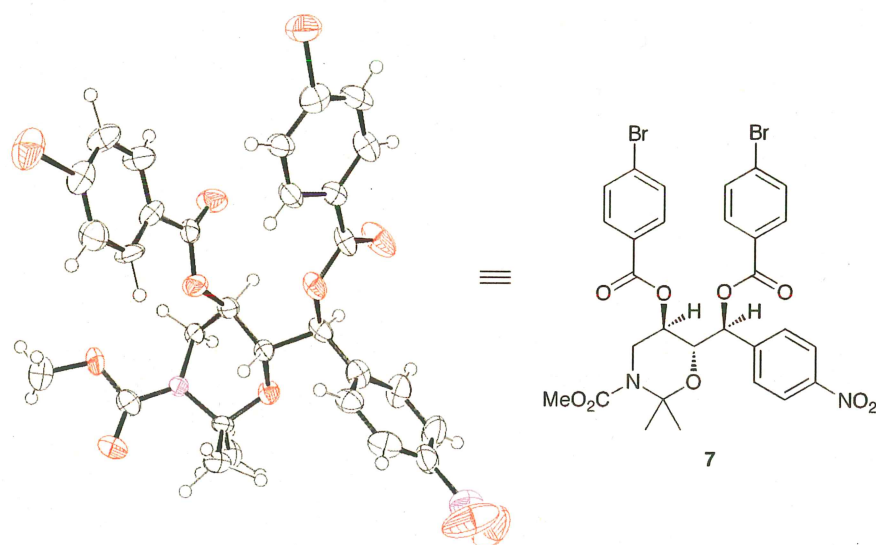
**Aminohydroxyacetone Synthons: Versatile Intermediates for the  
Organocatalytic Asymmetric Aldol Reaction**

Yoshiyuki Komatsu, Riki Watanabe, Hideaki Ikishima, Keiji Nakano,  
Yoshiyasu Ichikawa, and Hiyoshizo Kotsuki\*

*Laboratory of Natural Products Chemistry, Faculty of Science, Kochi University,  
Akebono-cho, Kochi 780-8520, Japan  
kotsuki@kochi-u.ac.jp*

**X-Ray Crystal &  $^1\text{H}$  &  $^{13}\text{C}$  NMR Data  
(52 Pages)**

### X-Ray Crystal Data for Compound 7.



#### Datablock:

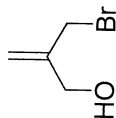
Empirical formula	C <sub>29</sub> H <sub>26</sub> Br <sub>2</sub> N <sub>2</sub> O <sub>9</sub>
Formula weight	706.34
Temperature	173 K
Radiation	CuKα (λ = 1.54187Å)
Crystal system	Orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> (#19)
Lattice parameters	a = 6.64749(14) Å b = 13.2825(3) Å c = 33.3205(7) Å V = 2942.05(11) Å <sup>3</sup>
Z value	4
Density (calculated)	1.595 g / cm <sup>3</sup>
<i>F</i> <sub>(000)</sub>	1424.000
μ (CuKα)	39.886 cm <sup>-1</sup>
Crystal dimensions	0.30 × 0.30 × 0.30 mm
Reflections collected / unique	28423 / 5336 ( <i>R</i> <sub>int</sub> = 0.071)
Refinement method	Full-matrix least-squares on <i>F</i>
Residuals: <i>R</i> [ <i>I</i> > 2.00σ( <i>I</i> )]	0.0592
Residuals: <i>R</i> <sub>w</sub> [ <i>I</i> > 2.00σ( <i>I</i> )]	0.0723
Goodness-of-fit indicator	5.036
Max shift / error in final cycle	0.051
Maximum peak in final diff. map	7.18 e <sup>-</sup> /Å <sup>3</sup>
Minimum peak in final diff. map	-5.06 e <sup>-</sup> /Å <sup>3</sup>
CCDC deposition number	844613

DIBAL fr 17

DIBAL fr 17  
Wed May 28 17:33:17 2008  
1H  
non

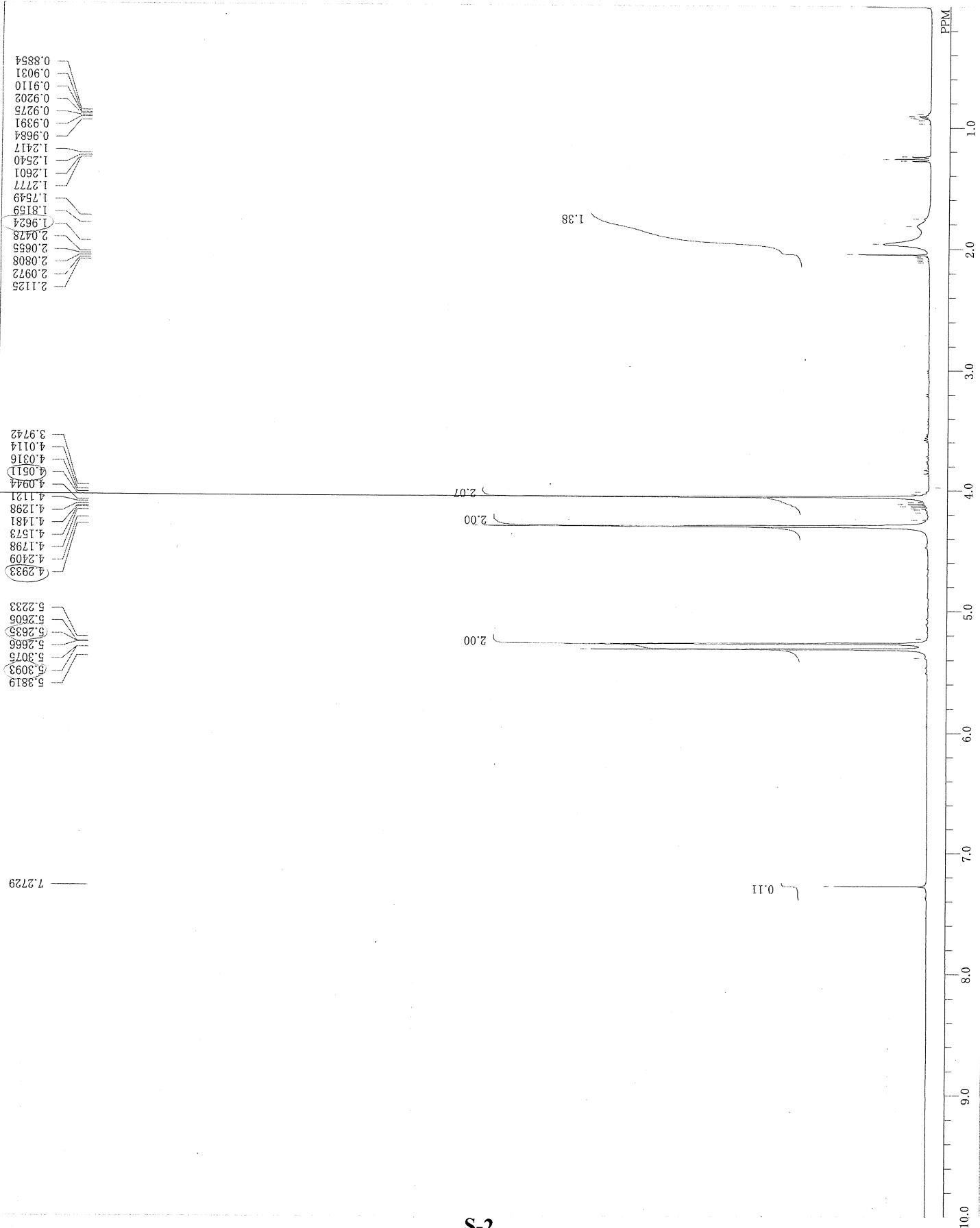
399.65 MHz  
130.00 KHz  
4300.00 Hz  
32768  
7993.60 Hz  
4  
4.0993 sec  
2.9007 sec  
5.25 usec  
1H  
23.2 c  
CDCl3  
0.00 ppm  
0.12 Hz  
20  
RGAIN

DFILE  
COMNT  
DATIM  
OBNUC  
EXMOD  
OBRQ  
OBSQ  
OBSQ  
POINT  
FREQU  
SCANS  
ACQTM  
PD  
PWI  
IRNUC  
CTEMP  
SLVNT  
EXREF  
BF  
RGAIN



1'

<sup>1</sup>H NMR  
(400 MHz, CDCl<sub>3</sub>)



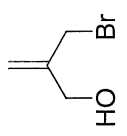
DIBAL-13C

S-3

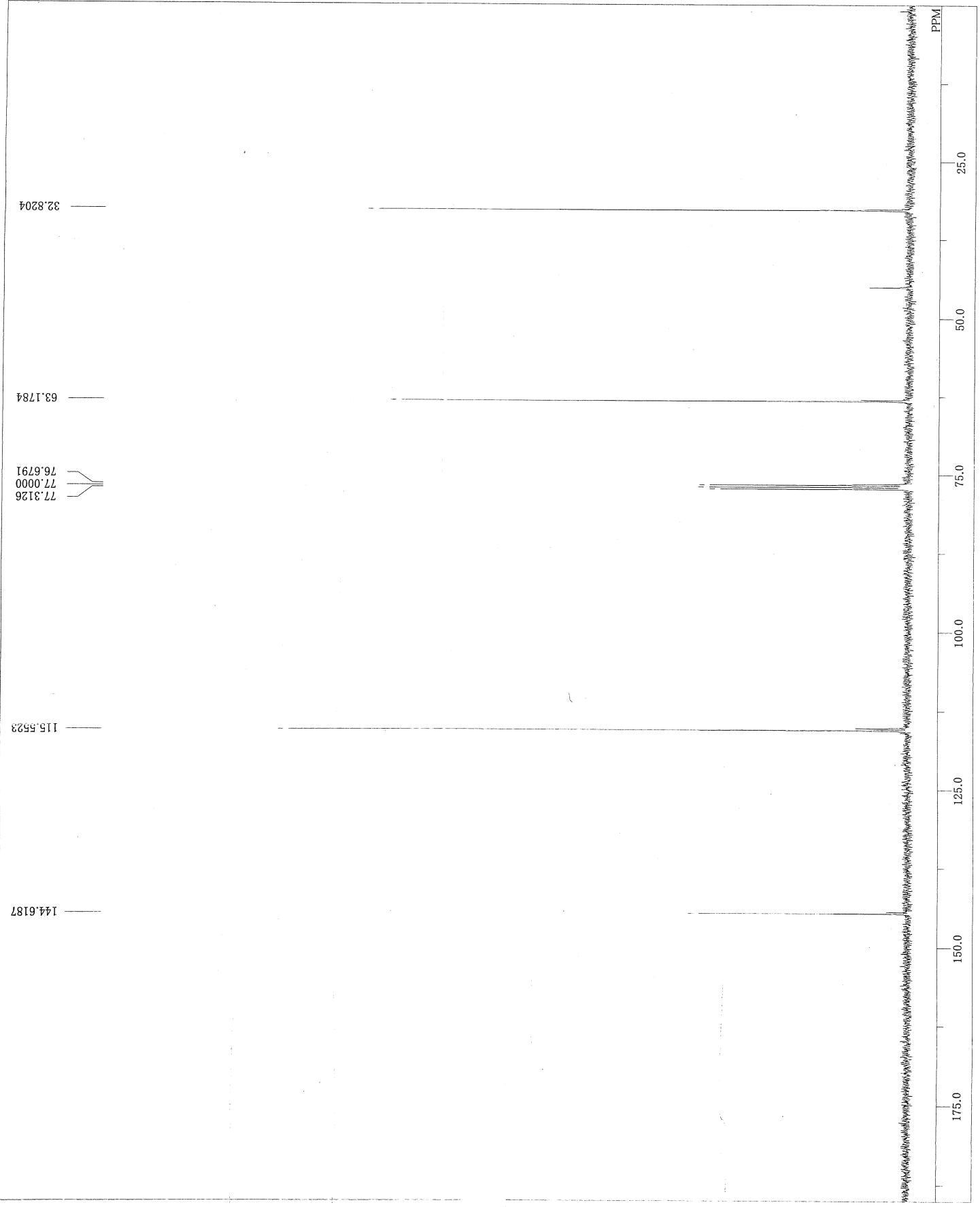
D1F1E  
COMNT  
DATIM  
OBNUC  
EXMOD  
OBFRRQ  
OBSET  
OBFIN  
POINT  
FREQU  
SCANS  
ACQTM  
PD  
PW1  
IRNUC  
CTEMP  
SLVNT  
EXREF  
BF  
RGAIN

DIBAL-13C.nmdata  
DIBAL-13C  
Sun Sep 13 17:04:46 2009  
13C  
bcm

100.40 MHz  
130.00 KHz  
5500.00 Hz  
32768  
27100.27 Hz  
240  
1.2091 sec  
1.7909 sec  
5.50 usec  
1H  
24.0 c  
CDCl3  
77.00 ppm  
0.22 Hz  
31



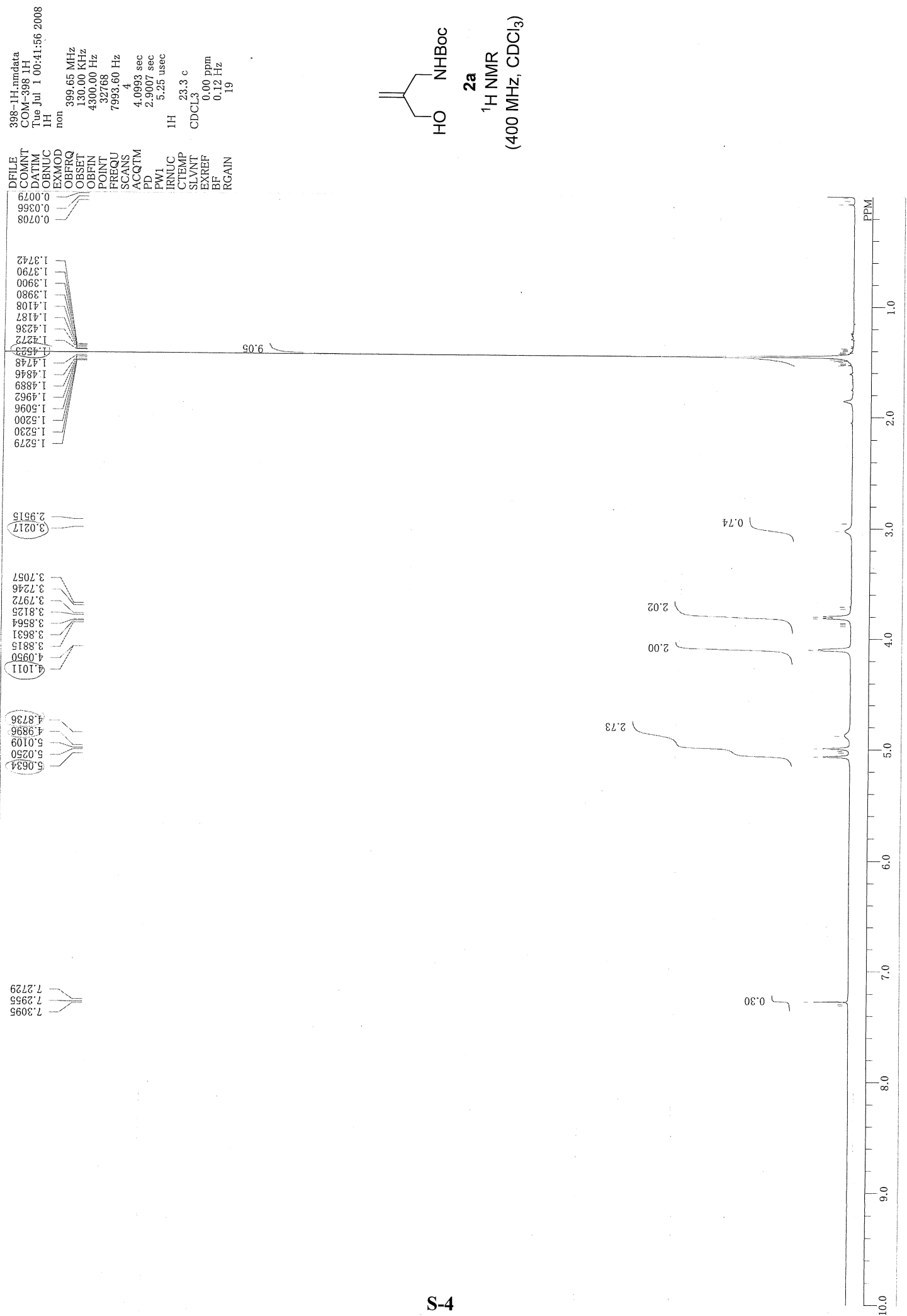
<sup>13</sup>C NMR  
(100 MHz, CDCl<sub>3</sub>)

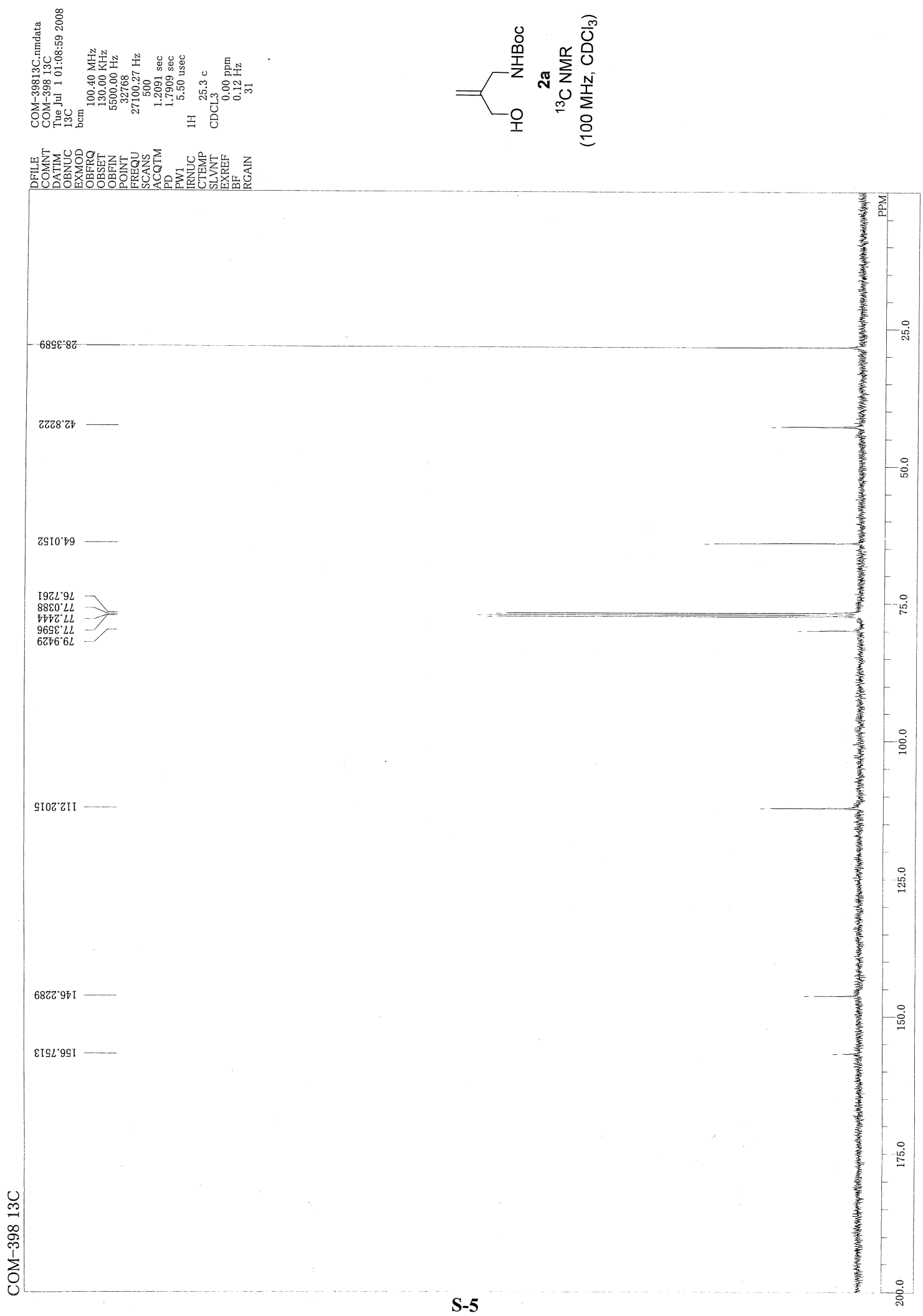




COM-398 1H

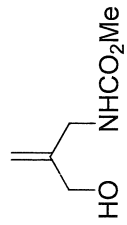
S-4



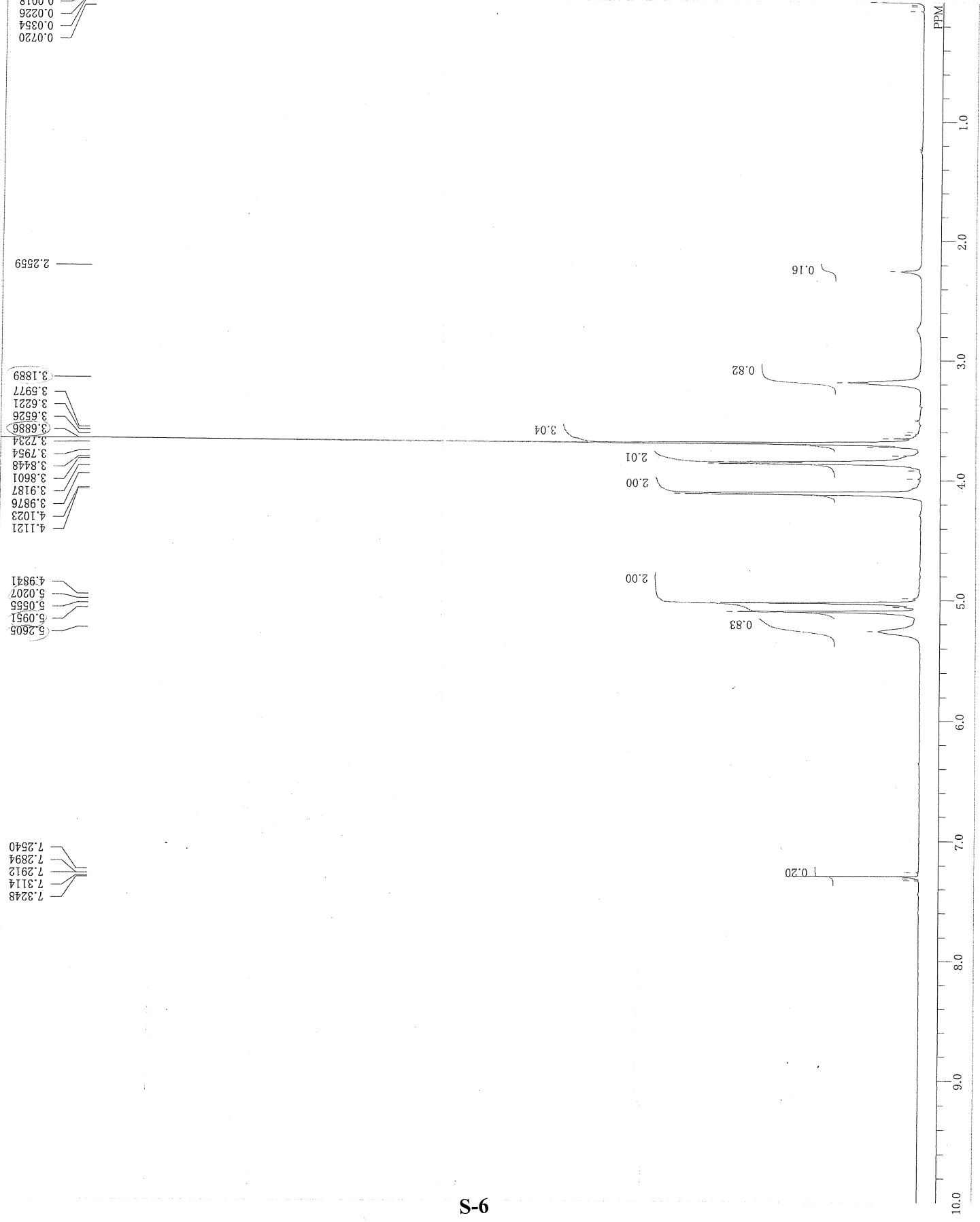


COM-541-1H

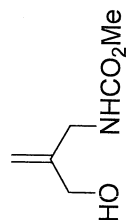
COM-541-1H.nmdata  
COM-541-1H  
Fri Jan 23 15:26:22 2009  
1H  
non  
399.65 MHz  
130.00 KHz  
4300.00 Hz  
32768  
7993.60 Hz  
4  
4.0993 sec  
2.9007 sec  
7.00 usec  
1H  
18.2 c  
CDCl<sub>3</sub>  
0.00 ppm  
0.12 Hz  
19  
DRIF  
COMET  
DATUM  
OBNUC  
EXMOD  
OBRQ  
OBSET  
OBFIN  
POINT  
FREQU  
SCANS  
ACQTM  
PD  
PW1  
IRNUC  
CTEMP  
SLVNT  
EXREF  
BF  
RGAIN



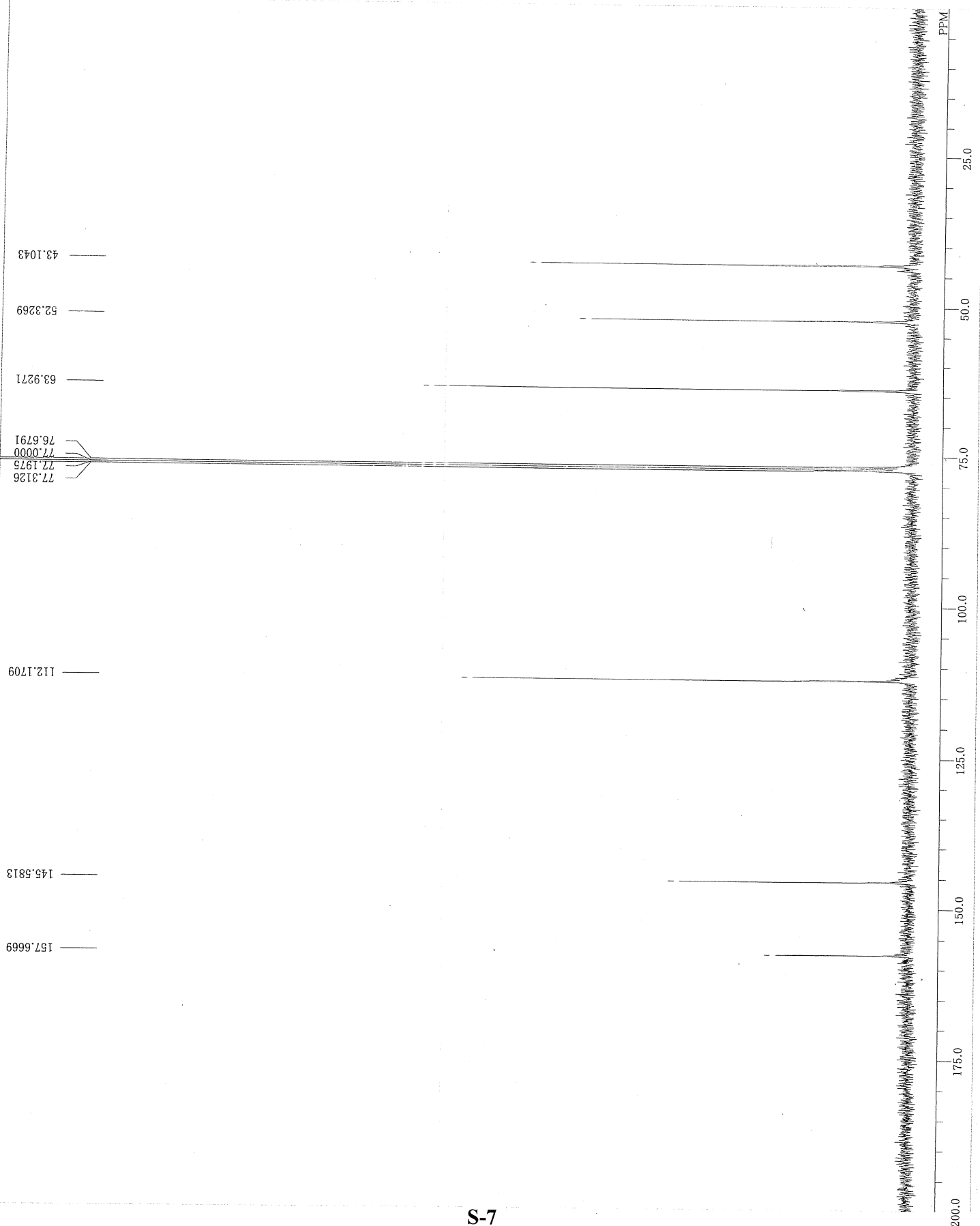
<sup>1</sup>H NMR  
(400 MHz, CDCl<sub>3</sub>)



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



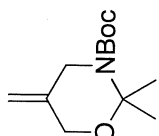
2b

<sup>13</sup>C NMR  
(100 MHz, CDCl<sub>3</sub>)

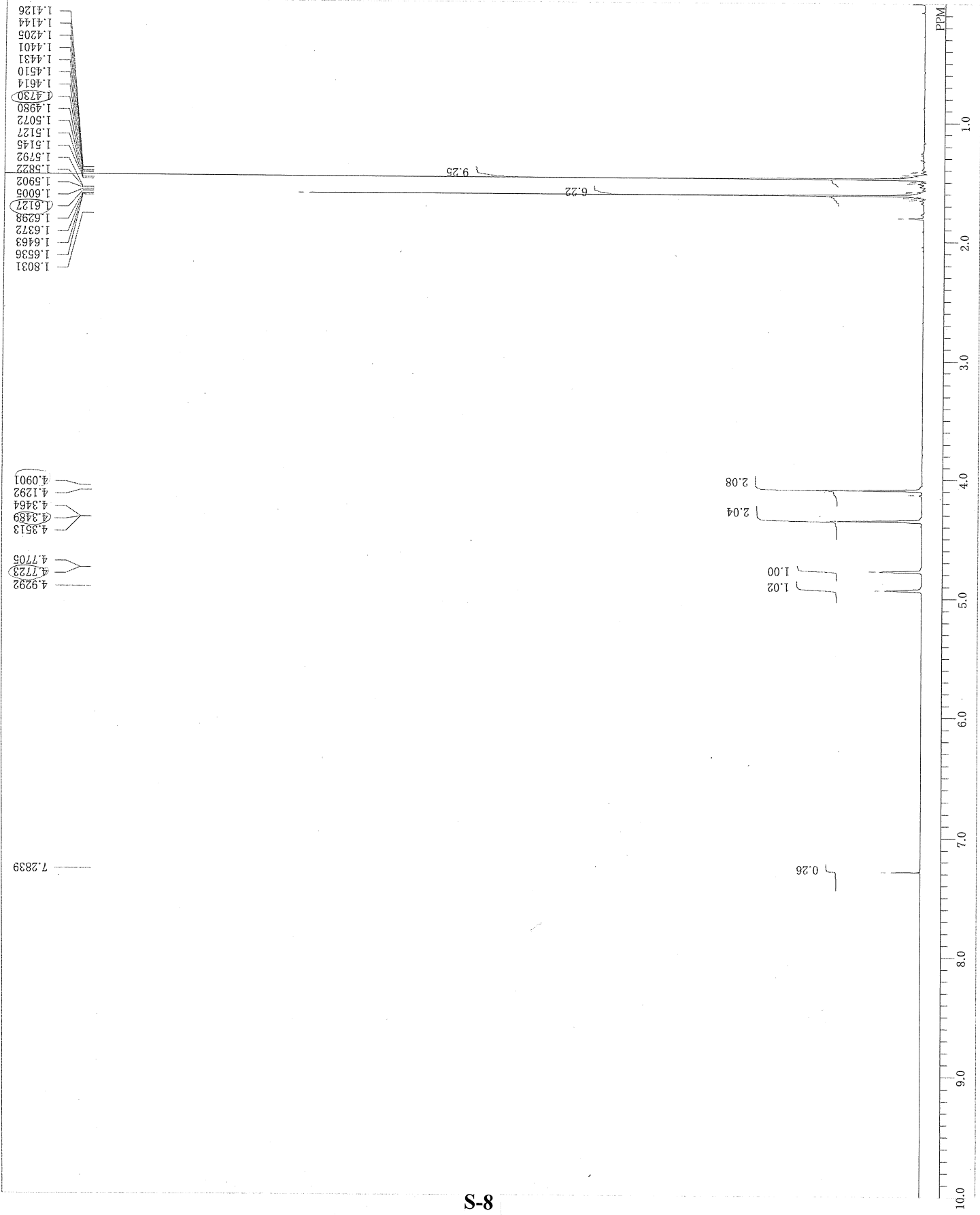
COM-429-1H

DRIF  
COMINT  
DATIM  
OBNUC  
EXMOD  
OBFRO  
OBFRO  
OBFRO  
OBFRO  
POINT  
FREQU  
SCANS  
ACQTM  
PD  
PW1  
IRNUC  
CTEMP  
SLVNT  
EXREF  
BF  
RGAIN

COM-429-fc2.3.mdata  
COM-429-1H  
Sun Jul 27 00:04:38 2008  
1H  
non  
399.65 MHz  
130.00 KHz  
4300.00 Hz  
32768  
7993.60 Hz  
4  
4.0993 sec  
2.9007 sec  
5.25 usec  
1H  
22.6 c  
CDCl3  
0.00 ppm  
0.12 Hz  
16

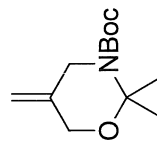


**3a**  
<sup>1</sup>H NMR  
(400 MHz, CDCl<sub>3</sub>)

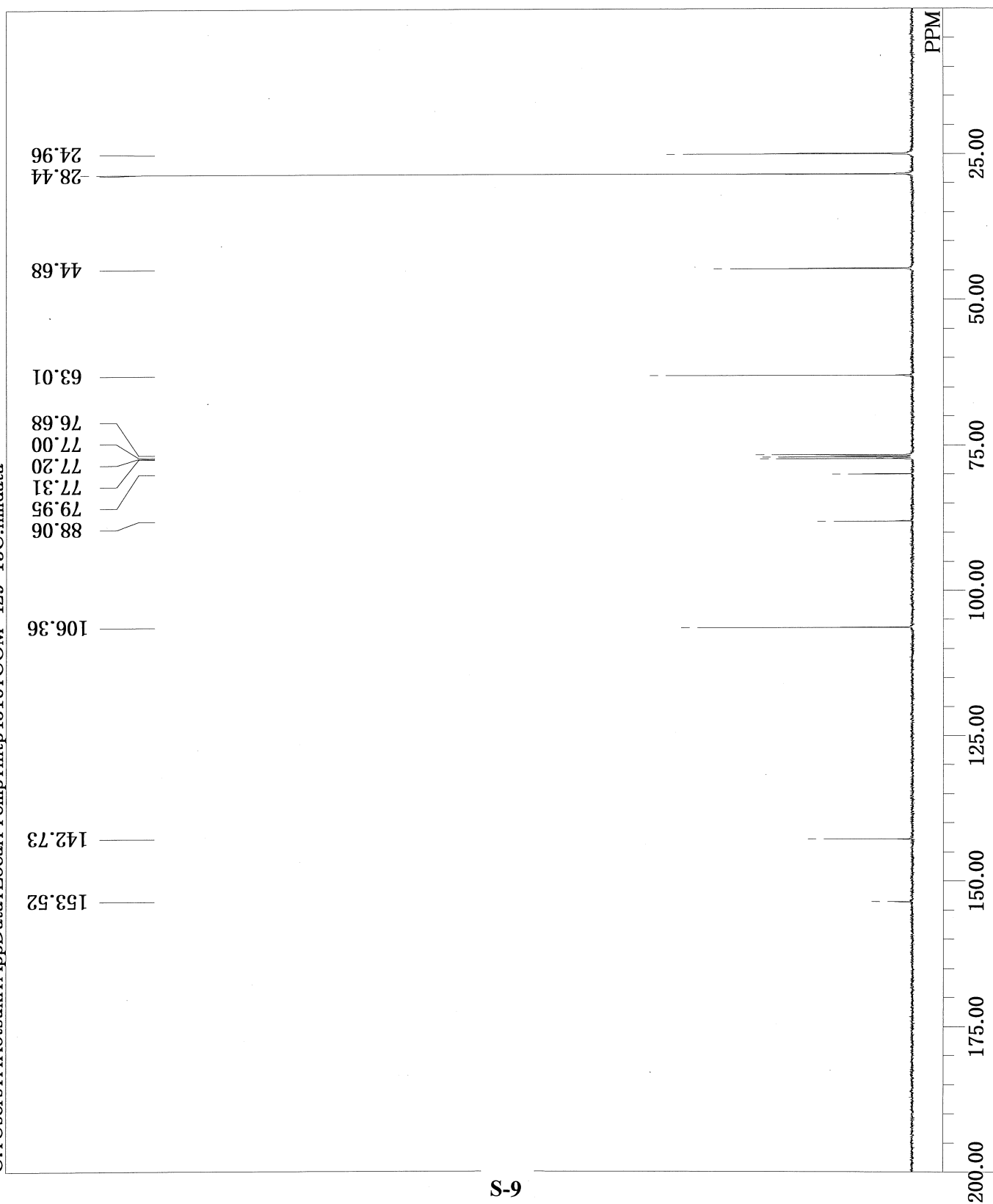


DFILE  
 COM-429-13C  
 COM-429-13C  
 DATIM  
 OBNUC  
 EXMOD  
 OBFRQ  
 OBSET  
 OBFIN  
 POINT  
 FREQU  
 SCANS  
 ACQTM  
 PD  
 PW1  
 IRNUC  
 CTEMP  
 SLVNT  
 EXREF  
 BF  
 RGAIN

COM-429-13C.nmdata  
 COM-429-13C  
 Sun Jul 27 00:58:26 2008  
 13C  
 bcm  
 100.40 MHz  
 130.00 KHz  
 5500.00 Hz  
 32768  
 27100.27 Hz  
 400  
 1.2091 sec  
 1.7909 sec  
 5.50 usec  
 1H  
 24.5 c  
 CDCL3  
 77.00 ppm  
 0.12 Hz  
 32

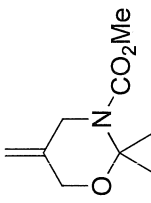


**3a**  
<sup>13</sup>C NMR  
 (100 MHz, CDCl<sub>3</sub>)

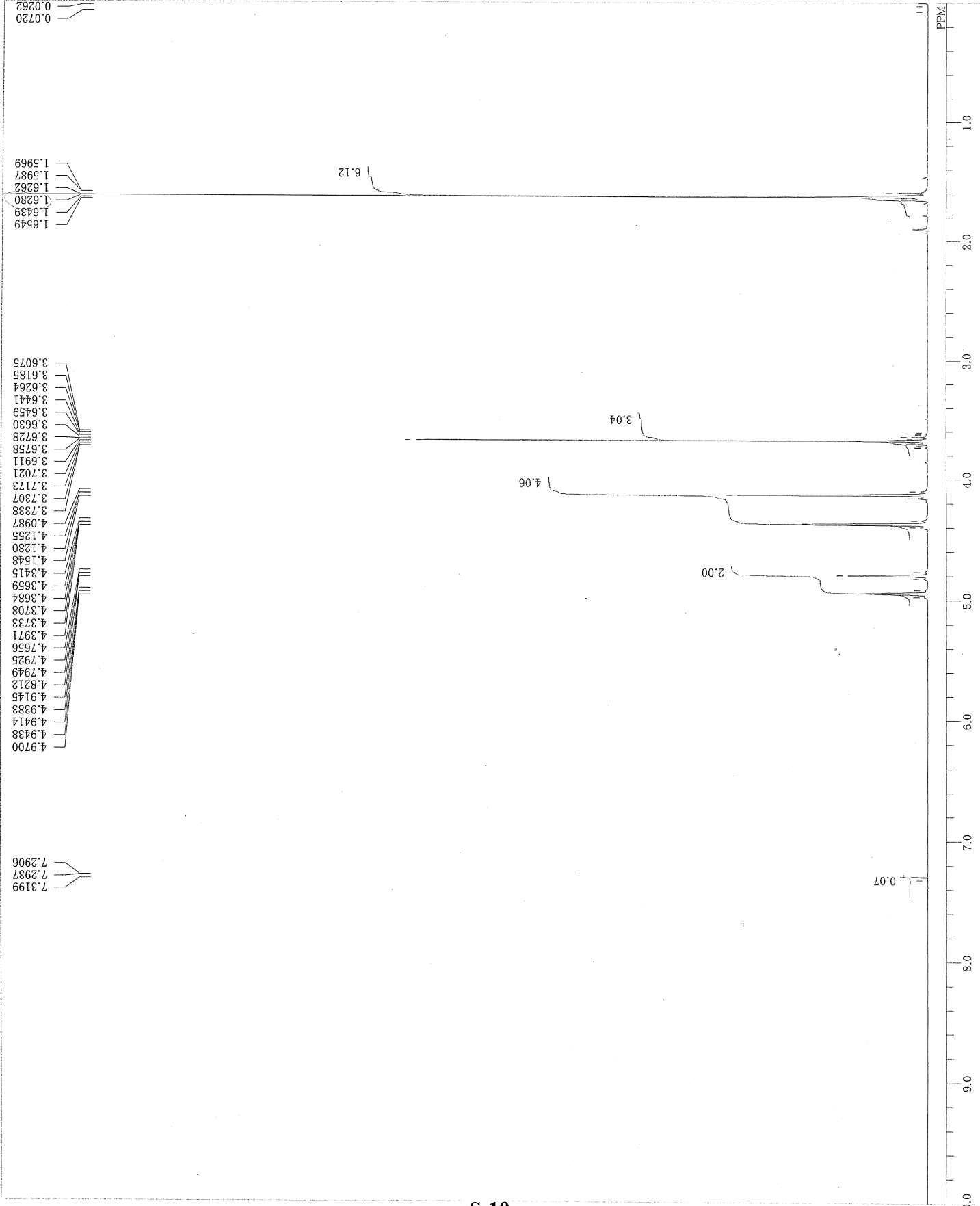


COM-542-1H

COM-542-1H.nmdata  
COM-542-1H  
Fri Jan 23 16:00:23 2009  
1H  
non  
399.65 MHz  
130.00 KHz  
4300.00 Hz  
32768  
7993.60 Hz  
4  
4.0993 sec  
2.9007 sec  
7.00 usec  
1H  
19.0 c  
CDCL<sub>3</sub>  
0.00 ppm  
0.12 Hz  
18  
RGAIN

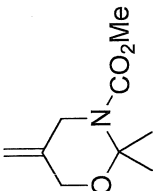


**3b**  
<sup>1</sup>H NMR  
(400 MHz, CDCl<sub>3</sub>)

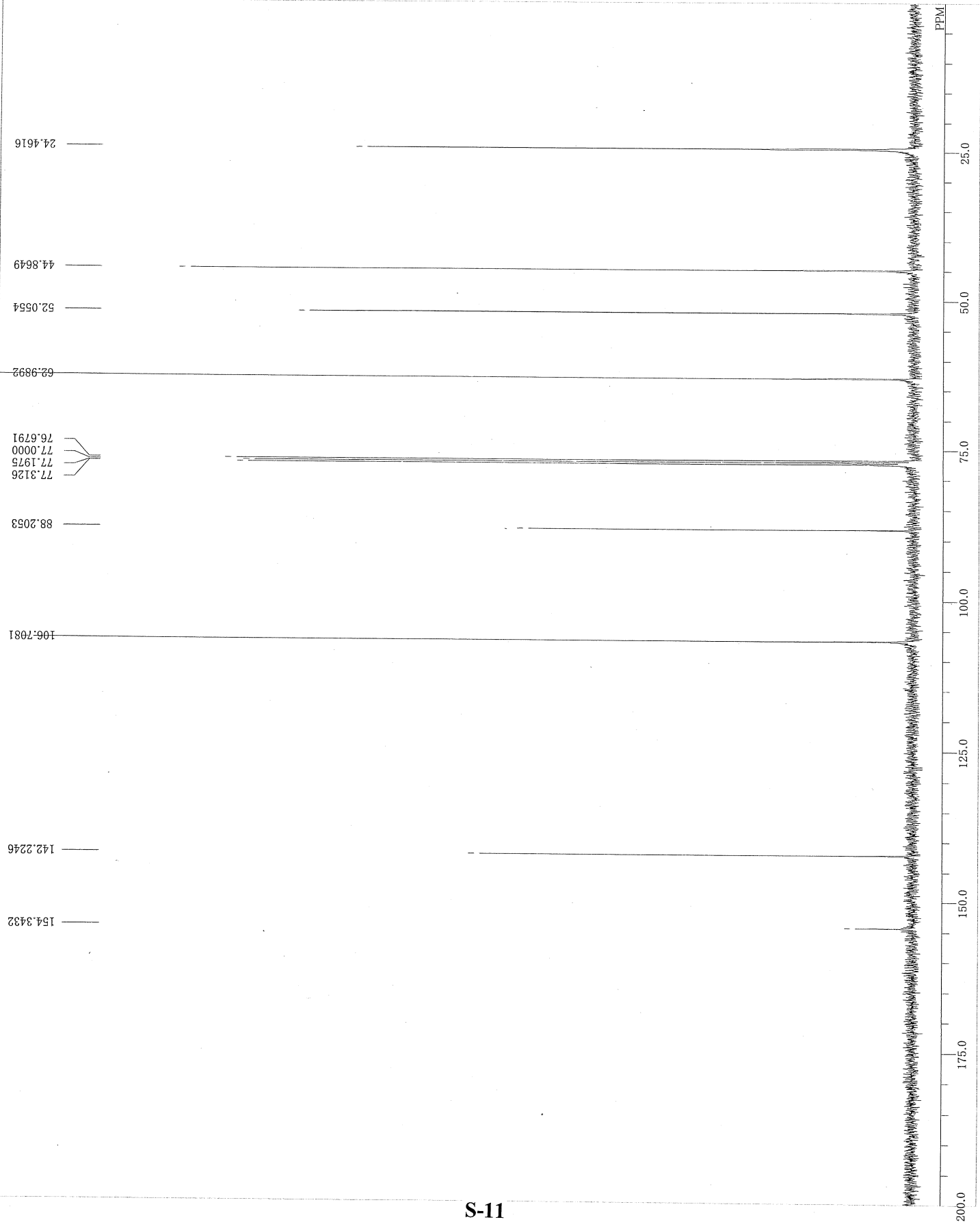


COM-542-13C

DFILE COM-542-13C.nmdata  
COMINT COM-542-13C  
DATIM Fri Jan 23 16:21:38 2009  
13C  
bcm  
EXMOD 100.40 MHz  
OBFRQ 130.00 KHz  
OBFIN 5500.00 Hz  
POINT 32768  
PREQU 27100.27 Hz  
SCANS 400  
ACQTM 1.2091 sec  
PD 1.7909 sec  
PW1 5.50 usec  
IRNUC 1H  
CTEMP 19.8 c  
SLVNT CDCL3  
EXREF 77.00 ppm  
BF 0.12 Hz  
RGAIN 33



**3b**  
<sup>13</sup>C NMR  
(100 MHz, CDCl<sub>3</sub>)

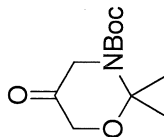




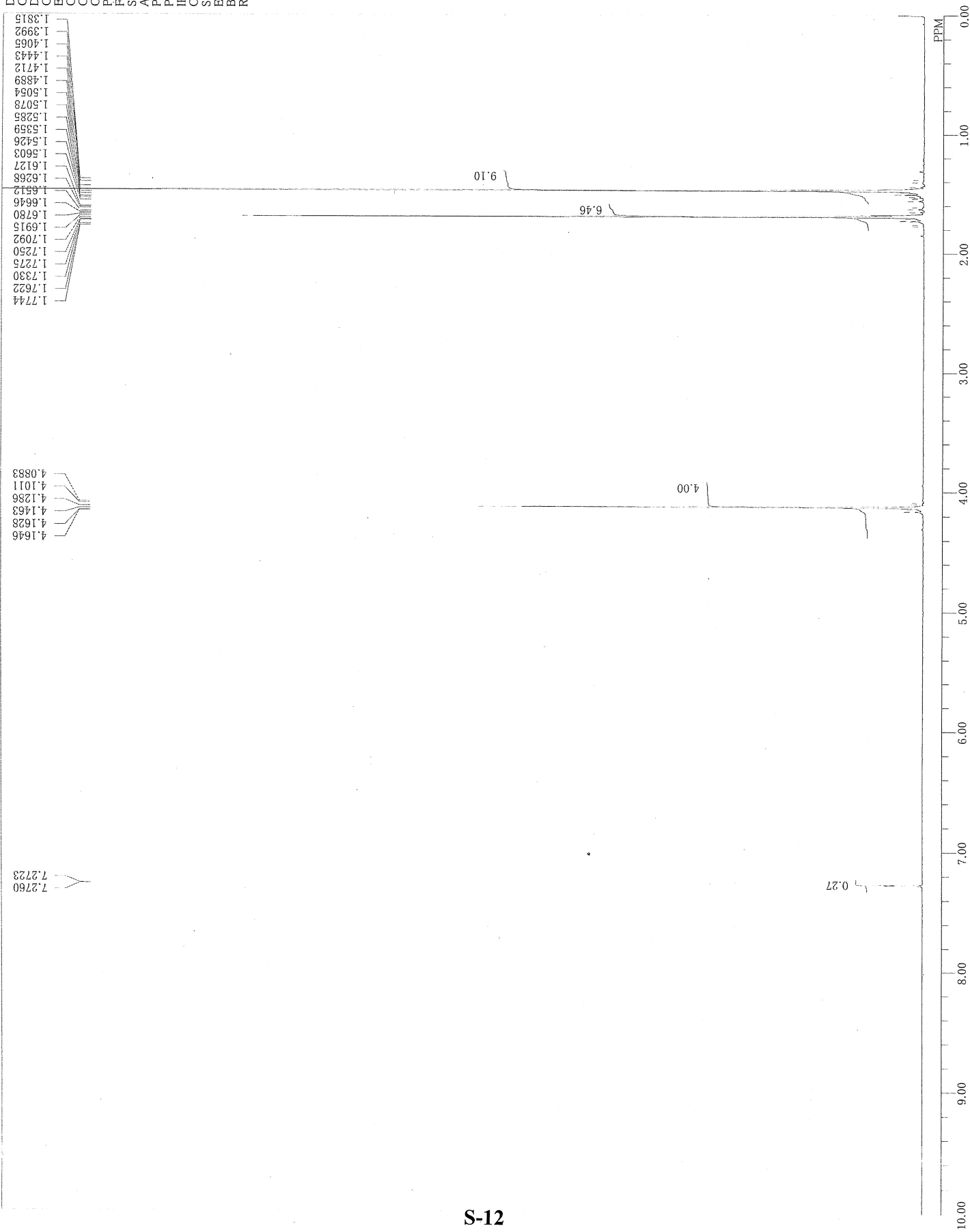
COM-433-1H

COM-433-1H.nmdata  
COM-433-1H  
Sat Aug 2 03:06:01 2008  
1H  
non  
399.65 MHz  
130.00 KHz  
4300.00 Hz  
32768  
7993.60 Hz  
4  
4.0993 sec  
2.9007 sec  
5.25 usec  
1H 23.1 c  
CDCl<sub>3</sub>  
0.00 ppm  
0.12 Hz  
18

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

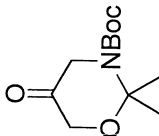


**4a**  
<sup>1</sup>H NMR  
(400 MHz, CDCl<sub>3</sub>)

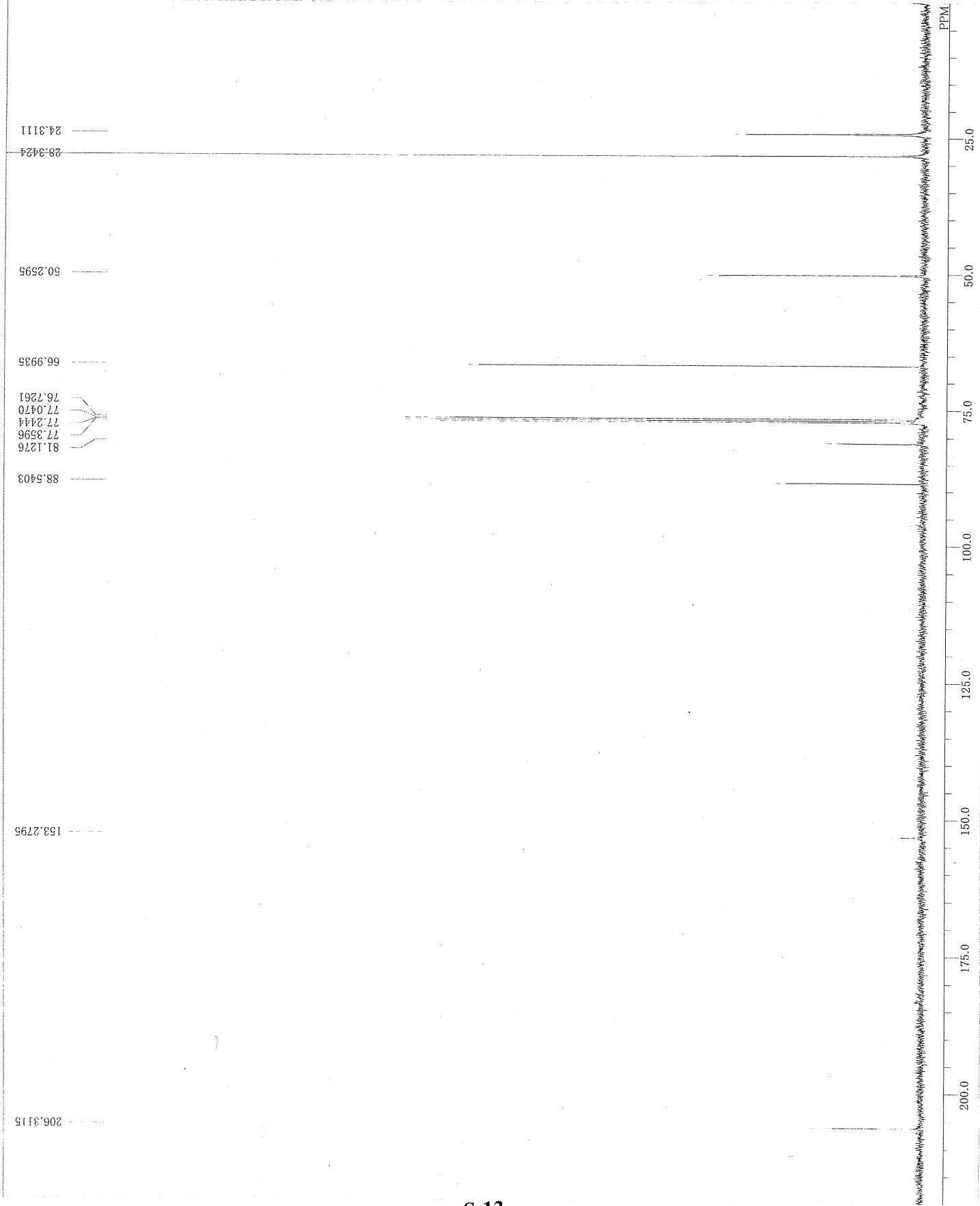


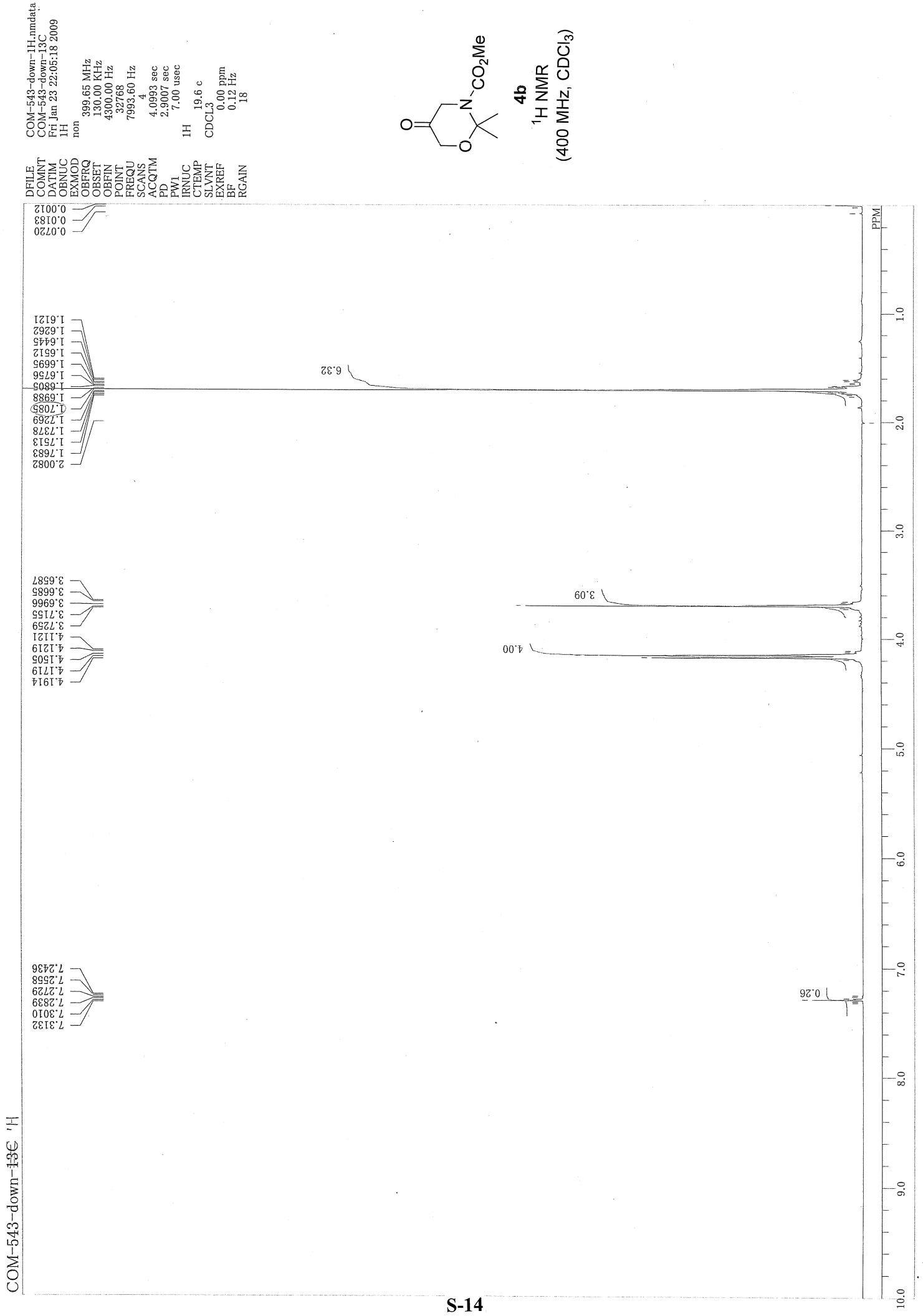
COM-433-13C

DFILE COM-433-13C.nmdata  
COM-433-13C  
DATIM Sat Aug 2 10:16:41 2008  
13C  
bcm  
EXMOD 100.40 MHz  
OBFRQ 130.00 KHz  
OBSET 5500.00 Hz  
OBFIN 32768  
POINT 27100.27 Hz  
FREQU 600  
SCANS 1.2091 sec  
ACQTM 1.7909 sec  
PD 5.50 usec  
PW1 1H  
IRNUC 24.7 c  
CTEMP CDCL3  
SLVNT 0.00 ppm  
EXREF 0.12 Hz  
BF 32  
RGAIN



**4a**  
<sup>13</sup>C NMR  
(100 MHz, CDCl<sub>3</sub>)

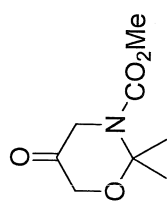




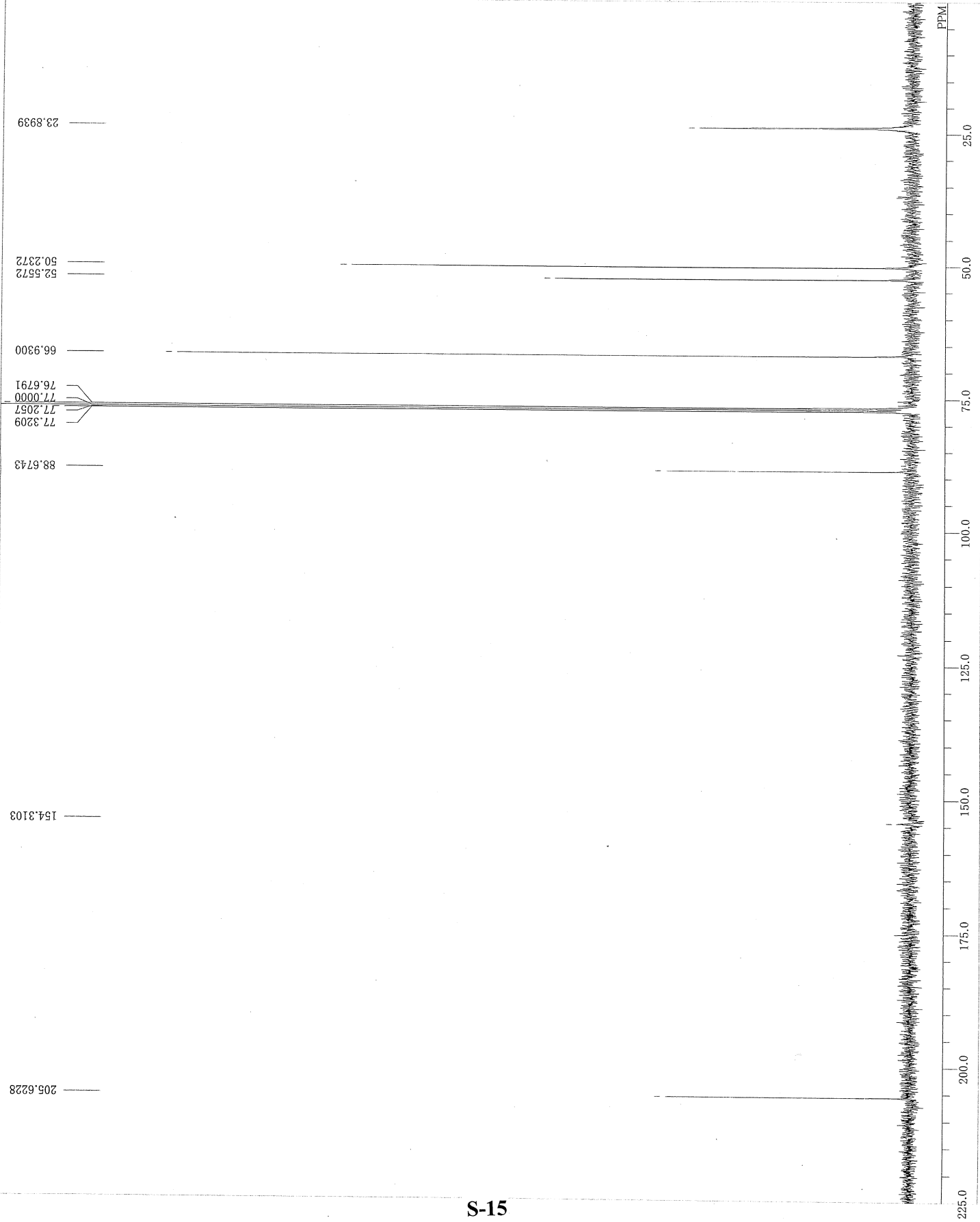
COM-543-down-13C

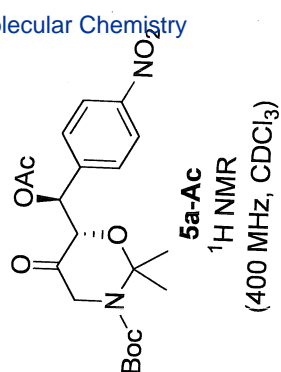
DFILE  
COMNT  
DATIM  
DENUM  
EXMOD  
OBFREQ  
OBFSET  
OBFIN  
POINT  
FREQ  
SCANS  
ACQTM  
PD  
FWI  
IRNUC  
CTEMP  
SLVNT  
EXREF  
BF  
RGAIN

COM-543-down-13C.nmdata  
COM-543-down-13C  
Fri Jan 23 22:32:02 2009  
13C  
bcm  
100.40 MHz  
130.00 KHz  
5500.00 Hz  
32768  
27100.27 Hz  
500  
1.2091 sec  
1.7909 sec  
5.50 usec  
1H  
20.5 c  
CDCL3  
77.00 ppm  
0.12 Hz  
32

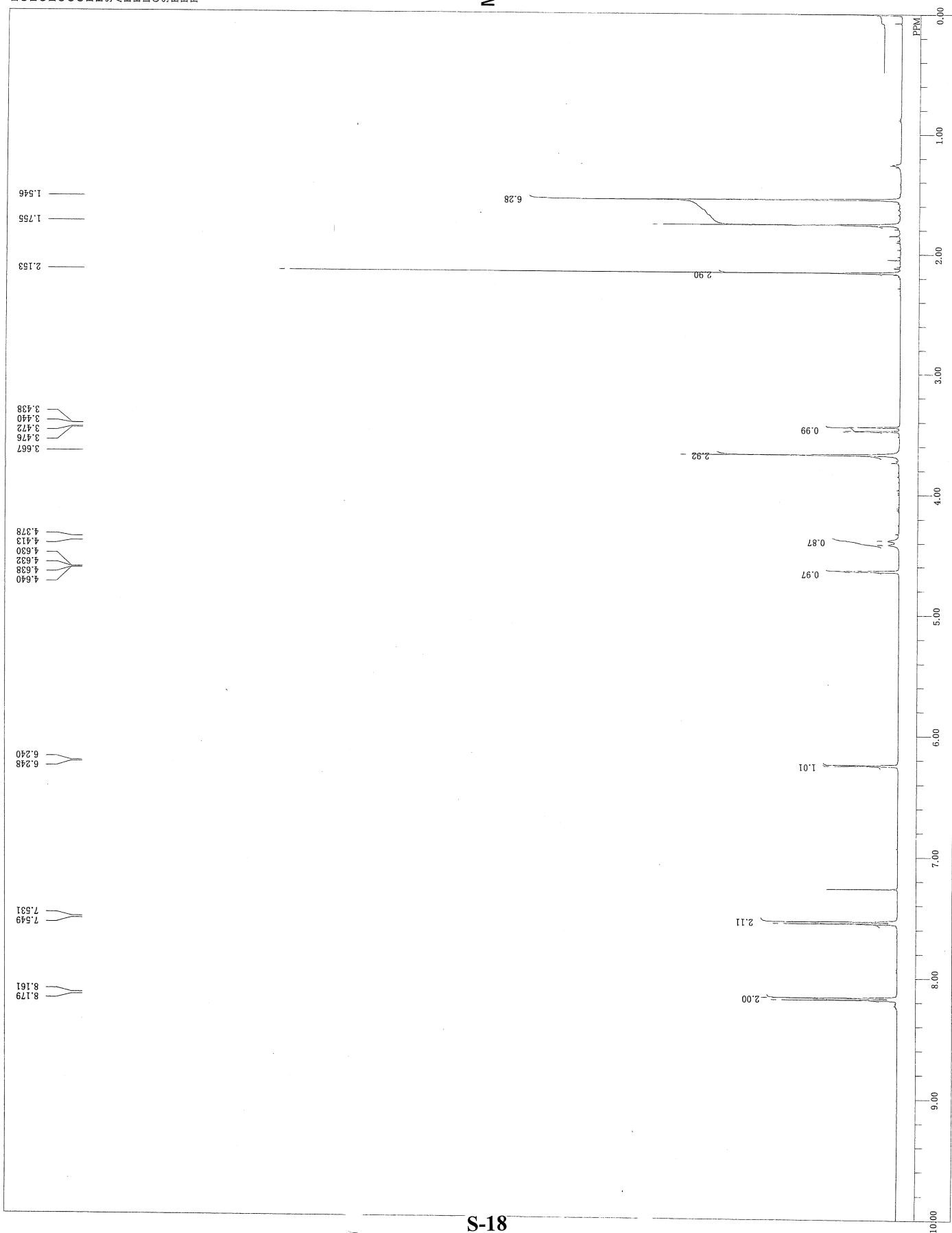
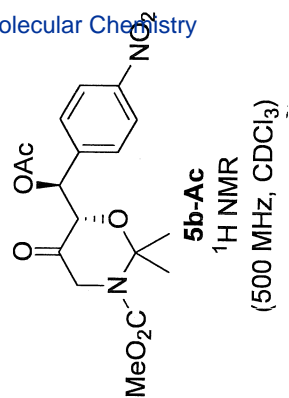


**4b**  
<sup>13</sup>C NMR  
(100 MHz, CDCl<sub>3</sub>)



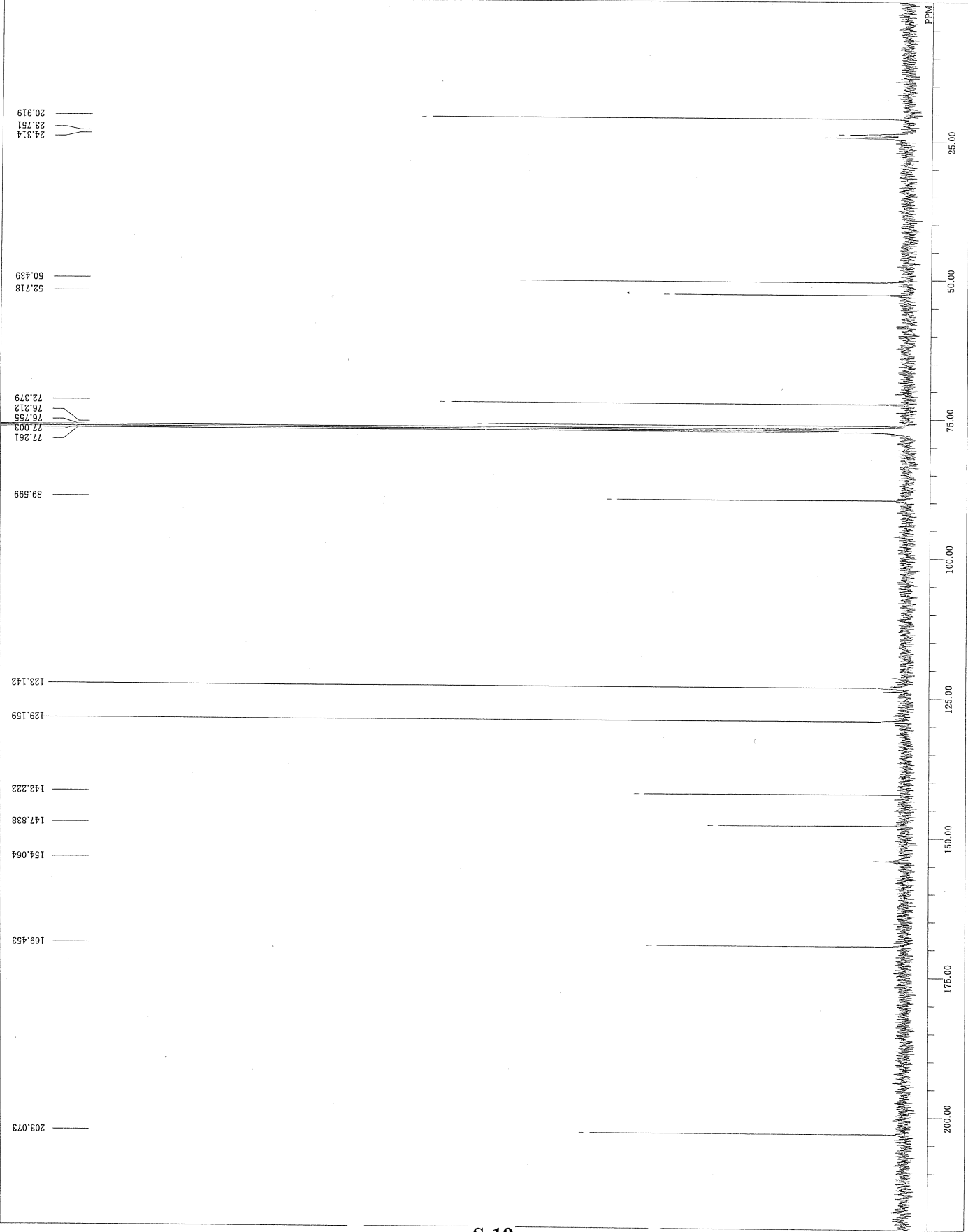
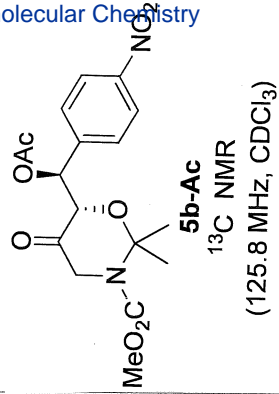






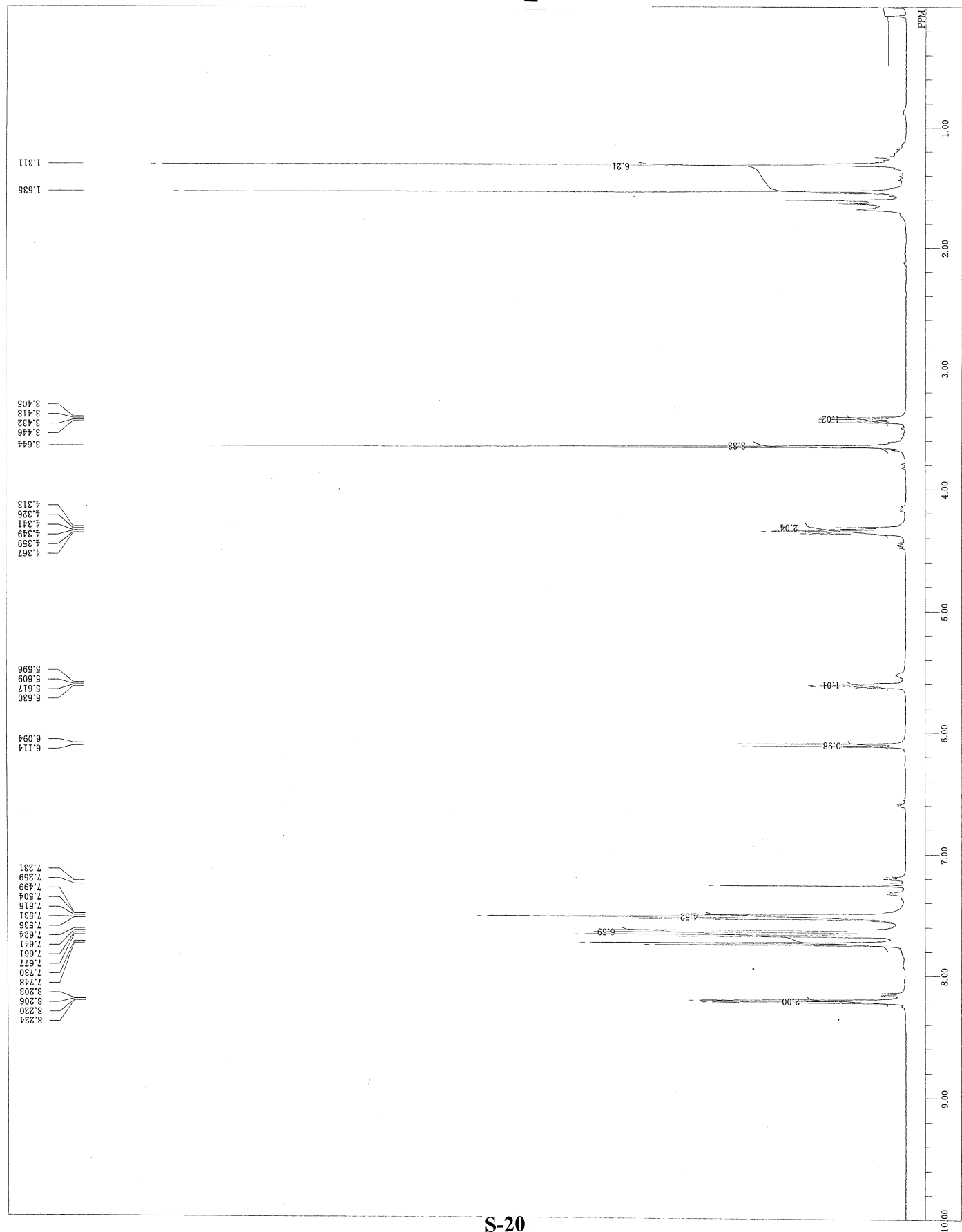
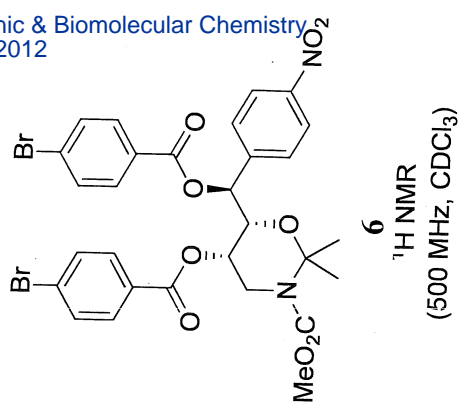
DFILE COMMT  
C:\msd\1\511-06-08 22:47:24  
13C  
carbon, 13p  
EXMOD 125.77 MHz  
OBFRQ 7.87 KHz  
OBSET 4.21 Hz  
POINT 26224  
FIDRES 31446.54 Hz  
SCANS 0.5336 sec  
AQTM 2.0000 sec  
PD 2.72 usec  
PW1 1H  
IRNUC 18.4 c  
CTEMP CDCl3  
SOLVENT 0.00 ppm  
F1REF 0.12 Hz  
RGAIN 50

20.919  
23.751  
24.314  
50.439  
52.718  
72.379  
76.212  
76.755  
77.003  
77.261  
89.599  
123.142  
129.159  
142.222  
147.838  
154.064  
169.453  
203.073





DELTA  
NAME  
COMPT  
DATE  
OBS  
OBS2  
OBS3  
OBS4  
OBS5  
OBS6  
OBS7  
OBS8  
OBS9  
OBS10  
OBS11  
OBS12  
OBS13  
OBS14  
OBS15  
OBS16  
OBS17  
OBS18  
OBS19  
OBS20  
OBS21  
OBS22  
OBS23  
OBS24  
OBS25  
OBS26  
OBS27  
OBS28  
OBS29  
OBS30  
OBS31  
OBS32  
OBS33  
OBS34  
OBS35  
OBS36  
OBS37  
OBS38  
OBS39  
OBS40  
OBS41  
OBS42  
OBS43  
OBS44  
OBS45  
OBS46  
OBS47  
OBS48  
OBS49  
OBS50  
OBS51  
OBS52  
OBS53  
OBS54  
OBS55  
OBS56  
OBS57  
OBS58  
OBS59  
OBS60  
OBS61  
OBS62  
OBS63  
OBS64  
OBS65  
OBS66  
OBS67  
OBS68  
OBS69  
OBS70  
OBS71  
OBS72  
OBS73  
OBS74  
OBS75  
OBS76  
OBS77  
OBS78  
OBS79  
OBS80  
OBS81  
OBS82  
OBS83  
OBS84  
OBS85  
OBS86  
OBS87  
OBS88  
OBS89  
OBS90  
OBS91  
OBS92  
OBS93  
OBS94  
OBS95  
OBS96  
OBS97  
OBS98  
OBS99  
OBS100  
OBS101  
OBS102  
OBS103  
OBS104  
OBS105  
OBS106  
OBS107  
OBS108  
OBS109  
OBS110  
OBS111  
OBS112  
OBS113  
OBS114  
OBS115  
OBS116  
OBS117  
OBS118  
OBS119  
OBS120  
OBS121  
OBS122  
OBS123  
OBS124  
OBS125  
OBS126  
OBS127  
OBS128  
OBS129  
OBS130  
OBS131  
OBS132  
OBS133  
OBS134  
OBS135  
OBS136  
OBS137  
OBS138  
OBS139  
OBS140  
OBS141  
OBS142  
OBS143  
OBS144  
OBS145  
OBS146  
OBS147  
OBS148  
OBS149  
OBS150  
OBS151  
OBS152  
OBS153  
OBS154  
OBS155  
OBS156  
OBS157  
OBS158  
OBS159  
OBS160  
OBS161  
OBS162  
OBS163  
OBS164  
OBS165  
OBS166  
OBS167  
OBS168  
OBS169  
OBS170  
OBS171  
OBS172  
OBS173  
OBS174  
OBS175  
OBS176  
OBS177  
OBS178  
OBS179  
OBS180  
OBS181  
OBS182  
OBS183  
OBS184  
OBS185  
OBS186  
OBS187  
OBS188  
OBS189  
OBS190  
OBS191  
OBS192  
OBS193  
OBS194  
OBS195  
OBS196  
OBS197  
OBS198  
OBS199  
OBS200  
OBS201  
OBS202  
OBS203  
OBS204  
OBS205  
OBS206  
OBS207  
OBS208  
OBS209  
OBS210  
OBS211  
OBS212  
OBS213  
OBS214  
OBS215  
OBS216  
OBS217  
OBS218  
OBS219  
OBS220  
OBS221  
OBS222  
OBS223  
OBS224  
OBS225  
OBS226  
OBS227  
OBS228  
OBS229  
OBS230  
OBS231  
OBS232  
OBS233  
OBS234  
OBS235  
OBS236  
OBS237  
OBS238  
OBS239  
OBS240  
OBS241  
OBS242  
OBS243  
OBS244  
OBS245  
OBS246  
OBS247  
OBS248  
OBS249  
OBS250  
OBS251  
OBS252  
OBS253  
OBS254  
OBS255  
OBS256  
OBS257  
OBS258  
OBS259  
OBS260  
OBS261  
OBS262  
OBS263  
OBS264  
OBS265  
OBS266  
OBS267  
OBS268  
OBS269  
OBS270  
OBS271  
OBS272  
OBS273  
OBS274  
OBS275  
OBS276  
OBS277  
OBS278  
OBS279  
OBS280  
OBS281  
OBS282  
OBS283  
OBS284  
OBS285  
OBS286  
OBS287  
OBS288  
OBS289  
OBS290  
OBS291  
OBS292  
OBS293  
OBS294  
OBS295  
OBS296  
OBS297  
OBS298  
OBS299  
OBS300  
OBS301  
OBS302  
OBS303  
OBS304  
OBS305  
OBS306  
OBS307  
OBS308  
OBS309  
OBS310  
OBS311  
OBS312  
OBS313  
OBS314  
OBS315  
OBS316  
OBS317  
OBS318  
OBS319  
OBS320  
OBS321  
OBS322  
OBS323  
OBS324  
OBS325  
OBS326  
OBS327  
OBS328  
OBS329  
OBS330  
OBS331  
OBS332  
OBS333  
OBS334  
OBS335  
OBS336  
OBS337  
OBS338  
OBS339  
OBS340  
OBS341  
OBS342  
OBS343  
OBS344  
OBS345  
OBS346  
OBS347  
OBS348  
OBS349  
OBS350  
OBS351  
OBS352  
OBS353  
OBS354  
OBS355  
OBS356  
OBS357  
OBS358  
OBS359  
OBS360  
OBS361  
OBS362  
OBS363  
OBS364  
OBS365  
OBS366  
OBS367  
OBS368  
OBS369  
OBS370  
OBS371  
OBS372  
OBS373  
OBS374  
OBS375  
OBS376  
OBS377  
OBS378  
OBS379  
OBS380  
OBS381  
OBS382  
OBS383  
OBS384  
OBS385  
OBS386  
OBS387  
OBS388  
OBS389  
OBS390  
OBS391  
OBS392  
OBS393  
OBS394  
OBS395  
OBS396  
OBS397  
OBS398  
OBS399  
OBS400  
OBS401  
OBS402  
OBS403  
OBS404  
OBS405  
OBS406  
OBS407  
OBS408  
OBS409  
OBS410  
OBS411  
OBS412  
OBS413  
OBS414  
OBS415  
OBS416  
OBS417  
OBS418  
OBS419  
OBS420  
OBS421  
OBS422  
OBS423  
OBS424  
OBS425  
OBS426  
OBS427  
OBS428  
OBS429  
OBS430  
OBS431  
OBS432  
OBS433  
OBS434  
OBS435  
OBS436  
OBS437  
OBS438  
OBS439  
OBS440  
OBS441  
OBS442  
OBS443  
OBS444  
OBS445  
OBS446  
OBS447  
OBS448  
OBS449  
OBS450  
OBS451  
OBS452  
OBS453  
OBS454  
OBS455  
OBS456  
OBS457  
OBS458  
OBS459  
OBS460  
OBS461  
OBS462  
OBS463  
OBS464  
OBS465  
OBS466  
OBS467  
OBS468  
OBS469  
OBS470  
OBS471  
OBS472  
OBS473  
OBS474  
OBS475  
OBS476  
OBS477  
OBS478  
OBS479  
OBS480  
OBS481  
OBS482  
OBS483  
OBS484  
OBS485  
OBS486  
OBS487  
OBS488  
OBS489  
OBS490  
OBS491  
OBS492  
OBS493  
OBS494  
OBS495  
OBS496  
OBS497  
OBS498  
OBS499  
OBS500  
OBS501  
OBS502  
OBS503  
OBS504  
OBS505  
OBS506  
OBS507  
OBS508  
OBS509  
OBS510  
OBS511  
OBS512  
OBS513  
OBS514  
OBS515  
OBS516  
OBS517  
OBS518  
OBS519  
OBS520  
OBS521  
OBS522  
OBS523  
OBS524  
OBS525  
OBS526  
OBS527  
OBS528  
OBS529  
OBS530  
OBS531  
OBS532  
OBS533  
OBS534  
OBS535  
OBS536  
OBS537  
OBS538  
OBS539  
OBS540  
OBS541  
OBS542  
OBS543  
OBS544  
OBS545  
OBS546  
OBS547  
OBS548  
OBS549  
OBS550  
OBS551  
OBS552  
OBS553  
OBS554  
OBS555  
OBS556  
OBS557  
OBS558  
OBS559  
OBS560  
OBS561  
OBS562  
OBS563  
OBS564  
OBS565  
OBS566  
OBS567  
OBS568  
OBS569  
OBS570  
OBS571  
OBS572  
OBS573  
OBS574  
OBS575  
OBS576  
OBS577  
OBS578  
OBS579  
OBS580  
OBS581  
OBS582  
OBS583  
OBS584  
OBS585  
OBS586  
OBS587  
OBS588  
OBS589  
OBS590  
OBS591  
OBS592  
OBS593  
OBS594  
OBS595  
OBS596  
OBS597  
OBS598  
OBS599  
OBS600  
OBS601  
OBS602  
OBS603  
OBS604  
OBS605  
OBS606  
OBS607  
OBS608  
OBS609  
OBS610  
OBS611  
OBS612  
OBS613  
OBS614  
OBS615  
OBS616  
OBS617  
OBS618  
OBS619  
OBS620  
OBS621  
OBS622  
OBS623  
OBS624  
OBS625  
OBS626  
OBS627  
OBS628  
OBS629  
OBS630  
OBS631  
OBS632  
OBS633  
OBS634  
OBS635  
OBS636  
OBS637  
OBS638  
OBS639  
OBS640  
OBS641  
OBS642  
OBS643  
OBS644  
OBS645  
OBS646  
OBS647  
OBS648  
OBS649  
OBS650  
OBS651  
OBS652  
OBS653  
OBS654  
OBS655  
OBS656  
OBS657  
OBS658  
OBS659  
OBS660  
OBS661  
OBS662  
OBS663  
OBS664  
OBS665  
OBS666  
OBS667  
OBS668  
OBS669  
OBS670  
OBS671  
OBS672  
OBS673  
OBS674  
OBS675  
OBS676  
OBS677  
OBS678  
OBS679  
OBS680  
OBS681  
OBS682  
OBS683  
OBS684  
OBS685  
OBS686  
OBS687  
OBS688  
OBS689  
OBS690  
OBS691  
OBS692  
OBS693  
OBS694  
OBS695  
OBS696  
OBS697  
OBS698  
OBS699  
OBS700  
OBS701  
OBS702  
OBS703  
OBS704  
OBS705  
OBS706  
OBS707  
OBS708  
OBS709  
OBS710  
OBS711  
OBS712  
OBS713  
OBS714  
OBS715  
OBS716  
OBS717  
OBS718  
OBS719  
OBS720  
OBS721  
OBS722  
OBS723  
OBS724  
OBS725  
OBS726  
OBS727  
OBS728  
OBS729  
OBS730  
OBS731  
OBS732  
OBS733  
OBS734  
OBS735  
OBS736  
OBS737  
OBS738  
OBS739  
OBS740  
OBS741  
OBS742  
OBS743  
OBS744  
OBS745  
OBS746  
OBS747  
OBS748  
OBS749  
OBS750  
OBS751  
OBS752  
OBS753  
OBS754  
OBS755  
OBS756  
OBS757  
OBS758  
OBS759  
OBS760  
OBS761  
OBS762  
OBS763  
OBS764  
OBS765  
OBS766  
OBS767  
OBS768  
OBS769  
OBS770  
OBS771  
OBS772  
OBS773  
OBS774  
OBS775  
OBS776  
OBS777  
OBS778  
OBS779  
OBS780  
OBS781  
OBS782  
OBS783  
OBS784  
OBS785  
OBS786  
OBS787  
OBS788  
OBS789  
OBS790  
OBS791  
OBS792  
OBS793  
OBS794  
OBS795  
OBS796  
OBS797  
OBS798  
OBS799  
OBS800  
OBS801  
OBS802  
OBS803  
OBS804  
OBS805  
OBS806  
OBS807  
OBS808  
OBS809  
OBS810  
OBS811  
OBS812  
OBS813  
OBS814  
OBS815  
OBS816  
OBS817  
OBS818  
OBS819  
OBS820  
OBS821  
OBS822  
OBS823  
OBS824  
OBS825  
OBS826  
OBS827  
OBS828  
OBS829  
OBS830  
OBS831  
OBS832  
OBS833  
OBS834  
OBS835  
OBS836  
OBS837  
OBS838  
OBS839  
OBS840  
OBS841  
OBS842  
OBS843  
OBS844  
OBS845  
OBS846  
OBS847  
OBS848  
OBS849  
OBS850  
OBS851  
OBS852  
OBS853  
OBS854  
OBS855  
OBS856  
OBS857  
OBS858  
OBS859  
OBS860  
OBS861  
OBS862  
OBS863  
OBS864  
OBS865  
OBS866  
OBS867  
OBS868  
OBS869  
OBS870  
OBS871  
OBS872  
OBS873  
OBS874  
OBS875  
OBS876  
OBS877  
OBS878  
OBS879  
OBS880  
OBS881  
OBS882  
OBS883  
OBS884  
OBS885  
OBS886  
OBS887  
OBS888  
OBS889  
OBS890  
OBS891  
OBS892  
OBS893  
OBS894  
OBS895  
OBS896  
OBS897  
OBS898  
OBS899  
OBS900  
OBS901  
OBS902  
OBS903  
OBS904  
OBS905  
OBS906  
OBS907  
OBS908  
OBS909  
OBS910  
OBS911  
OBS912  
OBS913  
OBS914  
OBS915  
OBS916  
OBS917  
OBS918  
OBS919  
OBS920  
OBS921  
OBS922  
OBS923  
OBS924  
OBS925  
OBS926  
OBS927  
OBS928  
OBS929  
OBS930  
OBS931  
OBS932  
OBS933  
OBS934  
OBS935  
OBS936  
OBS937  
OBS938  
OBS939  
OBS940  
OBS941  
OBS942  
OBS943  
OBS944  
OBS945  
OBS946  
OBS947  
OBS948  
OBS949  
OBS950  
OBS951  
OBS952  
OBS953  
OBS954  
OBS955  
OBS956  
OBS957  
OBS958  
OBS959  
OBS960  
OBS961  
OBS962  
OBS963  
OBS964  
OBS965  
OBS966  
OBS967  
OBS968  
OBS969  
OBS970  
OBS971  
OBS972  
OBS973  
OBS974  
OBS975  
OBS976  
OBS977  
OBS978  
OBS979  
OBS980  
OBS981  
OBS982  
OBS983  
OBS984  
OBS985  
OBS986  
OBS987  
OBS988  
OBS989  
OBS990  
OBS991  
OBS992  
OBS993  
OBS994  
OBS995  
OBS996  
OBS997  
OBS998  
OBS999  
OBS1000

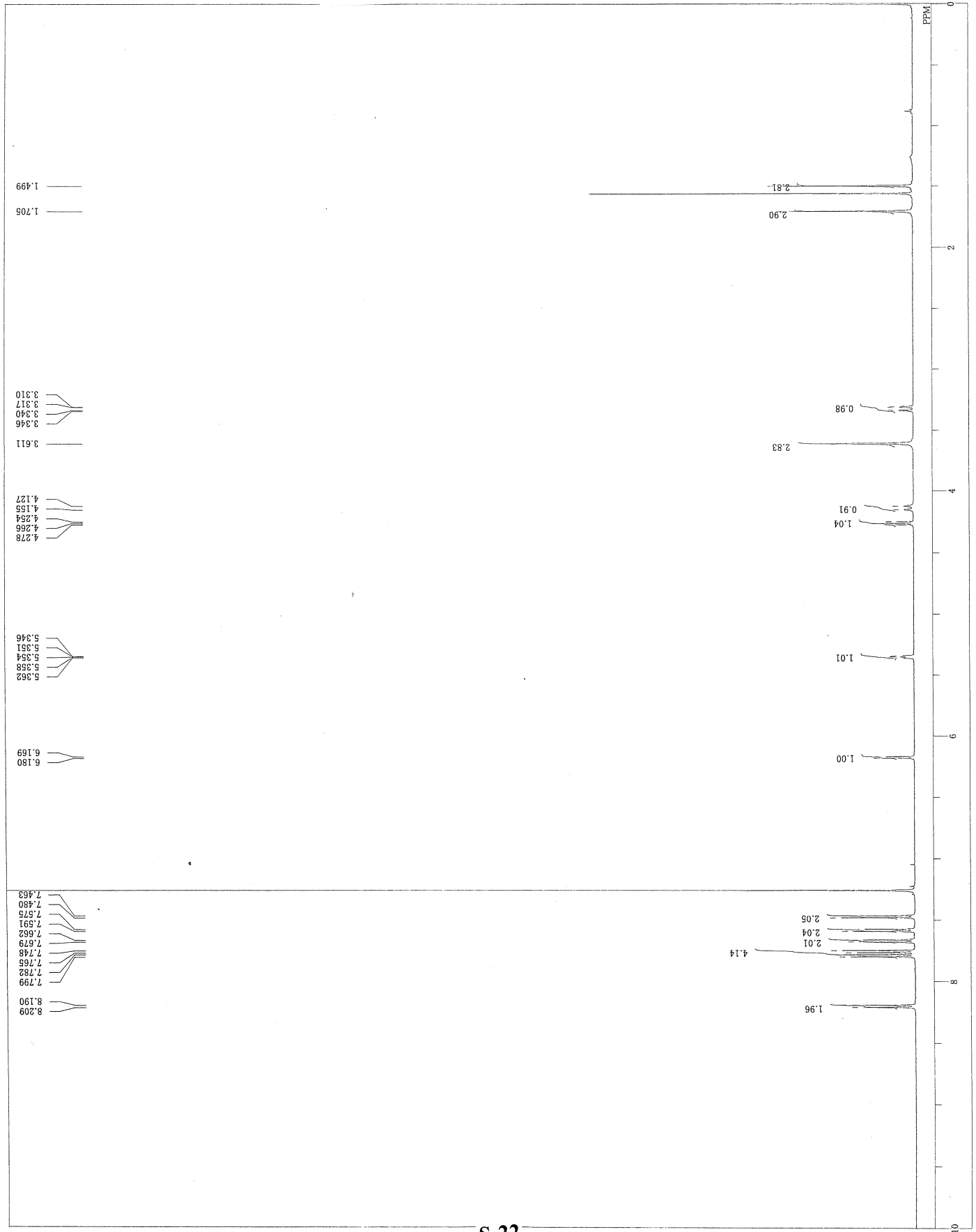
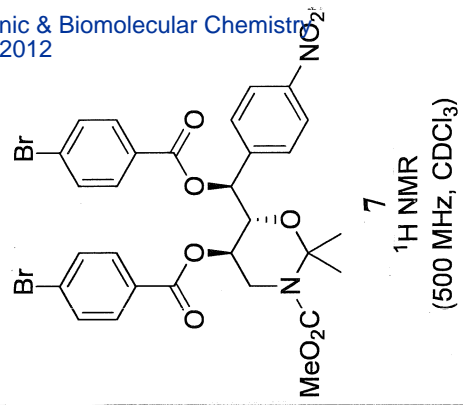


C:\DOCUMENT1\ADMINI\1\WINLOCALS\1\Temp\Hm2572\RIK-R-S-pure\_13C.als

DFILE COMMT  
DATIM  
EXPNO  
PROCNO  
F2  
F3  
F4  
F5  
F6  
F7  
F8  
F9  
F10  
F11  
F12  
F13  
F14  
F15  
F16  
F17  
F18  
F19  
F20  
F21  
F22  
F23  
F24  
F25  
F26  
F27  
F28  
F29  
F30  
F31  
F32  
F33  
F34  
F35  
F36  
F37  
F38  
F39  
F40  
F41  
F42  
F43  
F44  
F45  
F46  
F47  
F48  
F49  
F50  
F51  
F52  
F53  
F54  
F55  
F56  
F57  
F58  
F59  
F60  
F61  
F62  
F63  
F64  
F65  
F66  
F67  
F68  
F69  
F70  
F71  
F72  
F73  
F74  
F75  
F76  
F77  
F78  
F79  
F80  
F81  
F82  
F83  
F84  
F85  
F86  
F87  
F88  
F89  
F90  
F91  
F92  
F93  
F94  
F95  
F96  
F97  
F98  
F99  
F100  
F101  
F102  
F103  
F104  
F105  
F106  
F107  
F108  
F109  
F110  
F111  
F112  
F113  
F114  
F115  
F116  
F117  
F118  
F119  
F120  
F121  
F122  
F123  
F124  
F125  
F126  
F127  
F128  
F129  
F130  
F131  
F132  
F133  
F134  
F135  
F136  
F137  
F138  
F139  
F140  
F141  
F142  
F143  
F144  
F145  
F146  
F147  
F148  
F149  
F150  
F151  
F152  
F153  
F154  
F155  
F156  
F157  
F158  
F159  
F160  
F161  
F162  
F163  
F164  
F165  
F166  
F167  
F168  
F169  
F170  
F171  
F172  
F173  
F174  
F175  
F176  
F177  
F178  
F179  
F180  
F181  
F182  
F183  
F184  
F185  
F186  
F187  
F188  
F189  
F190  
F191  
F192  
F193  
F194  
F195  
F196  
F197  
F198  
F199  
F200  
F201  
F202  
F203  
F204  
F205  
F206  
F207  
F208  
F209  
F210  
F211  
F212  
F213  
F214  
F215  
F216  
F217  
F218  
F219  
F220  
F221  
F222  
F223  
F224  
F225  
F226  
F227  
F228  
F229  
F230  
F231  
F232  
F233  
F234  
F235  
F236  
F237  
F238  
F239  
F240  
F241  
F242  
F243  
F244  
F245  
F246  
F247  
F248  
F249  
F250  
F251  
F252  
F253  
F254  
F255  
F256  
F257  
F258  
F259  
F260  
F261  
F262  
F263  
F264  
F265  
F266  
F267  
F268  
F269  
F270  
F271  
F272  
F273  
F274  
F275  
F276  
F277  
F278  
F279  
F280  
F281  
F282  
F283  
F284  
F285  
F286  
F287  
F288  
F289  
F290  
F291  
F292  
F293  
F294  
F295  
F296  
F297  
F298  
F299  
F300  
F301  
F302  
F303  
F304  
F305  
F306  
F307  
F308  
F309  
F310  
F311  
F312  
F313  
F314  
F315  
F316  
F317  
F318  
F319  
F320  
F321  
F322  
F323  
F324  
F325  
F326  
F327  
F328  
F329  
F330  
F331  
F332  
F333  
F334  
F335  
F336  
F337  
F338  
F339  
F340  
F341  
F342  
F343  
F344  
F345  
F346  
F347  
F348  
F349  
F350  
F351  
F352  
F353  
F354  
F355  
F356  
F357  
F358  
F359  
F360  
F361  
F362  
F363  
F364  
F365  
F366  
F367  
F368  
F369  
F370  
F371  
F372  
F373  
F374  
F375  
F376  
F377  
F378  
F379  
F380  
F381  
F382  
F383  
F384  
F385  
F386  
F387  
F388  
F389  
F390  
F391  
F392  
F393  
F394  
F395  
F396  
F397  
F398  
F399  
F400  
F401  
F402  
F403  
F404  
F405  
F406  
F407  
F408  
F409  
F410  
F411  
F412  
F413  
F414  
F415  
F416  
F417  
F418  
F419  
F420  
F421  
F422  
F423  
F424  
F425  
F426  
F427  
F428  
F429  
F430  
F431  
F432  
F433  
F434  
F435  
F436  
F437  
F438  
F439  
F440  
F441  
F442  
F443  
F444  
F445  
F446  
F447  
F448  
F449  
F450  
F451  
F452  
F453  
F454  
F455  
F456  
F457  
F458  
F459  
F460  
F461  
F462  
F463  
F464  
F465  
F466  
F467  
F468  
F469  
F470  
F471  
F472  
F473  
F474  
F475  
F476  
F477  
F478  
F479  
F480  
F481  
F482  
F483  
F484  
F485  
F486  
F487  
F488  
F489  
F490  
F491  
F492  
F493  
F494  
F495  
F496  
F497  
F498  
F499  
F500  
F501  
F502  
F503  
F504  
F505  
F506  
F507  
F508  
F509  
F510  
F511  
F512  
F513  
F514  
F515  
F516  
F517  
F518  
F519  
F520  
F521  
F522  
F523  
F524  
F525  
F526  
F527  
F528  
F529  
F530  
F531  
F532  
F533  
F534  
F535  
F536  
F537  
F538  
F539  
F540  
F541  
F542  
F543  
F544  
F545  
F546  
F547  
F548  
F549  
F550  
F551  
F552  
F553  
F554  
F555  
F556  
F557  
F558  
F559  
F560  
F561  
F562  
F563  
F564  
F565  
F566  
F567  
F568  
F569  
F570  
F571  
F572  
F573  
F574  
F575  
F576  
F577  
F578  
F579  
F580  
F581  
F582  
F583  
F584  
F585  
F586  
F587  
F588  
F589  
F590  
F591  
F592  
F593  
F594  
F595  
F596  
F597  
F598  
F599  
F600  
F601  
F602  
F603  
F604  
F605  
F606  
F607  
F608  
F609  
F610  
F611  
F612  
F613  
F614  
F615  
F616  
F617  
F618  
F619  
F620  
F621  
F622  
F623  
F624  
F625  
F626  
F627  
F628  
F629  
F630  
F631  
F632  
F633  
F634  
F635  
F636  
F637  
F638  
F639  
F640  
F641  
F642  
F643  
F644  
F645  
F646  
F647  
F648  
F649  
F650  
F651  
F652  
F653  
F654  
F655  
F656  
F657  
F658  
F659  
F660  
F661  
F662  
F663  
F664  
F665  
F666  
F667  
F668  
F669  
F670  
F671  
F672  
F673  
F674  
F675  
F676  
F677  
F678  
F679  
F680  
F681  
F682  
F683  
F684  
F685  
F686  
F687  
F688  
F689  
F690  
F691  
F692  
F693  
F694  
F695  
F696  
F697  
F698  
F699  
F700  
F701  
F702  
F703  
F704  
F705  
F706  
F707  
F708  
F709  
F710  
F711  
F712  
F713  
F714  
F715  
F716  
F717  
F718  
F719  
F720  
F721  
F722  
F723  
F724  
F725  
F726  
F727  
F728  
F729  
F730  
F731  
F732  
F733  
F734  
F735  
F736  
F737  
F738  
F739  
F740  
F741  
F742  
F743  
F744  
F745  
F746  
F747  
F748  
F749  
F750  
F751  
F752  
F753  
F754  
F755  
F756  
F757  
F758  
F759  
F760  
F761  
F762  
F763  
F764  
F765  
F766  
F767  
F768  
F769  
F770  
F771  
F772  
F773  
F774  
F775  
F776  
F777  
F778  
F779  
F780  
F781  
F782  
F783  
F784  
F785  
F786  
F787  
F788  
F789  
F790  
F791  
F792  
F793  
F794  
F795  
F796  
F797  
F798  
F799  
F800  
F801  
F802  
F803  
F804  
F805  
F806  
F807  
F808  
F809  
F810  
F811  
F812  
F813  
F814  
F815  
F816  
F817  
F818  
F819  
F820  
F821  
F822  
F823  
F824  
F825  
F826  
F827  
F828  
F829  
F830  
F831  
F832  
F833  
F834  
F835  
F836  
F837  
F838  
F839  
F840  
F841  
F842  
F843  
F844  
F845  
F846  
F847  
F848  
F849  
F850  
F851  
F852  
F853  
F854  
F855  
F856  
F857  
F858  
F859  
F860  
F861  
F862  
F863  
F864  
F865  
F866  
F867  
F868  
F869  
F870  
F871  
F872  
F873  
F874  
F875  
F876  
F877  
F878  
F879  
F880  
F881  
F882  
F883  
F884  
F885  
F886  
F887  
F888  
F889  
F890  
F891  
F892  
F893  
F894  
F895  
F896  
F897  
F898  
F899  
F900  
F901  
F902  
F903  
F904  
F905  
F906  
F907  
F908  
F909  
F910  
F911  
F912  
F913  
F914  
F915  
F916  
F917  
F918  
F919  
F920  
F921  
F922  
F923  
F924  
F925  
F926  
F927  
F928  
F929  
F930  
F931  
F932  
F933  
F934  
F935  
F936  
F937  
F938  
F939  
F940  
F941  
F942  
F943  
F944  
F945  
F946  
F947  
F948  
F949  
F950  
F951  
F952  
F953  
F954  
F955  
F956  
F957  
F958  
F959  
F960  
F961  
F962  
F963  
F964  
F965  
F966  
F967  
F968  
F969  
F970  
F971  
F972  
F973  
F974  
F975  
F976  
F977  
F978  
F979  
F980  
F981  
F982  
F983  
F984  
F985  
F986  
F987  
F988  
F989  
F990  
F991  
F992  
F993  
F994  
F995  
F996  
F997  
F998  
F999  
F1000  
F1001  
F1002  
F1003  
F1004  
F1005  
F1006  
F1007  
F1008  
F1009  
F1010  
F1011  
F1012  
F1013  
F1014  
F1015  
F1016  
F1017  
F1018  
F1019  
F1020  
F1021  
F1022  
F1023  
F1024  
F1025  
F1026  
F1027  
F1028  
F1029  
F1030  
F1031  
F1032  
F1033  
F1034  
F1035  
F1036  
F1037  
F1038  
F1039  
F1040  
F1041  
F1042  
F1043  
F1044  
F1045  
F1046  
F1047  
F1048  
F1049  
F1050  
F1051  
F1052  
F1053  
F1054  
F1055  
F1056  
F1057  
F1058  
F1059  
F1060  
F1061  
F1062  
F1063  
F1064  
F1065  
F1066  
F1067  
F1068  
F1069  
F1070  
F1071  
F1072  
F1073  
F1074  
F1075  
F1076  
F1077  
F1078  
F1079  
F1080  
F1081  
F1082  
F1083  
F1084  
F1085  
F1086  
F1087  
F1088  
F1089  
F1090  
F1091  
F1092  
F1093  
F1094  
F1095  
F1096  
F1097  
F1098  
F1099  
F1100  
F1101  
F1102  
F1103  
F1104  
F1105  
F1106  
F1107  
F1108  
F1109  
F1110  
F1111  
F1112  
F1113  
F1114  
F1115  
F1116  
F1117  
F1118  
F1119  
F1120  
F1121  
F1122  
F1123  
F1124  
F1125  
F1126  
F1127  
F1128  
F1129  
F1130  
F1131  
F1132  
F1133  
F1134  
F1135  
F1136  
F1137  
F1138  
F1139  
F1140  
F1141  
F1142  
F1143  
F1144  
F1145  
F1146  
F1147  
F1148  
F1149  
F1150  
F1151  
F1152  
F1153  
F1154  
F1155  
F1156  
F1157  
F1158  
F1159  
F1160  
F1161  
F1162  
F1163  
F1164  
F1165  
F1166  
F1167  
F1168  
F1169  
F1170  
F1171  
F1172  
F1173  
F1174  
F1175  
F1176  
F1177  
F1178  
F1179  
F1180  
F1181  
F1182  
F1183  
F1184  
F1185  
F1186  
F1187  
F1188  
F1189  
F1190  
F1191  
F1192  
F1193  
F1194  
F1195  
F1196  
F1197  
F1198  
F1199  
F1200  
F1201  
F1202  
F1203  
F1204  
F1205  
F1206  
F1207  
F1208  
F1209  
F1210  
F1211  
F1212  
F1213  
F1214  
F1215  
F1216  
F1217  
F1218  
F1219  
F1220  
F1221  
F1222  
F1223  
F1224  
F1225  
F1226  
F1227  
F1228  
F1229  
F1230  
F1231  
F1232  
F1233  
F1234  
F1235  
F1236  
F1237  
F1238  
F1239  
F1240  
F1241  
F1242  
F1243  
F1244  
F1245  
F1246  
F1247  
F1248  
F1249  
F1250  
F1251  
F1252  
F1253  
F1254  
F1255  
F1256  
F1257  
F1258  
F1259  
F1260  
F1261  
F1262  
F1263  
F1264  
F1265  
F1266  
F1267  
F1268  
F1269  
F1270  
F1271  
F1272  
F1273  
F1274  
F1275  
F1276  
F1277  
F1278  
F1279  
F1280  
F1281  
F1282  
F1283  
F1284  
F1285  
F1286  
F1287  
F1288  
F1289  
F1290  
F1291  
F1292  
F1293  
F1294  
F1295  
F1296  
F1297  
F1298  
F1299  
F1300  
F1301  
F1302  
F1303  
F1304  
F1305  
F1306  
F1307  
F1308  
F1309  
F1310  
F1311  
F1312  
F1313  
F1314  
F1315  
F1316  
F1317  
F1318  
F1319  
F1320  
F1321  
F1322  
F1323  
F1324  
F1325  
F1326  
F1327  
F1328  
F1329  
F1330  
F1331  
F1332  
F1333  
F1334  
F1335  
F1336  
F1337  
F1338  
F1339  
F1340  
F1341  
F1342  
F1343  
F1344  
F1345  
F1346  
F1347  
F1348  
F1349  
F1350  
F1351  
F1352  
F1353  
F1354  
F1355  
F1356  
F1357  
F1358  
F1359  
F1360  
F1361  
F1362  
F1363  
F1364  
F1365  
F1366  
F1367  
F1368  
F1369  
F1370  
F1371  
F1372  
F1373  
F1374  
F1375  
F1376  
F1377  
F1378  
F1379  
F1380  
F1381  
F1382  
F1383  
F1384  
F1385  
F1386  
F1387  
F1388  
F1389  
F1390  
F1391  
F1392  
F1393  
F1394  
F1395  
F1396  
F1397  
F1398  
F1399  
F1400  
F1401  
F1402  
F1403  
F1404  
F1405  
F1406  
F1407  
F1408  
F1409  
F1410  
F1411  
F1412  
F1413  
F1414  
F1415  
F1416  
F1417  
F1418  
F1419  
F1420  
F1421  
F1422  
F1423  
F1424  
F1425  
F1426  
F1427  
F1428  
F1429  
F1430  
F1431  
F1432  
F1433  
F1434  
F1435  
F1436  
F1437  
F1438  
F1439  
F1440  
F1441  
F1442  
F1443  
F1444  
F1445  
F1446  
F1447  
F1448  
F1449  
F1450  
F1451  
F1452  
F1453  
F1454  
F1455  
F1456  
F1457  
F1458  
F1459  
F1460  
F1461  
F1462  
F1463  
F1464  
F1465  
F1466  
F1467  
F1468  
F1469  
F1470  
F1471  
F1472  
F1473  
F1474  
F1475  
F1476  
F1477  
F1478  
F1479  
F1480  
F1481  
F1482  
F1483  
F1484  
F1485  
F1486  
F1487  
F1488  
F1489  
F1490  
F1491  
F1492  
F1493  
F1494  
F1495  
F1496  
F1497  
F1498  
F1499  
F1500  
F1501  
F1502  
F1503  
F1504  
F1505  
F1506  
F1507  
F1508  
F1509  
F1510  
F1511  
F1512  
F1513  
F1514  
F1515  
F1516  
F1517  
F1518  
F1519  
F1520  
F1521  
F1522  
F1523  
F1524  
F1525  
F1526  
F1527  
F1528  
F1529  
F1530  
F1531  
F1532  
F1533  
F1534  
F1535  
F1536  
F1537  
F1538  
F1539  
F1540  
F1541  
F1542  
F1543  
F1544  
F1545  
F1546  
F1547  
F1548  
F1549  
F1550  
F1551  
F1552  
F1553  
F1554  
F1555  
F1556  
F1557  
F1558  
F1559  
F1560  
F1561  
F1562  
F1563  
F1564  
F1565  
F1566  
F1567  
F1568  
F1569  
F1570  
F1571  
F1572  
F1573  
F1574  
F1575  
F1576  
F1577  
F1578  
F1579  
F1580  
F1581  
F1582  
F1583  
F1584  
F1585  
F1586  
F1587  
F1588  
F1589  
F1590  
F1591  
F1592  
F1593  
F1594  
F1595  
F1596  
F1597  
F1598  
F1599  
F1600  
F1601  
F1602  
F1603  
F1604  
F1605  
F1606  
F1607  
F1608  
F1609  
F1610  
F1611  
F1612  
F1613  
F1614  
F1615  
F1616  
F1617  
F1618  
F1619  
F1620  
F1621  
F1622  
F1623  
F1624  
F1625  
F1626  
F1627  
F1628  
F1629  
F1630  
F1631  
F1632  
F1633  
F1634  
F1635  
F1636  
F1637  
F1638  
F1639  
F1640  
F1641  
F1642  
F1643  
F1644  
F1645  
F1646  
F1647  
F1648  
F1649  
F1650  
F1651  
F1652  
F1653  
F1654  
F1655  
F1656  
F1657  
F1658  
F1659  
F1660  
F1661  
F1662  
F1663  
F1664  
F1665  
F1666  
F1667  
F1668  
F1669  
F1670  
F1671  
F1672  
F1673  
F1674  
F1675  
F1676  
F1677  
F1678  
F1679  
F1680  
F1681  
F1682  
F1683  
F1684  
F1685  
F1686  
F1687  
F1688  
F1689  
F1690  
F1691  
F1692  
F1693  
F1694  
F1695  
F1696  
F1697  
F1698  
F1699  
F1700  
F1701  
F1702  
F1703  
F1704  
F1705  
F1706  
F1707  
F1708  
F1709  
F1710  
F1711  
F1712  
F1713  
F1714  
F1715  
F1716  
F1717  
F1718  
F1719  
F1720  
F1721  
F1722  
F1723  
F1724  
F1725  
F1726  
F1727  
F1728  
F1729  
F1730  
F1731  
F1732  
F1733  
F1734  
F1735  
F1736  
F1737  
F1738  
F1739  
F1740  
F1741  
F1742  
F1743  
F1744  
F1745  
F1746  
F1747  
F1748  
F1749  
F1750  
F1751  
F1752  
F1753  
F1754  
F1755  
F1756  
F1757  
F1758  
F1759  
F1760  
F1761  
F1762  
F1763  
F1764  
F1765  
F1766  
F1767  
F1768  
F1769  
F1770  
F1771  
F1772  
F1773  
F1774  
F1775  
F1776  
F1777  
F1778  
F1779  
F1780  
F1781  
F1782  
F1783  
F1784  
F1785  
F1786  
F1787  
F1788  
F1789  
F1790  
F1791  
F1792  
F1793  
F1794  
F1795  
F1796  
F1797  
F1798  
F1799  
F1800  
F1801  
F1802  
F1803  
F1804  
F1805  
F1806  
F1807  
F1808  
F1809  
F1810  
F1811  
F1812  
F1813  
F1814  
F1815  
F1816  
F1817  
F1818  
F1819  
F1820  
F1821  
F1822  
F1823  
F1824  
F1825  
F1826  
F1827  
F1828  
F1829  
F1830  
F1831  
F1832  
F1833  
F1834  
F1835  
F1836  
F1837  
F1838  
F1839  
F1840  
F1841  
F1842  
F1843  
F1844  
F1845  
F1846  
F1847  
F1848  
F1849  
F1850  
F1851  
F1852  
F1853  
F1854  
F1855  
F1856  
F1857  
F1858  
F1859  
F1860  
F1861  
F1862  
F1863  
F1864  
F1865  
F1866  
F1867  
F1868  
F1869  
F1870  
F1871  
F1872  
F1873  
F1874  
F1875  
F1876  
F1877  
F1878  
F1879  
F1880  
F1881  
F1882  
F1883  
F1884  
F1885  
F1886  
F1887  
F1888  
F1889  
F1890  
F1891  
F1892  
F1893  
F1894  
F1895  
F1896  
F1897  
F1898  
F1899  
F1900  
F1901  
F1902  
F1903  
F

DFILE  
COMET  
NAME  
ORNUC  
EXMOD  
OBFRQ  
OBFTN  
POINT  
PULSE  
SCANS  
ACQTM  
PD  
PWL  
IRNUC  
CTEMP  
SLANT  
SHEF  
RGAIN

diem, proton-1, als  
single\_pulse  
111-01-31 15:43:18  
1H  
proton, bp  
500.16 MHz  
2.41 KHz  
13120  
750751 Hz  
1.7459 sec  
5.0000 sec  
4.68 usec  
1H  
16.7 c  
CDCL3  
0.00 ppm  
1.00 Hz  
50



```

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

```

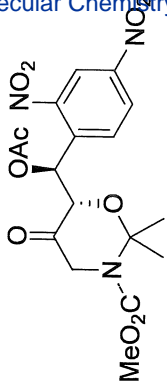


(125.8 MHz, CDCl<sub>3</sub>)

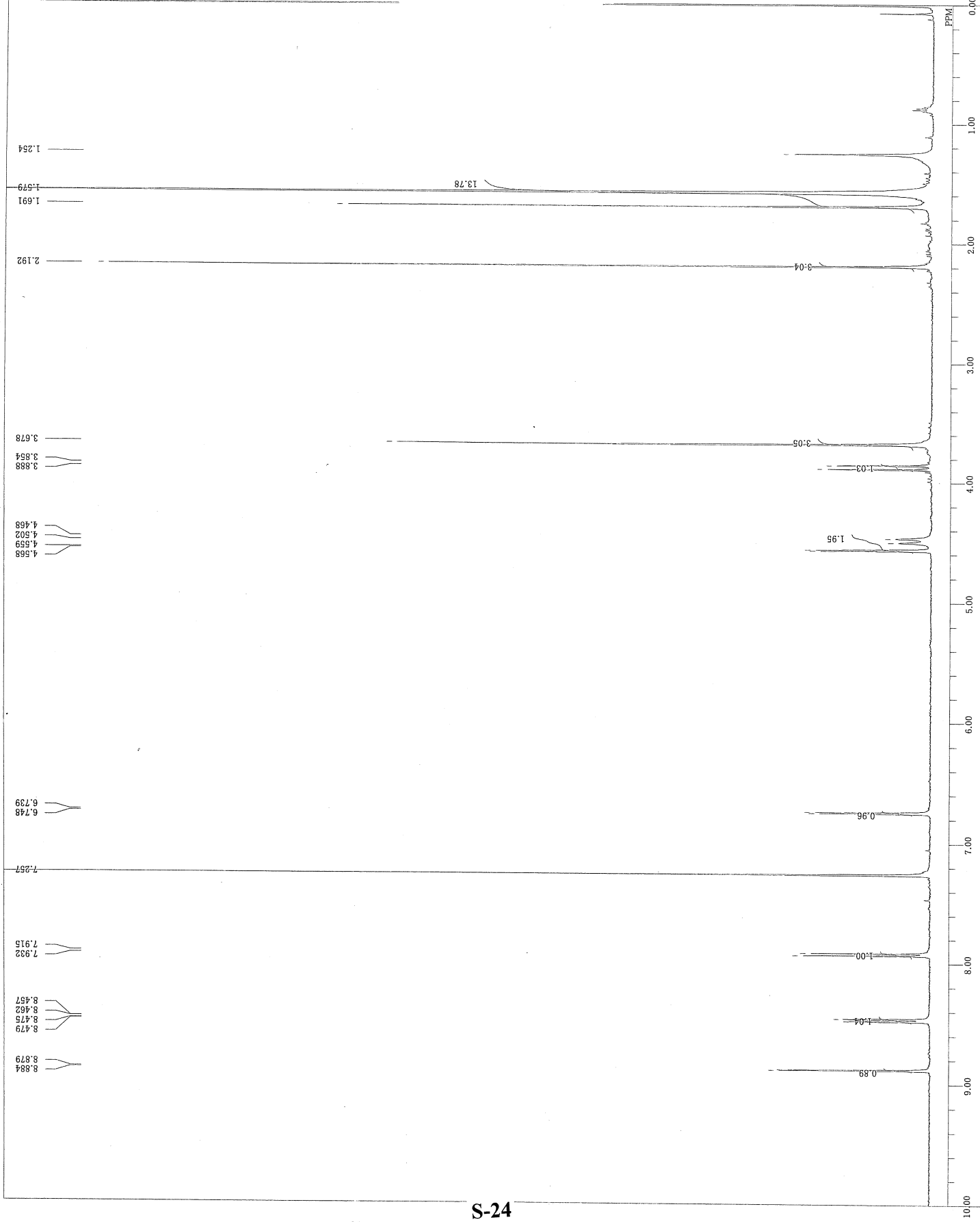


FILE  
NAME  
DATE  
TIME  
PROB  
PULP  
PROG  
F2  
F3  
F4  
F5  
F6  
F7  
F8  
F9  
F10  
F11  
F12  
F13  
F14  
F15  
F16  
F17  
F18  
F19  
F20  
F21  
F22  
F23  
F24  
F25  
F26  
F27  
F28  
F29  
F30  
F31  
F32  
F33  
F34  
F35  
F36  
F37  
F38  
F39  
F40  
F41  
F42  
F43  
F44  
F45  
F46  
F47  
F48  
F49  
F50  
F51  
F52  
F53  
F54  
F55  
F56  
F57  
F58  
F59  
F60  
F61  
F62  
F63  
F64  
F65  
F66  
F67  
F68  
F69  
F70  
F71  
F72  
F73  
F74  
F75  
F76  
F77  
F78  
F79  
F80  
F81  
F82  
F83  
F84  
F85  
F86  
F87  
F88  
F89  
F90  
F91  
F92  
F93  
F94  
F95  
F96  
F97  
F98  
F99  
F100

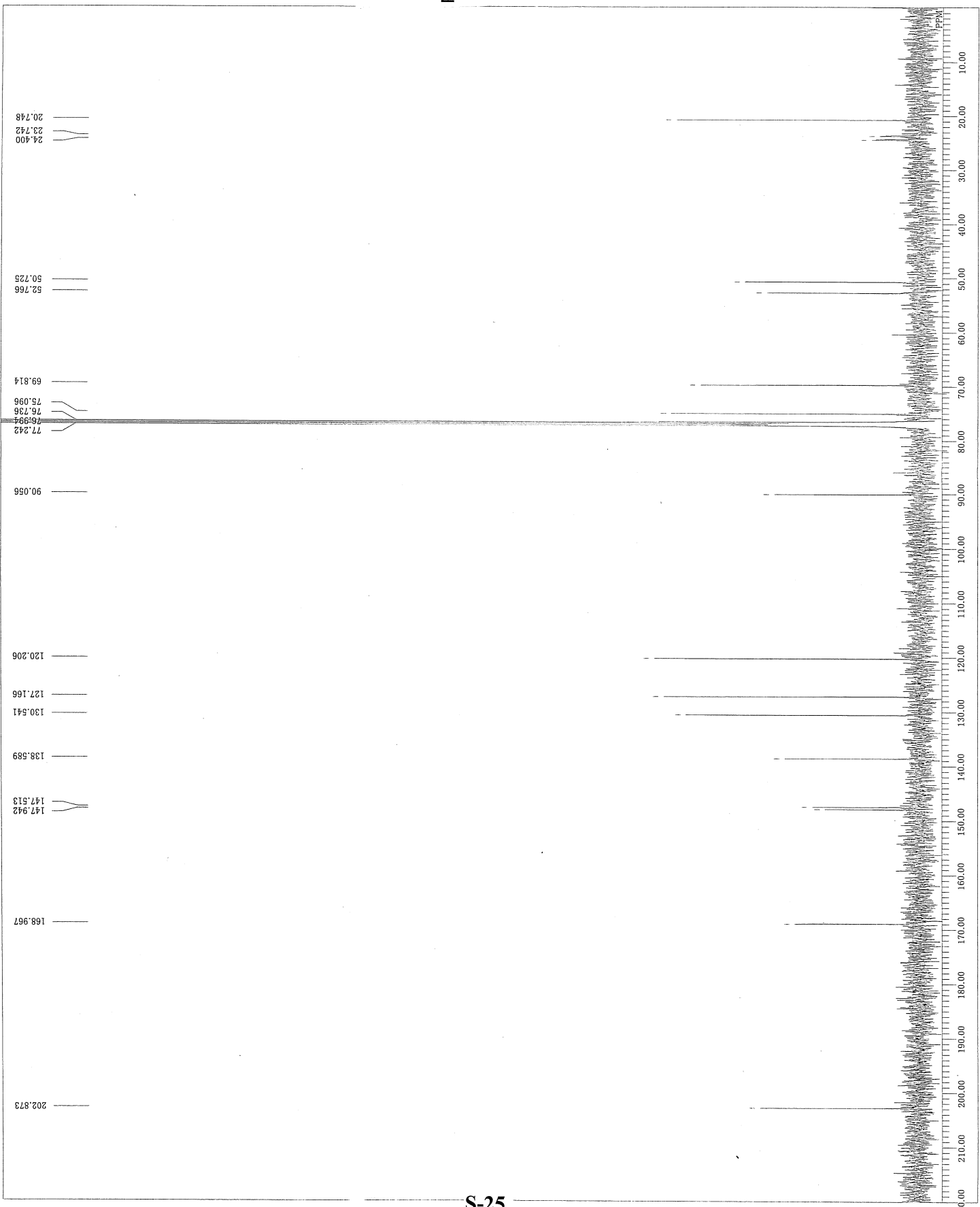
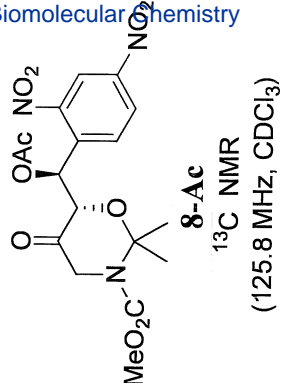
RIK-298-c, proton-1-1.jf  
2011-07-26 22:13:36  
500.16 MHz  
2.41 KHz  
6.01 Hz  
16400  
9864338 Hz  
8  
1.7459 sec  
5.0000 sec  
4.68 usec  
19.6 c  
19.6 c  
0.00 ppm  
0.12 Hz  
54



8-Ac  
<sup>1</sup>H NMR  
(500 MHz, CDCl<sub>3</sub>)



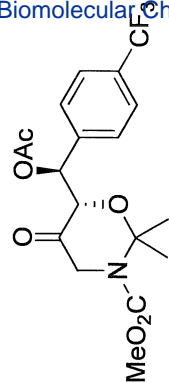
FILE RIK-298pure\_Carbon-2-1\_als  
NAME 8-Ac  
PULSE single pulse decoupled gated NOE  
DATE 2011-06-21 22:35:15  
PROC 13C  
INSTR carbon,kp  
P1 125.77 MHz  
P2 7.87 KHz  
P3 4.21 Hz  
P4 4.21 Hz  
P5 4.21 Hz  
P6 31465.54 Hz  
P7 1024  
P8 0.83336 sec  
P9 2.0000 sec  
P10 2.72 usec  
P11 1H  
P12 19.8 c  
P13 CDCl3  
P14 0.00 ppm  
P15 0.12 Hz  
P16 60  
P17 RGAIN



RHPLC-661-Ac-1H

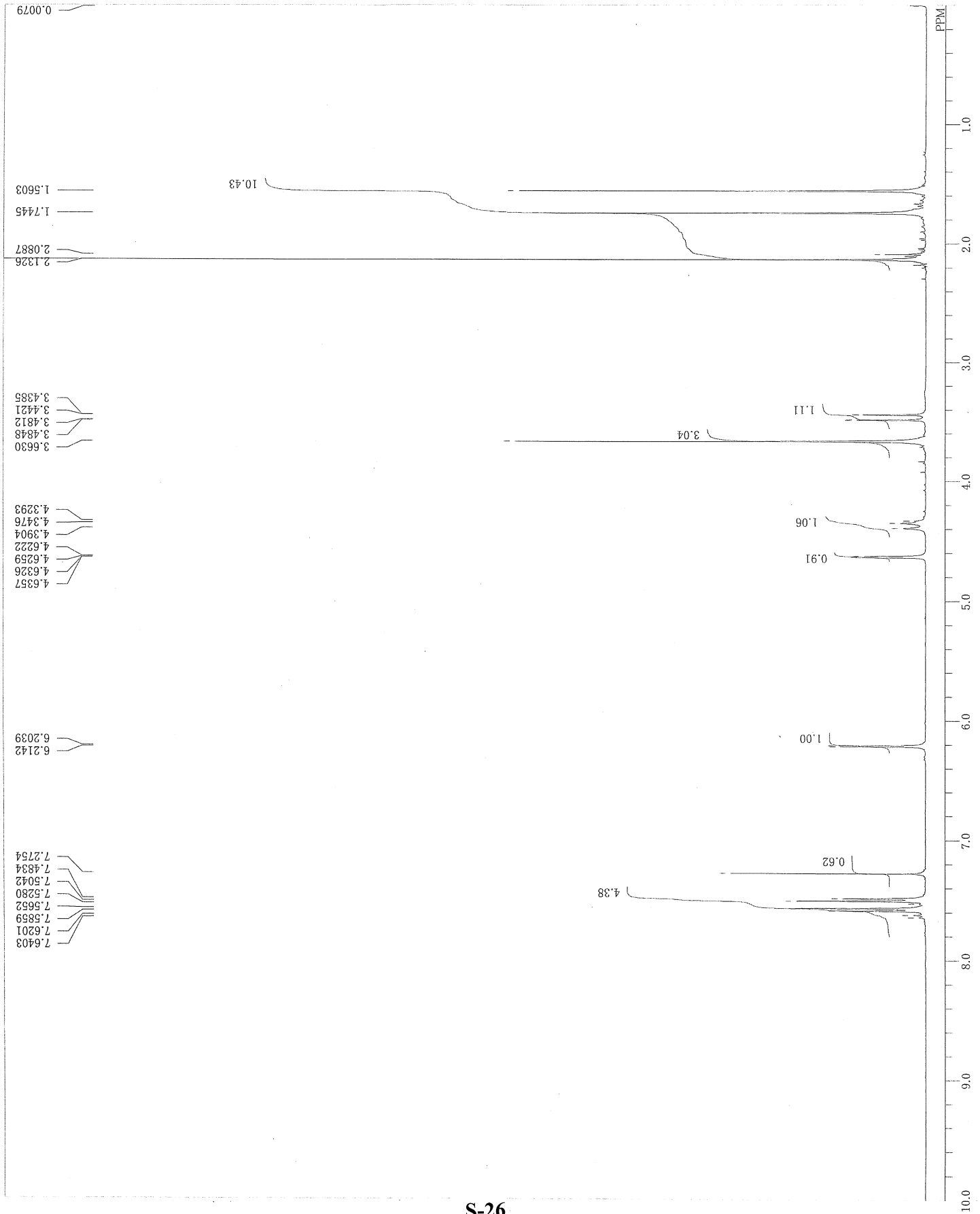
DFILE  
COMINT  
DATUM  
OBNUC  
EXMOD  
OBFREQ  
OBSET  
OBFIN  
POINT  
FREQ  
SCANS  
ACQTM  
PD  
PW1  
IRNUC  
CTEMP  
SLVNT  
EXREF  
BF  
RGAIN

RHPLC-661-Ac-1H.nmdata  
RHPLC-661-Ac-1H  
Thu Nov 19 01:35:25 2009  
1H  
non  
399.65 MHz  
130.00 KHz  
4300.00 Hz  
32768  
7993.60 Hz  
4  
4.0933 sec  
2.9007 sec  
7.00 usec  
1H  
23.8 c  
CDCl<sub>3</sub>  
0.00 ppm  
0.12 Hz  
16



9-Ac

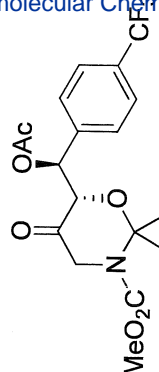
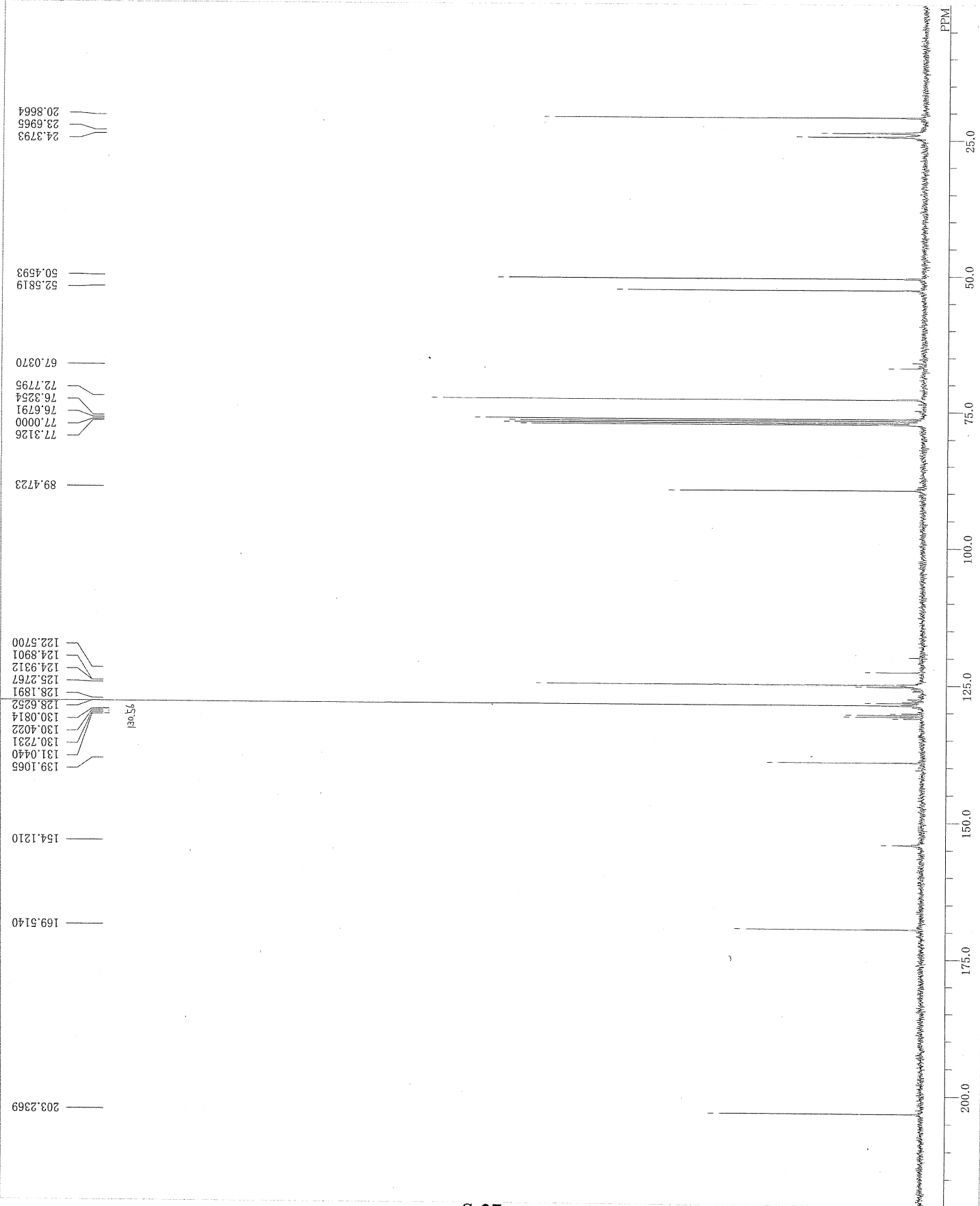
<sup>1</sup>H NMR  
(400 MHz, CDCl<sub>3</sub>)



RHPLC-661-Ac-13C

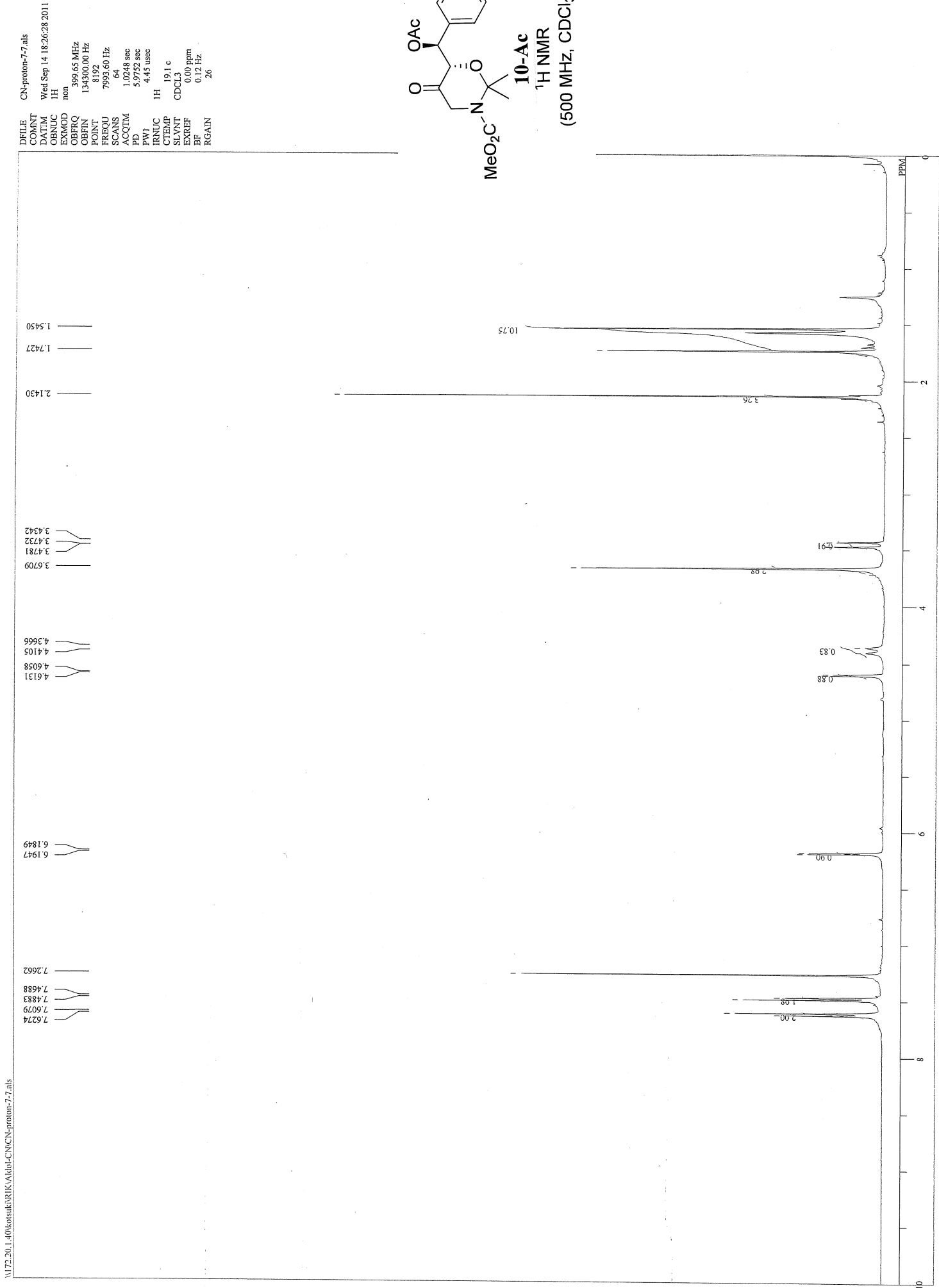
DFILE  
COMNT  
DATIM  
OBNUC  
EXMOD  
OBFRC  
OBSER  
OBFIN  
POINT  
FREQU  
SCANS  
ACQTM  
PD  
PW1  
IRNUC  
CTEMP  
SLVNT  
EXREF  
BF  
RGAIN

RHPLC-661-Ac-13C.nmdata  
RHPLC-661-Ac-13C  
Thu Nov 19 10:53:05 2009  
13C  
bcm  
100.40 MHz  
130.00 KHz  
5500.00 Hz  
32768  
27100.27 Hz  
1000  
1.2091 sec  
1.7909 sec  
5.50 usec  
1H  
25.6 c  
CDCl<sub>3</sub>  
77.00 ppm  
0.12 Hz  
31

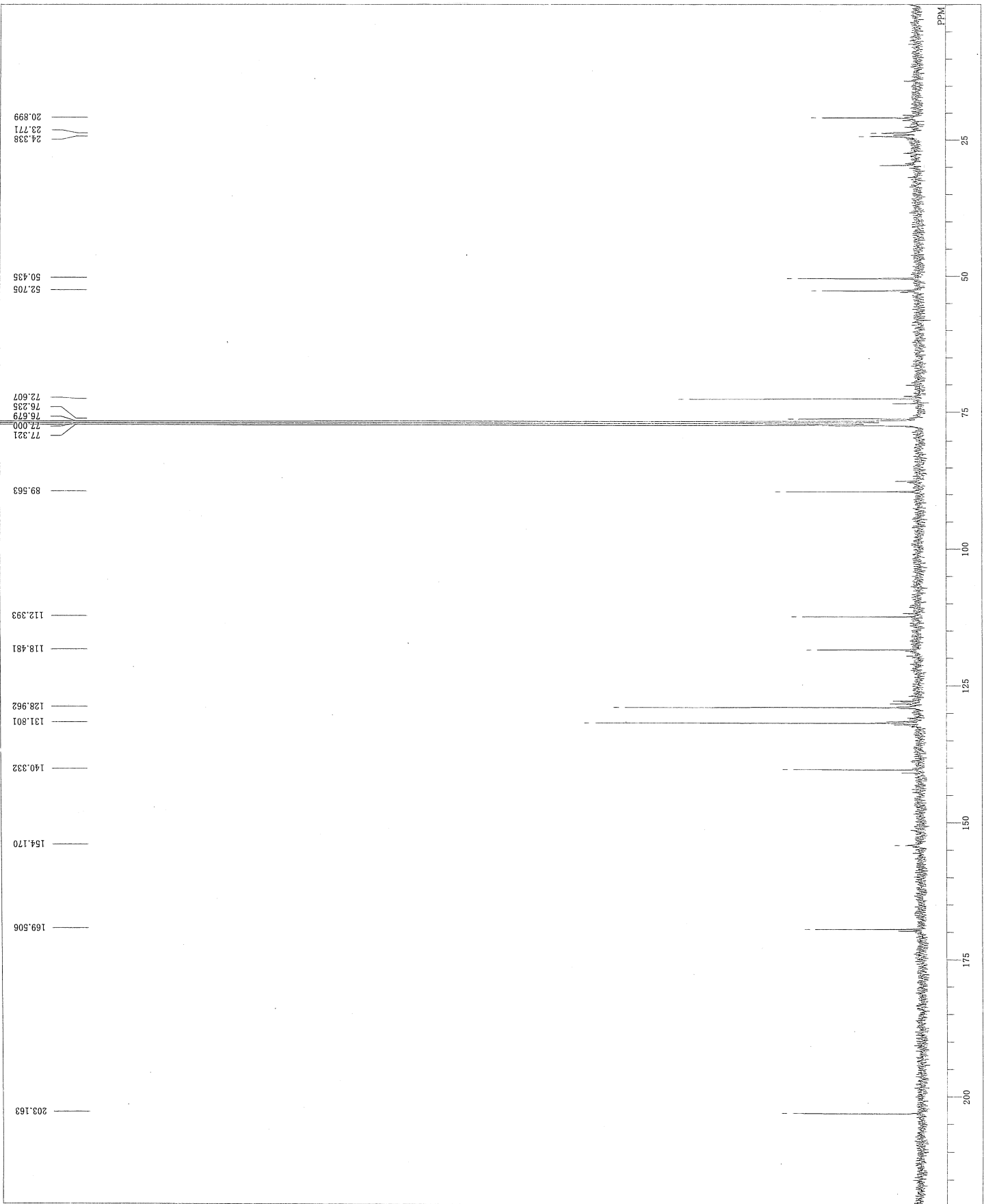
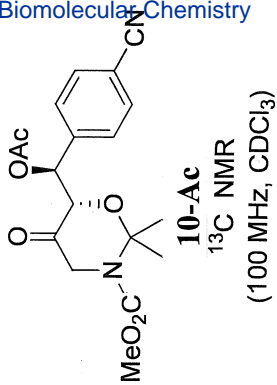


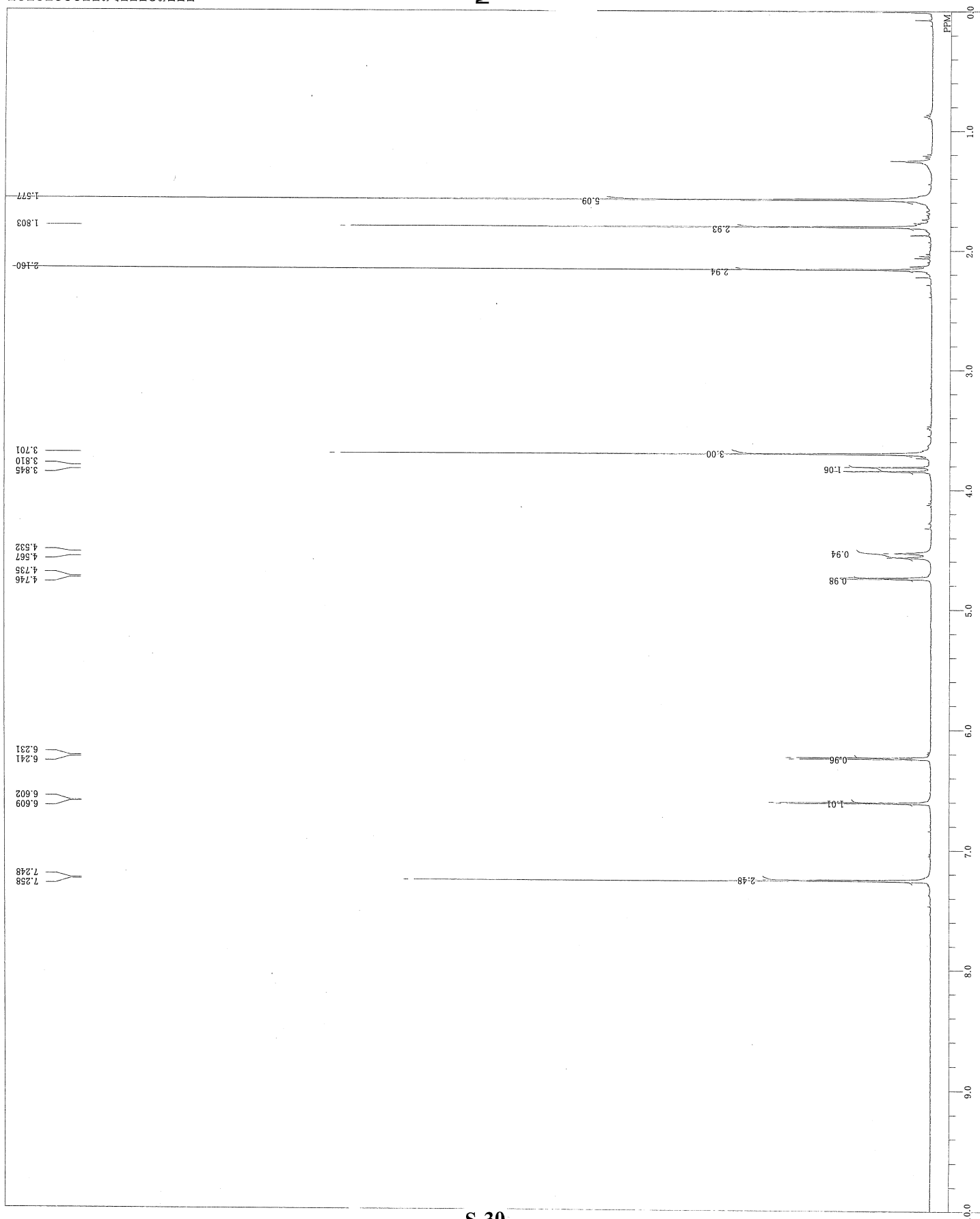
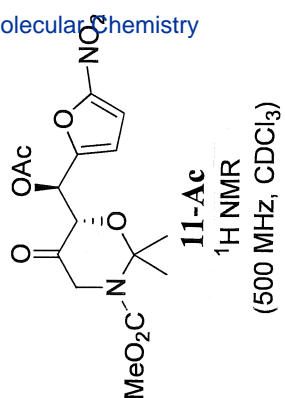
**9-Ac**  
<sup>13</sup>C NMR  
(100 MHz, CDCl<sub>3</sub>)

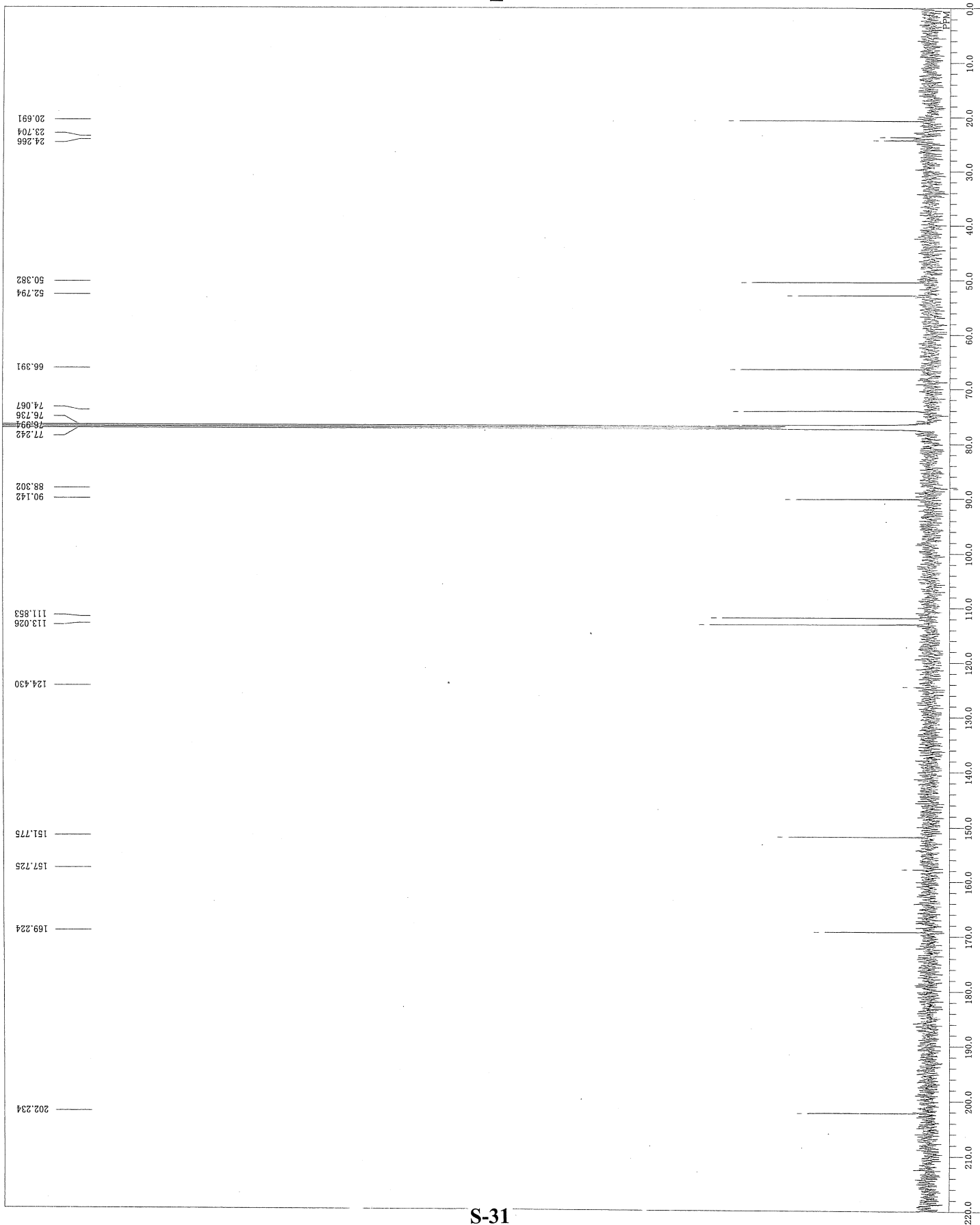
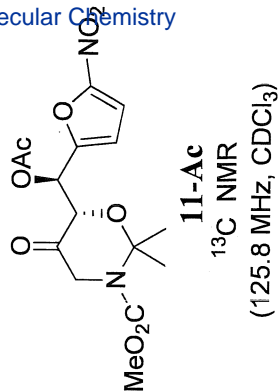




DFILE RIK-CNAc7\_1913C.als  
COMET  
DATE\_01  
ORNUC 13C  
EXMOD 15C  
OBFREQ 100.40 MHz  
OBSSET 0.00 KHz  
OBFIN 135500.00 Hz  
POINT 32768  
PULSE 271.0027 Hz  
SCANS 1063  
ACQTM 1.2091 sec  
PD 1.7909 sec  
PWL 5.45 usec  
IRNUC 1H  
CTEMP 19.6 c  
VARY CDCL3  
EXREF 17.00 ppm  
BF 1.20 Hz  
RGAIN 29





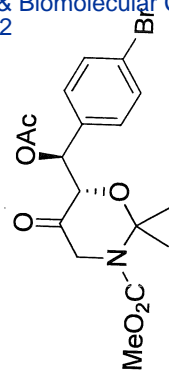


COM-660-Ac-1H

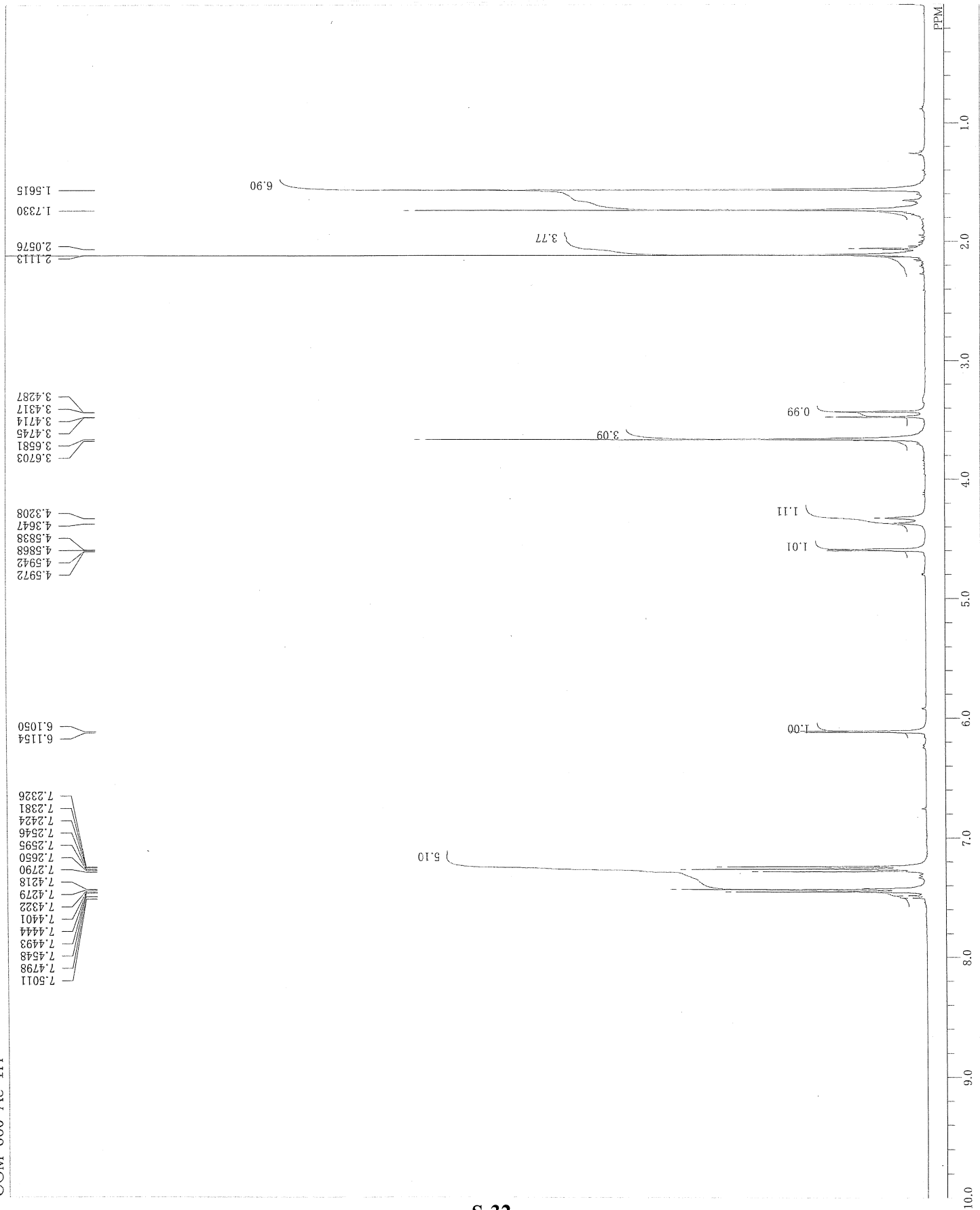
DFILE  
COMNT  
DATIM  
OBNUC  
EXMOD  
OBFRO  
OBSET  
OBFIN  
POINT  
FREQU  
SCANS  
ACQTM  
PD  
PW1  
IRNUC  
CTEMP  
SLVNT  
EXREF  
BF  
RGAIN

COM-660-Ac-1H.nmdata  
COM-660-Ac-1H  
Sat Nov 21 17:15:47 2009  
1H  
non

399.65 MHz  
130.00 KHz  
4300.00 Hz  
32768  
7993.60 Hz  
4  
4.0993 sec  
2.9007 sec  
7.00 usec  
1H  
24.0 c  
CDCL3  
0.00 ppm  
0.12 Hz  
16

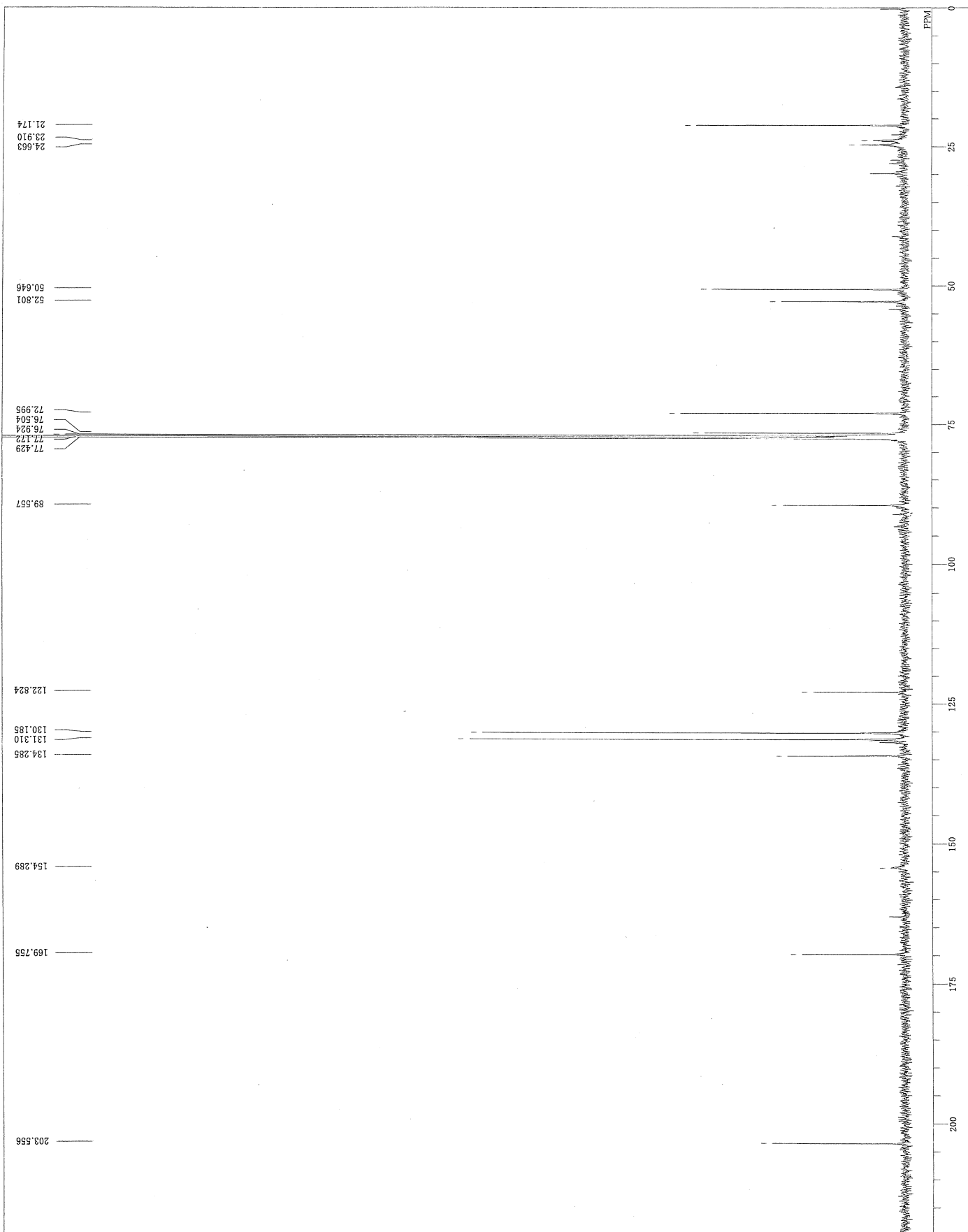
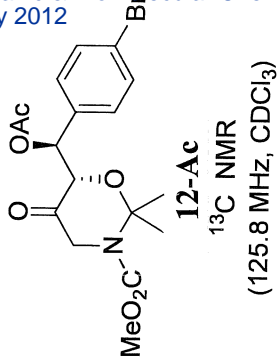


**12-Ac**  
<sup>1</sup>H NMR  
(400 MHz, CDCl<sub>3</sub>)

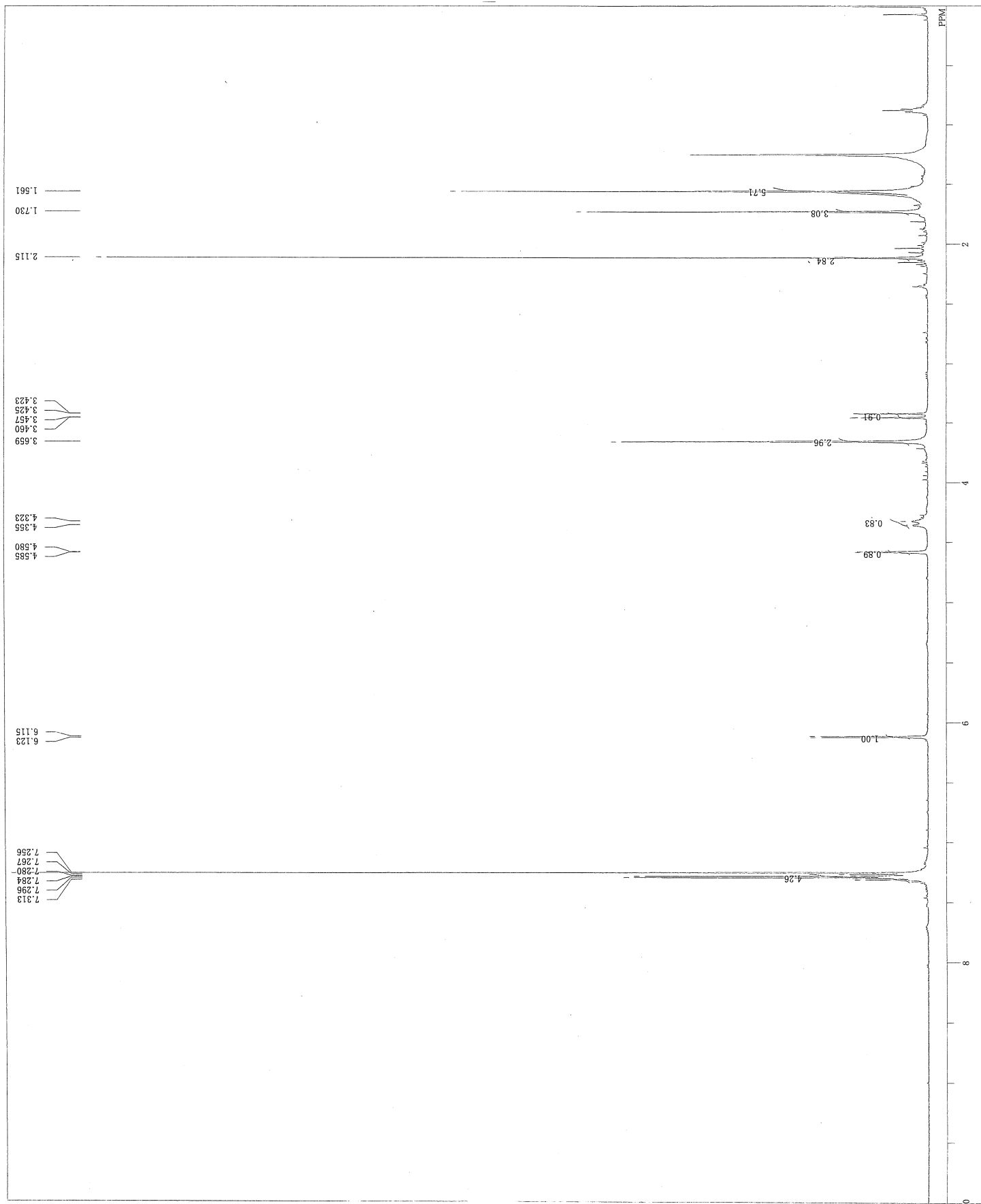
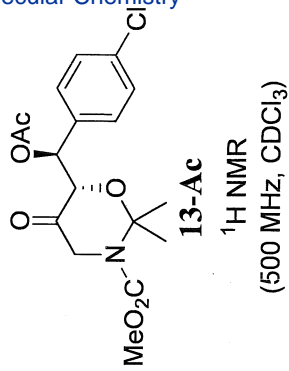


DFILE COMNT  
DATM  
OBNUC  
EXMOD  
ORSET  
OBSF  
POINT  
FREQU  
SCANS  
ACQTM  
PUL  
IRNLC  
CTEMP  
SLVNT  
EXREF  
BF  
RGAIN

single pulse decoupled gated NOE  
2011-06-23 17:11:41  
13C  
carbon\_1p  
125.77 MHz  
7.87 Hz  
4.21 Hz  
32780  
39308.18 Hz  
2048  
0.8336 sec  
2.0000 sec  
2.72 usec  
1H 20.6 c  
CDCl3  
225.02 ppm  
0.12 Hz  
60



DFILE RIX-ClAc7.19.proton-1-1.als  
COMINT single-pulse  
NAME 1311-07-20 00:09:19  
PROCNO 1  
PULPROG zgpg30  
PROTONS 1  
PULPROG 500.16 MHz  
EXMOD 2.41 KHz  
OBPRQ 6.01 Hz  
OBSFQ 13120  
POINT 7507.51 Hz  
PRGCU 1.7459 sec  
SCANS 5.0000 sec  
AQCTM 4.68 usec  
PD 1H  
PWL 20.1 c  
IRNUC CDCL3  
CTEMP 0.100 ppm  
SLVNT 0.12 Hz  
BK 50  
RGAIN

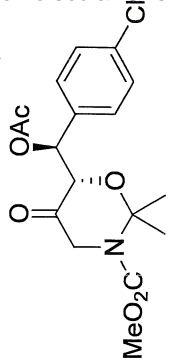


COM-670-Ac-13C

DFILE  
COMNT  
DATIM  
OBNUC  
EXMOD  
OBFQ  
OBSF  
OBFN  
POINT  
FREQU  
SCANS  
ACQTM  
PD  
PW1  
IRNUC  
CTEMP  
SLVNT  
EXREF  
BF  
RGAIN

COM-670-Ac-13C.nmdata  
COM-670-Ac-13C  
Sat Nov 21 01:09:11 2009  
13C  
bcm

100.40 MHz  
130.00 KHz  
5500.00 Hz  
32768  
27100.27 Hz  
1000  
1.2091 sec  
1.7909 sec  
5.50 usec  
1H  
25.2 c  
CDCL3  
77.00 ppm  
0.12 Hz  
32

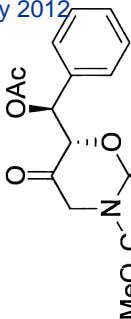


**13-Ac**  
<sup>13</sup>C NMR  
(100 MHz, CDCl<sub>3</sub>)



PPM



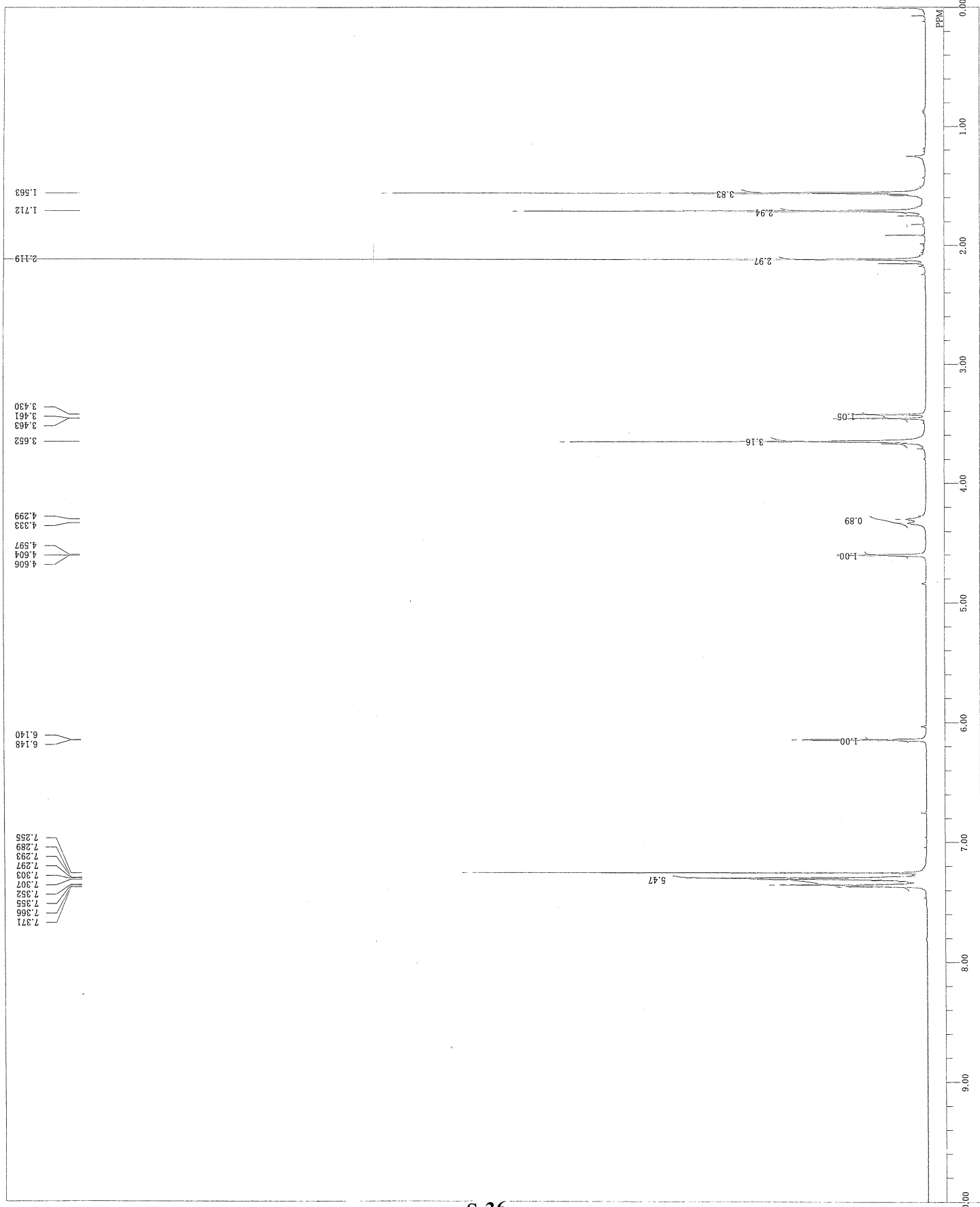


14-Ac

<sup>1</sup>H NMR  
(500 MHz, CDCl<sub>3</sub>)

DFILF  
COMNT  
DATM  
OBNUC  
EXMOD  
OBSFQ  
OBSFQ  
OBSFQ  
POINT  
FREQU  
SCANS  
ACQTM  
PULP  
PULP  
IRNLC  
CTEMP  
SLVNT  
EXREF  
BF  
RGAIN

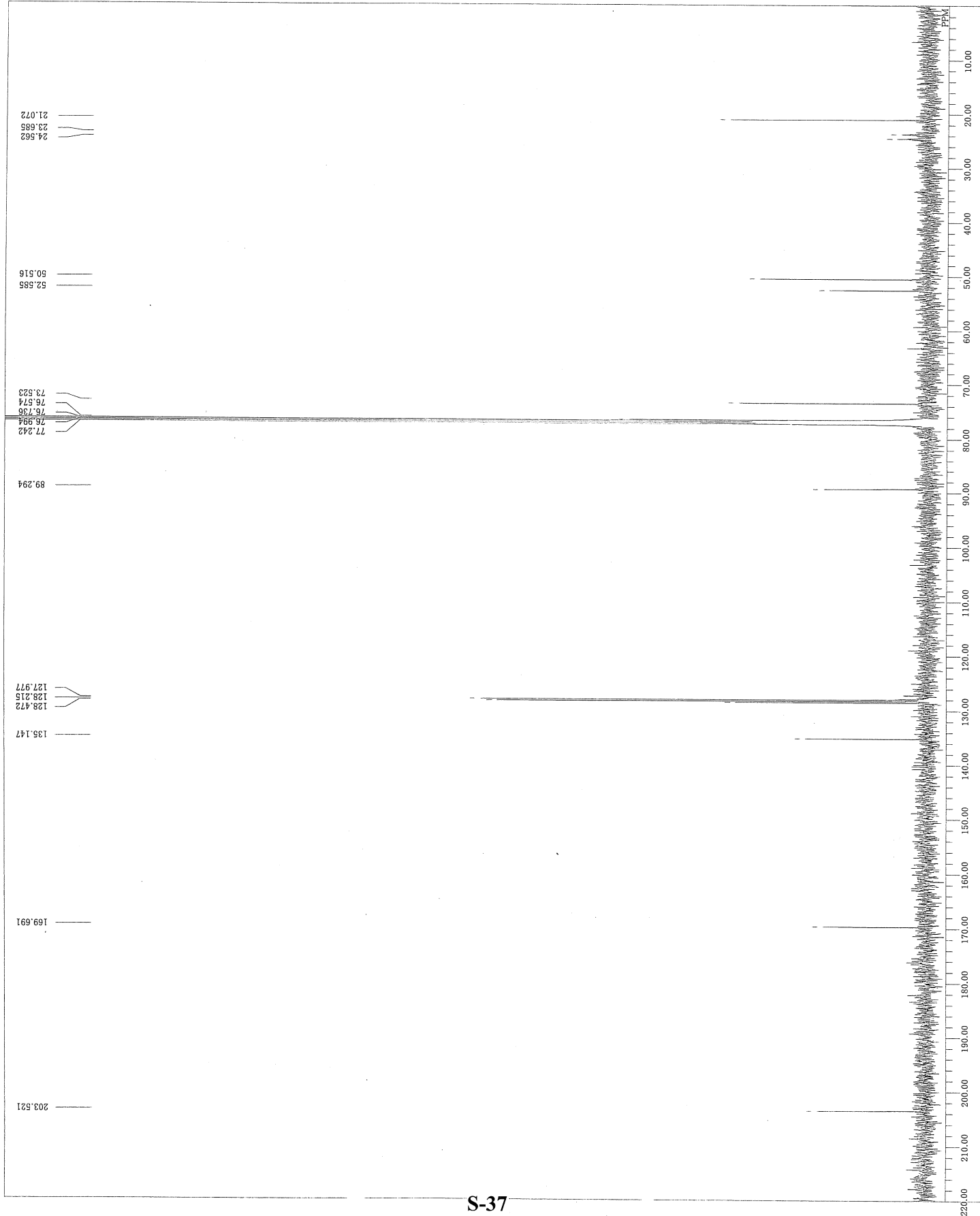
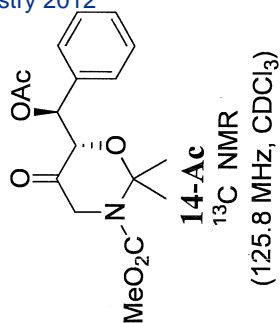
RIK-292Acquire, proton-1-1, df  
single pulse  
2011-07-01 12:27:25  
1H  
proton, 1p  
500.16 MHz  
4.11 Hz  
6.01 Hz  
16400  
9384.38 Hz  
16  
1.7459 sec  
5.000 sec  
4.66 usec  
1H  
20.9 c  
CDCl<sub>3</sub>  
0.00 ppm  
0.12 Hz  
50



```

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

```



RHPLC-662-AC-1H.nmdata  
RHPLC-662-AC-1H  
Wed Nov 18 17:22:45 2009

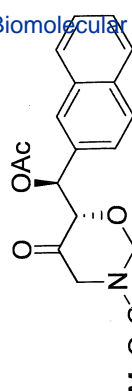
RHPL  
 RHPL  
 Wed  
 1H  
 non

399.65 MHz  
130.00 KHz  
4300.00 Hz  
32768  
7993.60 Hz

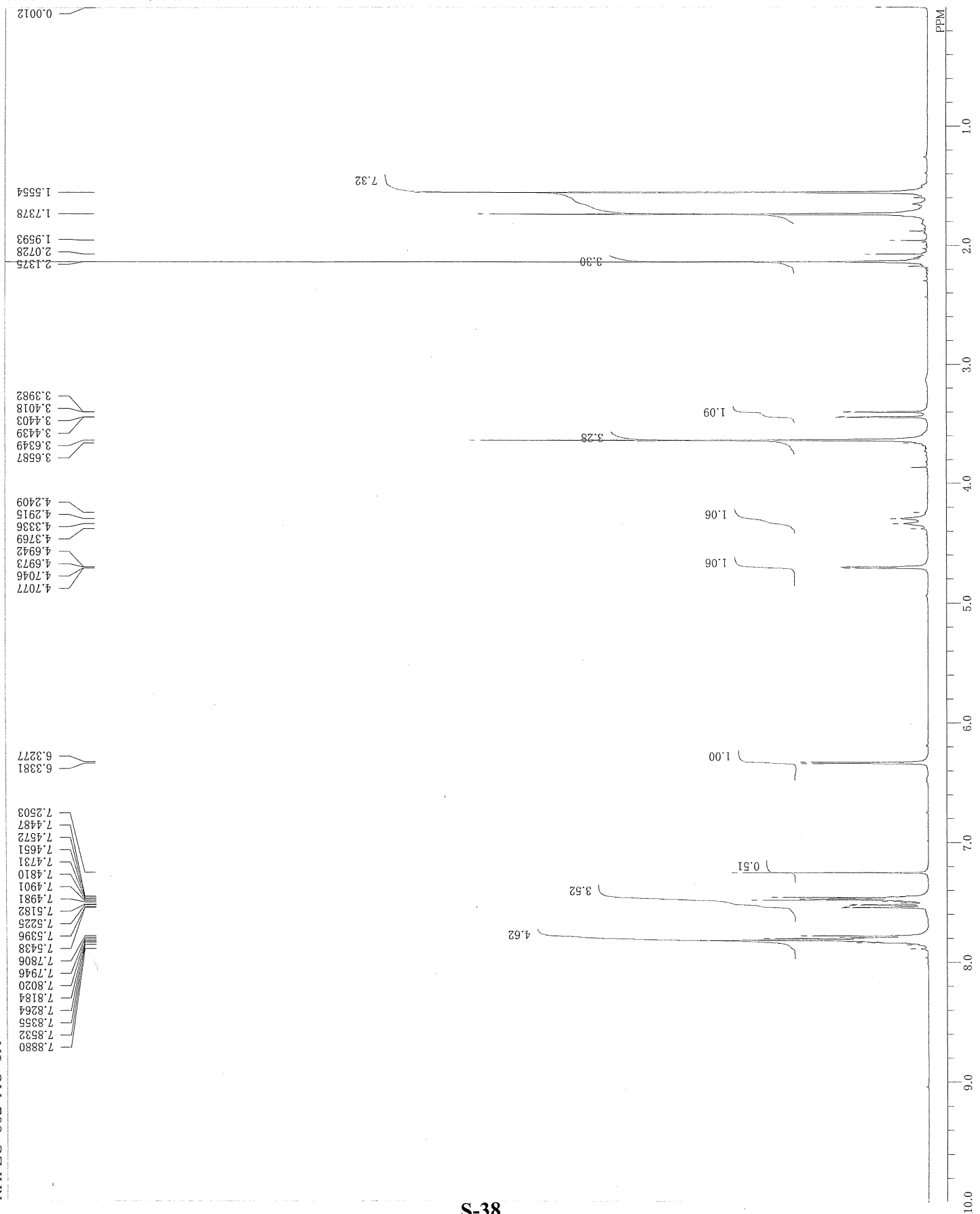
4  
4.0993 sec  
2.9007 sec  
7.00 usec

CL3  
23.8 c  
1.00 usec

0.00 ppm  
0.12 Hz  
16



**15-Ac**  
<sup>1</sup>H NMR  
(400 MHz, CDCl<sub>3</sub>)



RHPLC-662-AC-13C

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

RHPLC-662-AC-13C.nmdata  
RHPLC-662-AC-13C  
Wed Nov 18 18:14:13 2009  
13C  
bcm

100.40 MHz  
130.00 KHz  
5500.00 Hz  
32768  
27100.27 Hz  
1000  
1.2091 sec  
1.7909 sec  
5.50 usec  
1H  
25.4 c  
CDCL3  
77.00 ppm  
0.12 Hz  
32

21.0062  
23.6553  
24.5192

50.4675  
52.4996

73.6433  
76.6874  
76.7038  
77.0000  
77.3209

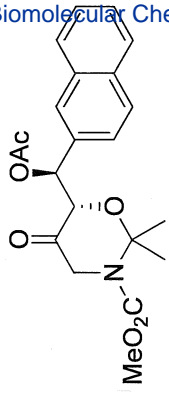
89.3078

125.6716  
126.0665  
126.3216  
127.5145  
127.6050  
127.7778  
128.1891  
132.6236  
132.7058  
133.2077

154.0799

169.6621

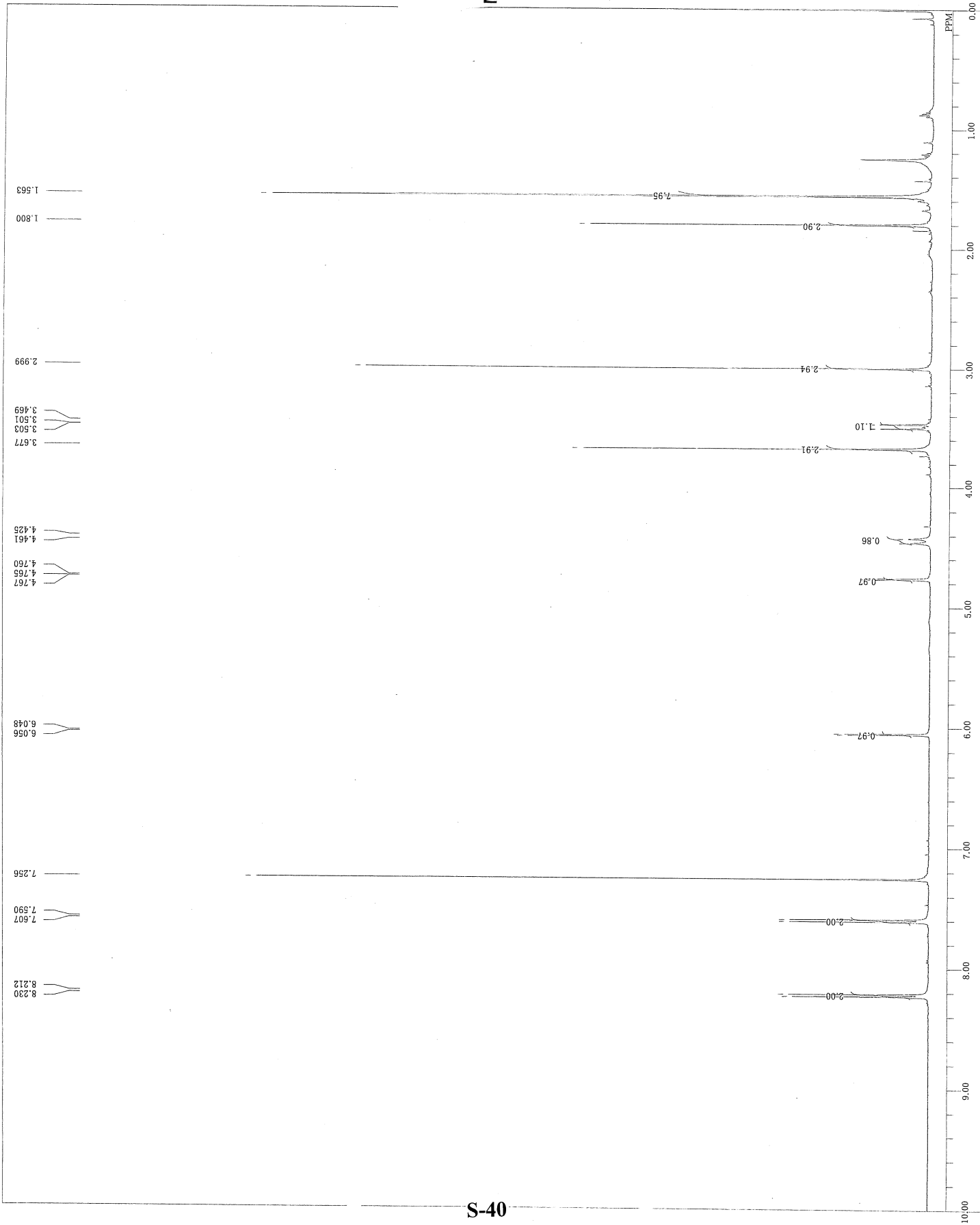
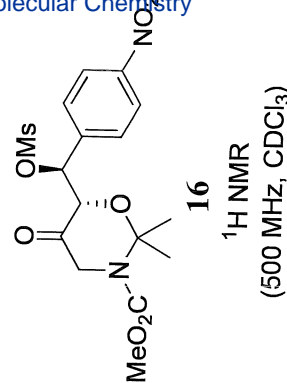
203.5249

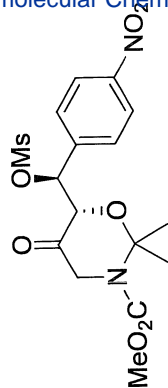
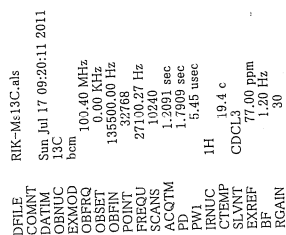


15-Ac

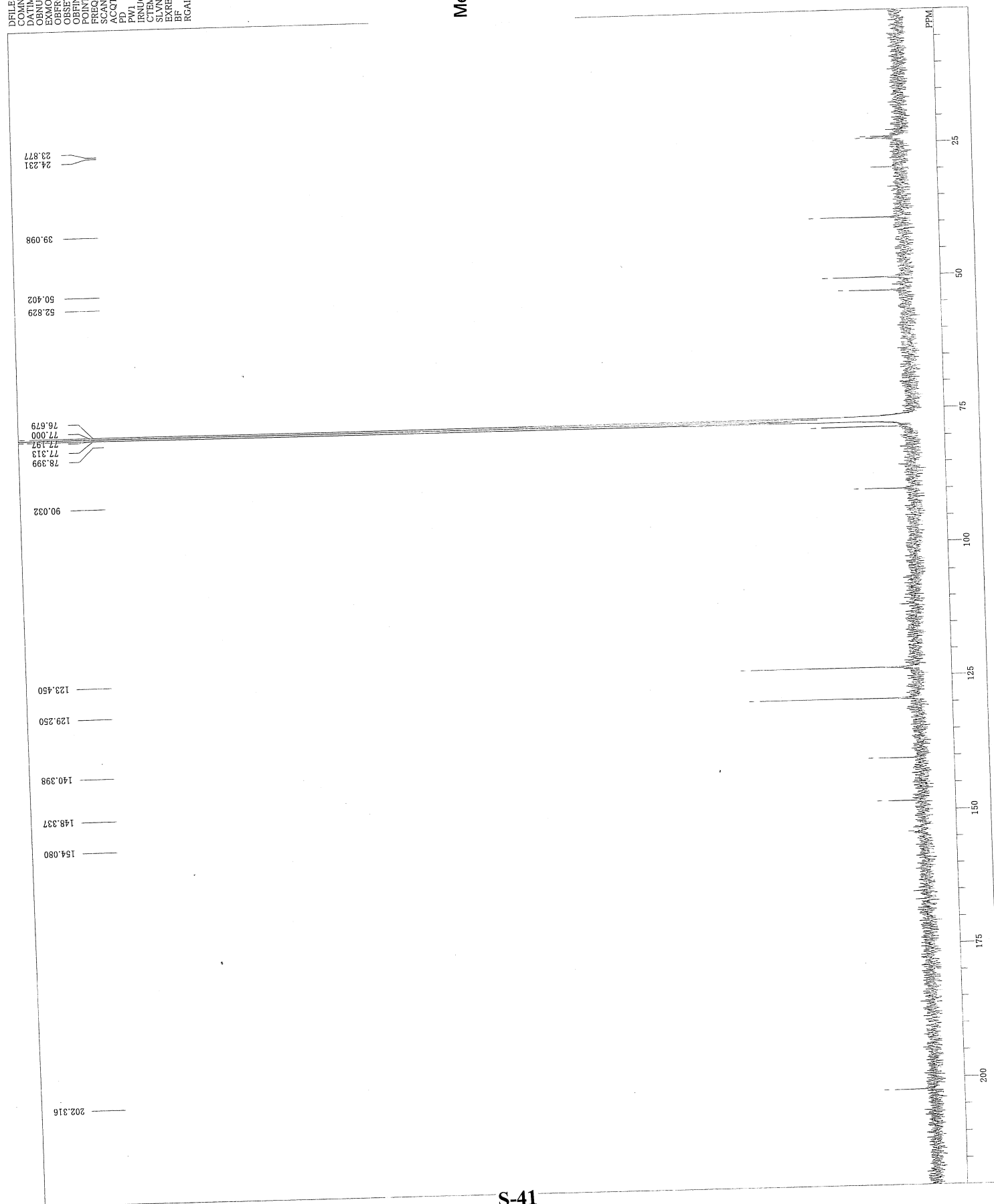
<sup>13</sup>C NMR  
(100 MHz, CDCl<sub>3</sub>)

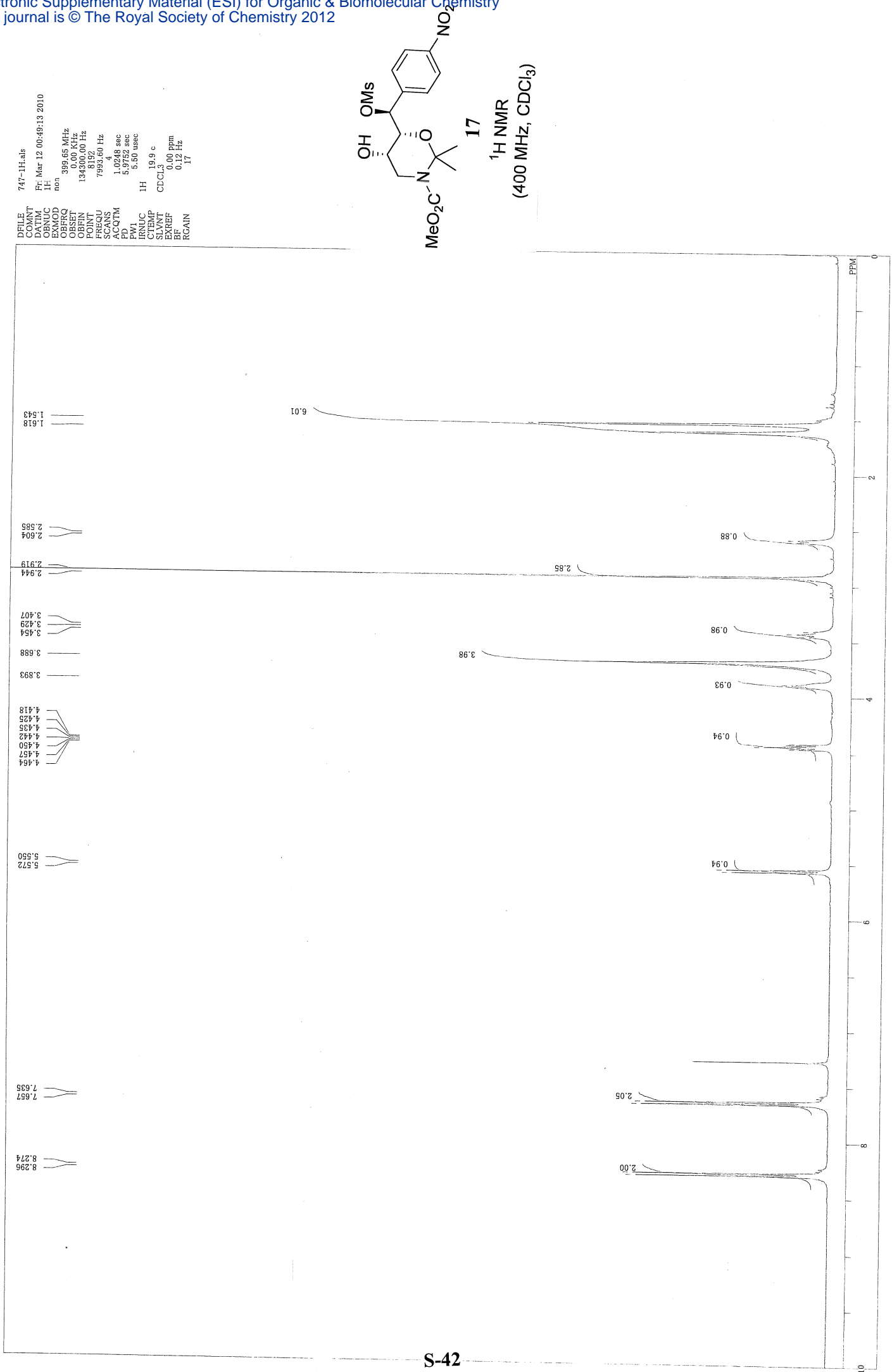
Ms-f00 proton-2-1.jdf  
Date\_ 2011-07-09 21:29:03  
1H  
proton.jxp  
500.16 MHz  
2.41 KHz  
16.01 Hz  
1.44 sec  
9384.38 Hz  
SCANS 8  
ACQTM 1.7459 sec  
PD 5.0000 sec  
4.68 usec  
1H 21.0 c  
IRNUC  
CDCl3  
0.00 ppm  
BF 0.12 Hz  
RGAIN 54

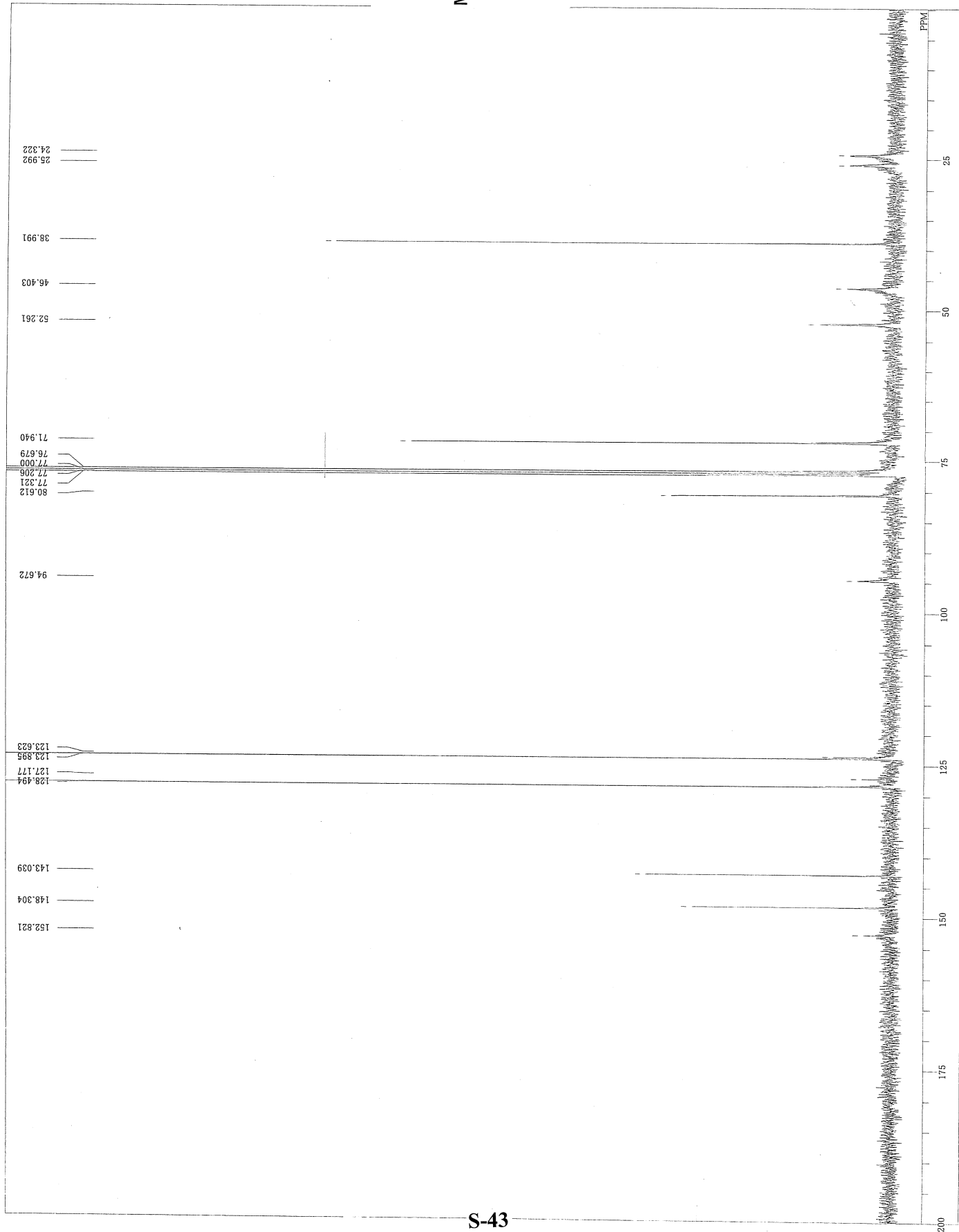
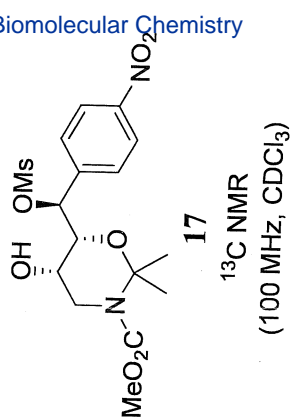




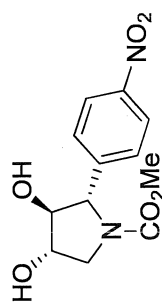
**16**  
**<sup>13</sup>C NMR**  
**(100 MHz, CDCl<sub>3</sub>)**



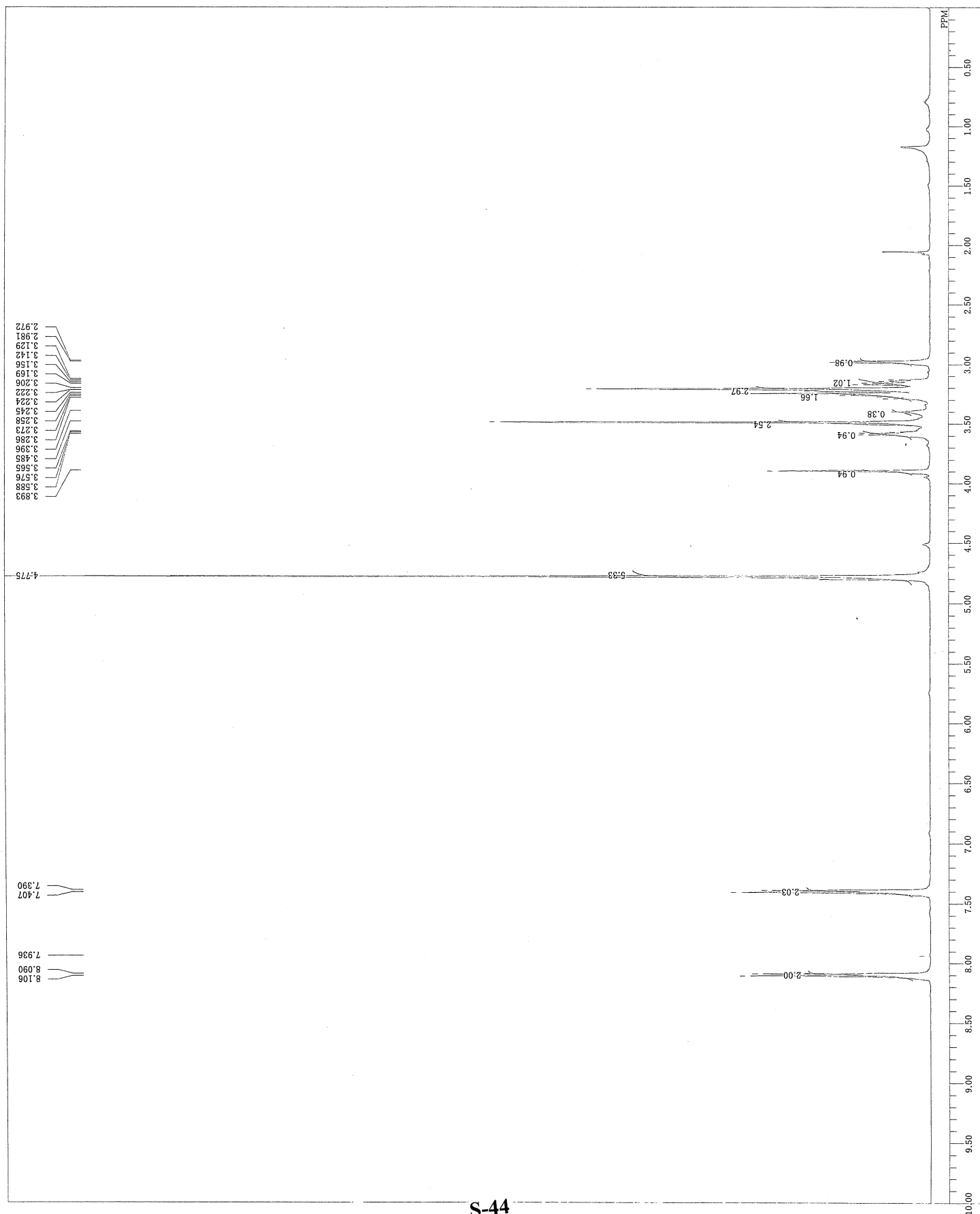






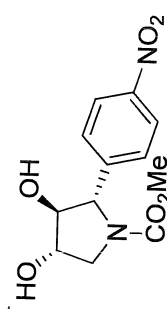


**18**  
 $^1\text{H}$  NMR  
(500 MHz,  $\text{CD}_3\text{OD}$ )



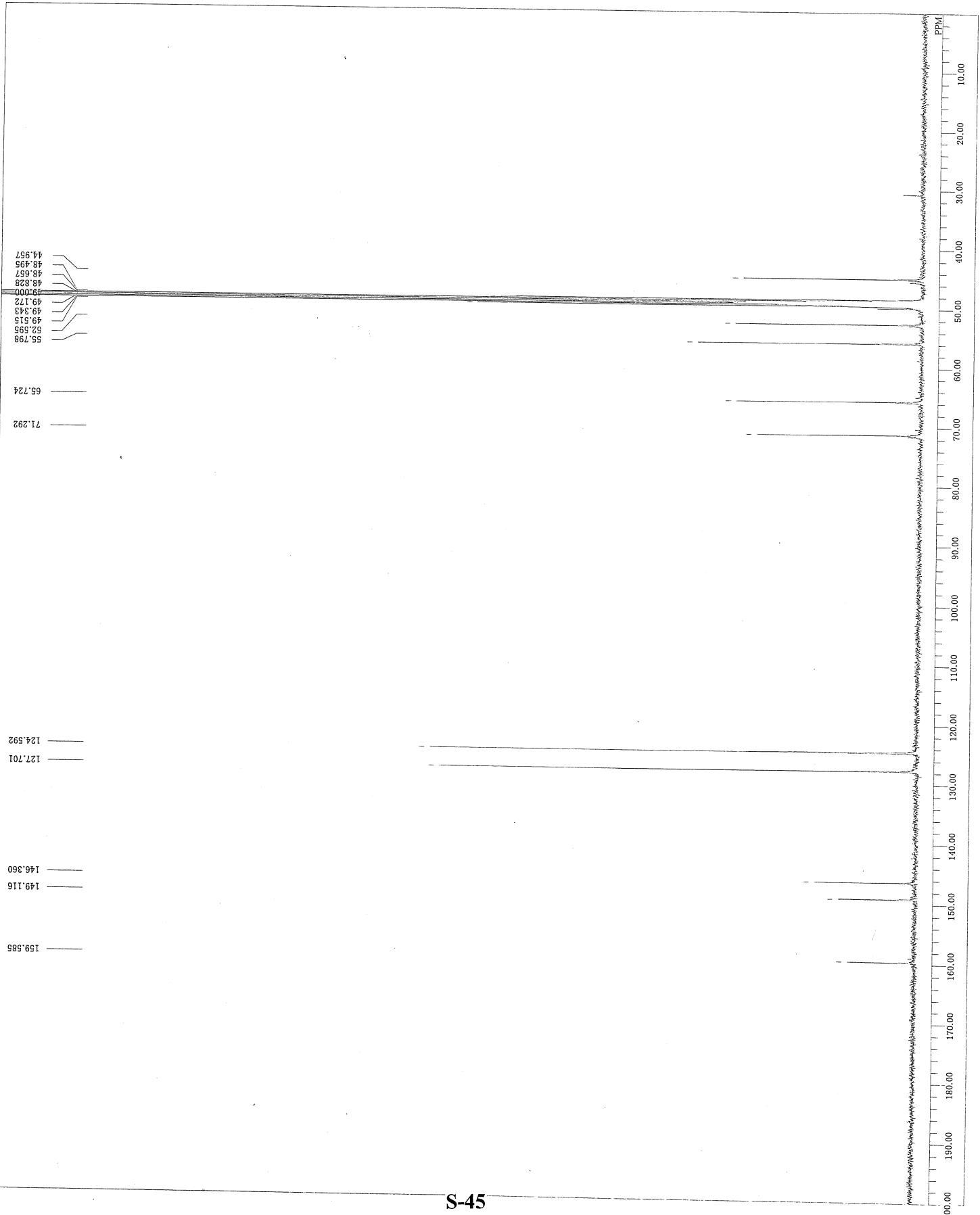
RIK-aza, Carbon-3-1, jif  
single pulse decoupled gated NOE  
2011-09-07 00:12:06  
13C  
canton\_jip  
EXMOD 125.77 MHz  
OBFRQ 7.87 KHz  
OBSET 4.21 Hz  
OBFIN 32780  
POINT 39308.18 Hz  
FREQU 2048  
SCANS 2  
AQ-TIM 2.0036 sec  
PD 2.00 sec  
PW1 2.72 msec  
1H 20.1 e  
CD3OD 49.00 ppm  
EXREF 0.12 Hz  
RGAIN 60

DFILE  
COMNT  
DATIM  
EXMOD  
EXREF  
OBFRQ  
OBSET  
OBFIN  
POINT  
FREQU  
SCANS  
AQ-TIM  
PD  
PW1  
IRNUC  
CTEMP  
SLVNT  
EXREF  
RGAIN

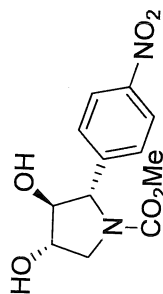


18

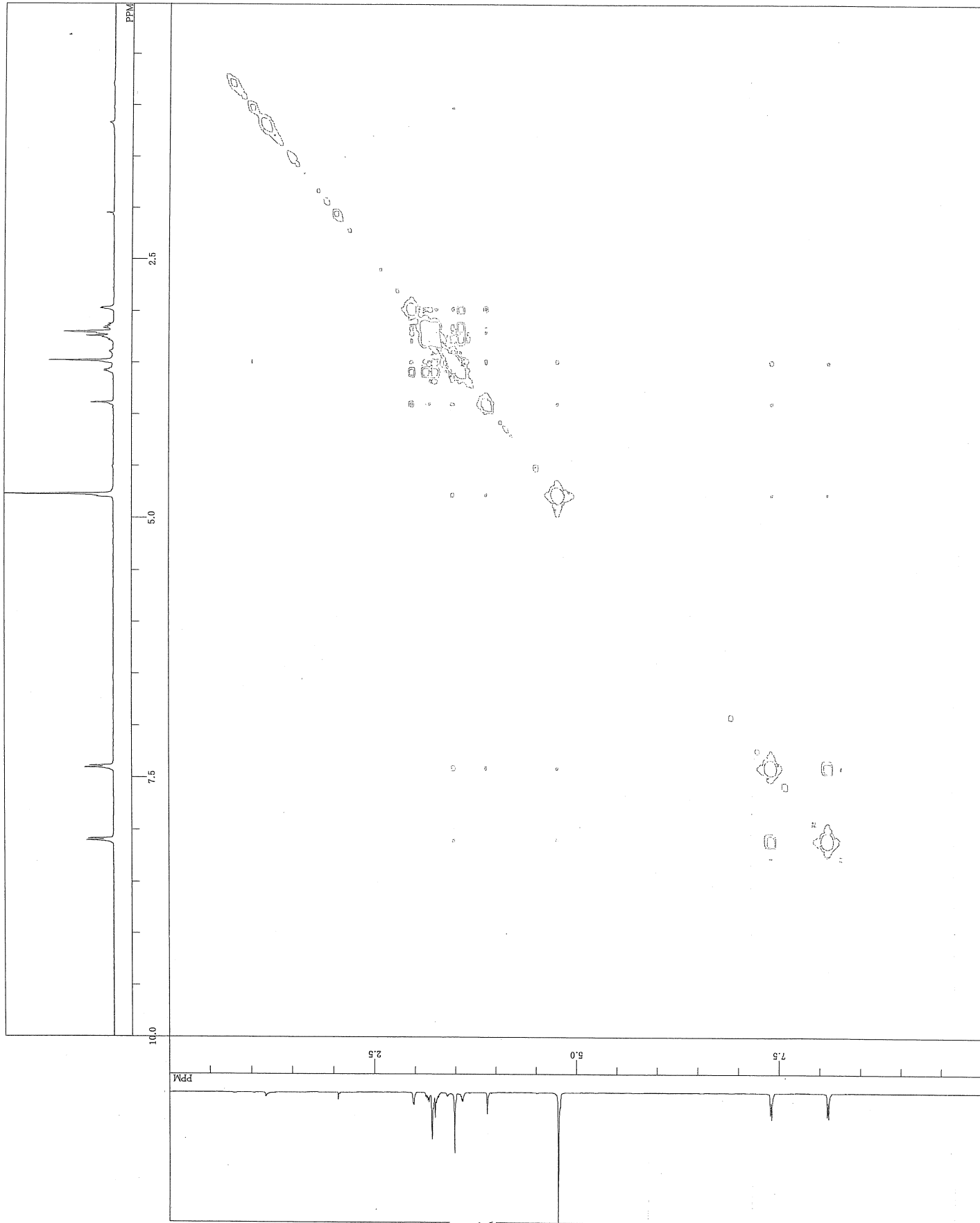
<sup>13</sup>C NMR  
(125.8 MHz, CD<sub>3</sub>OD)



RIX-nza-cosy-4-2.xls  
gradient absolute value cosy  
cosy\_bp  
1H 500.16 MHz  
OBSFQ 2.21 kHz  
OBSF1 6.01 Hz  
POINT 1024  
FREQ1 7507.51 Hz  
CLPNT 1024  
TODAT 256  
SOLV1 CD3OD  
ACQTM 7504.13 Hz  
PD 0.1364 sec  
PW1 9.35 usec  
PW2 0.00 usec  
PW3 0.00 usec  
P11 0.0000 msec  
P12 0.0000 msec  
P13 0.0000 msec  
IRNUC 1H 20.0 c  
CTEMP CD3OD  
SLVNT 0.00 ppm  
EXREF 0.00  
CLEXR 46  
RGAIN



H-H COSY  
(500 MHz, CD<sub>3</sub>OD)

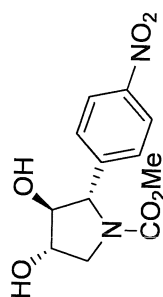




```

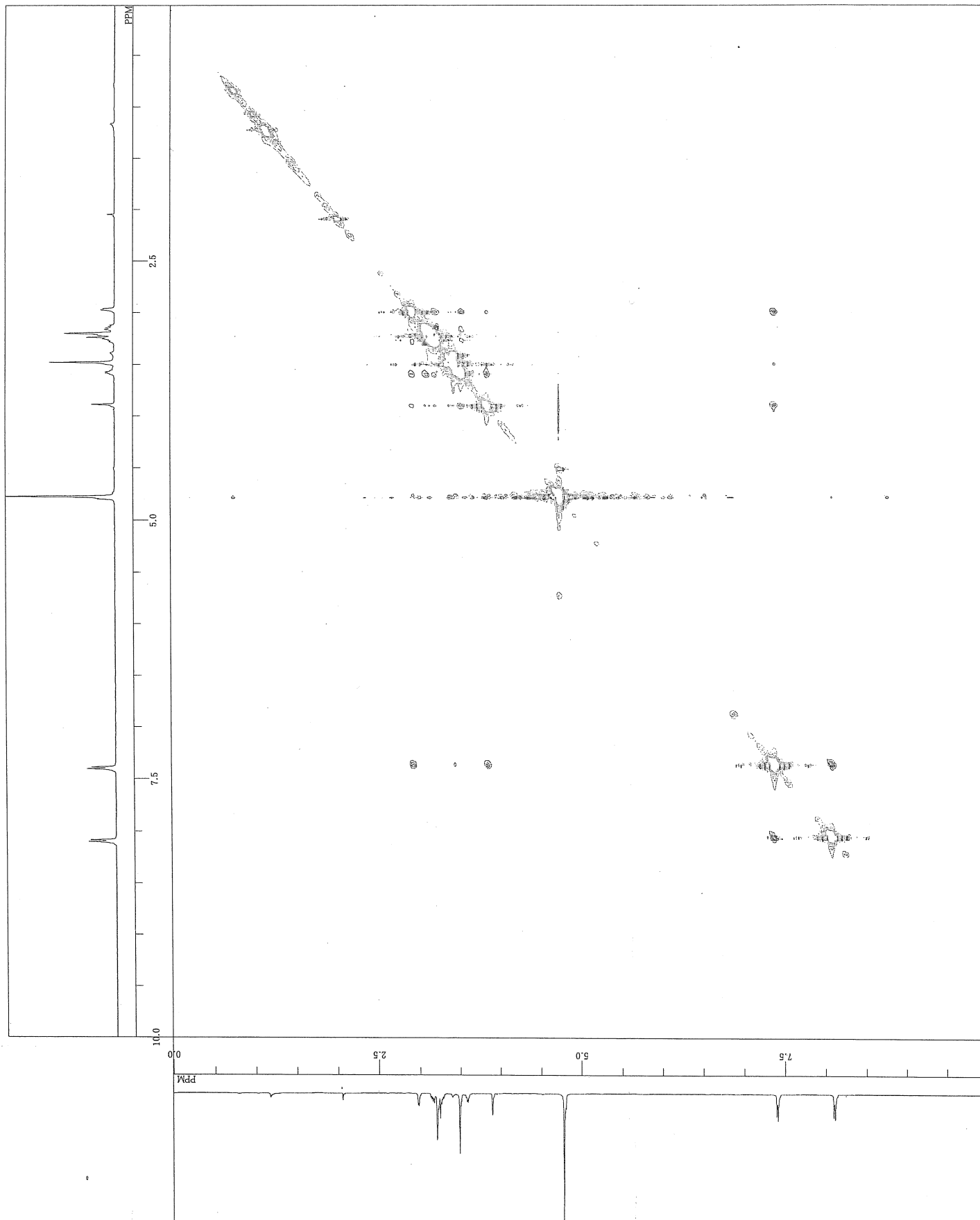
DFILE  COMNT  DATIM  EXMOD  OBNUC  OBFRQ  OBSET  OBFIN  POINT  FREQU  CLPNT  TODAT  CLFRQ  SCANS  ACQTM
PD      PW1    PW2    PW3    P11    P12    P13    IRNUC  CTEMP  SLVNT  EXREF  CLEXR  RGAIN

```



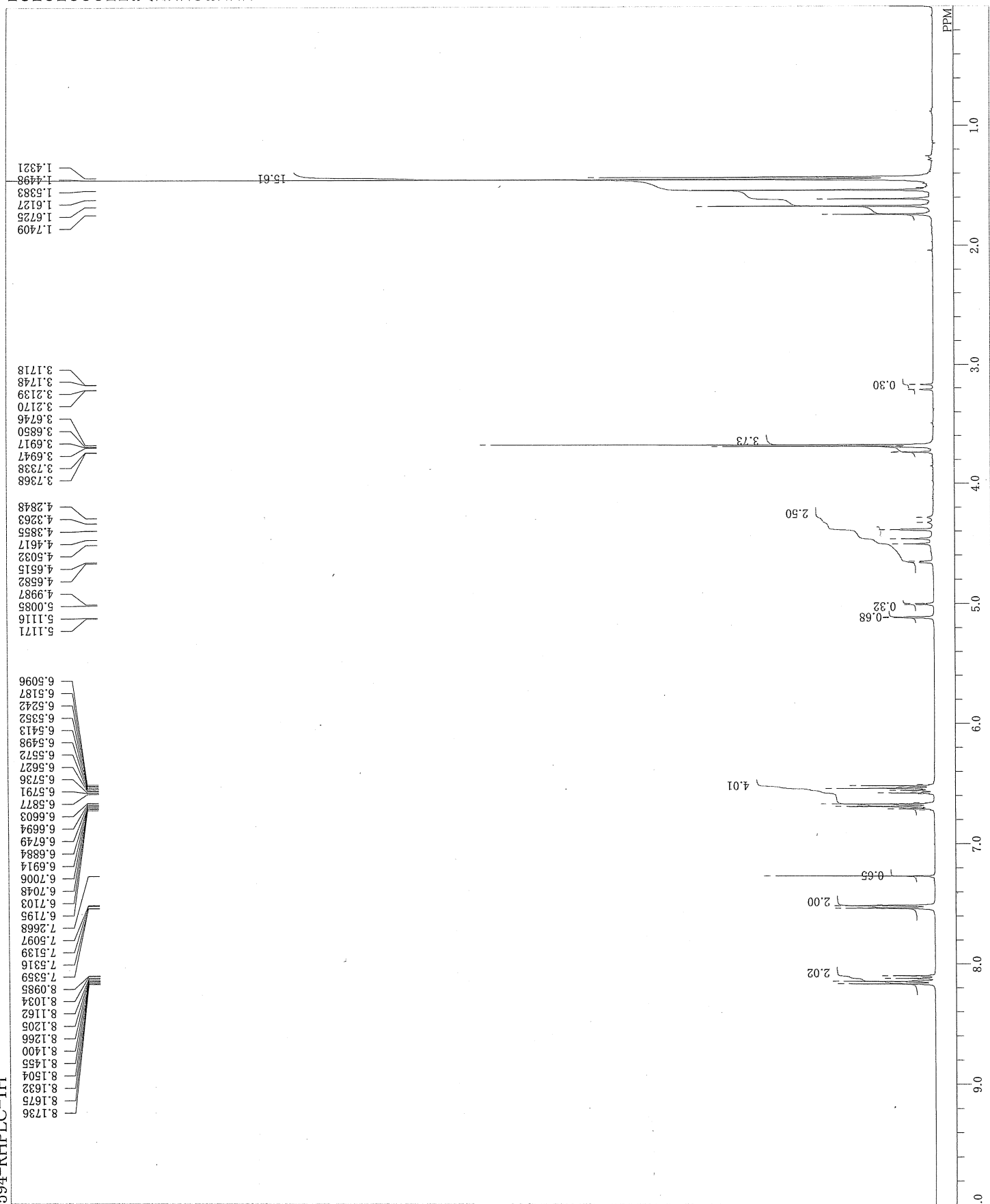
18

NOESY  
(500 MHz, CD<sub>3</sub>OD)

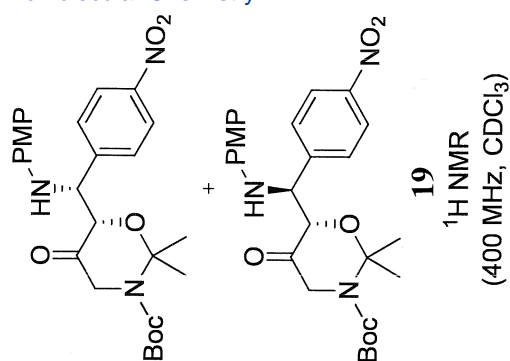


594-RHPLC-1H

S-49



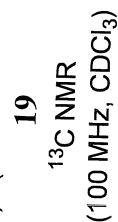
594-RHPLC-1H.mnmda  
594-RHPLC-1H  
Wed Apr 15 20:22:43 2009  
1H  
non  
399.65 MHz  
130.00 KHz  
4300.00 Hz  
32768  
7993.60 Hz  
4  
4.0933 sec  
2.9007 sec  
PD  
7.00 usec  
1H  
22.9 c  
CDCL3  
0.00 ppm  
0.22 Hz  
18  
RGAIN

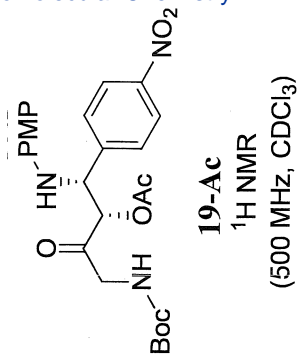
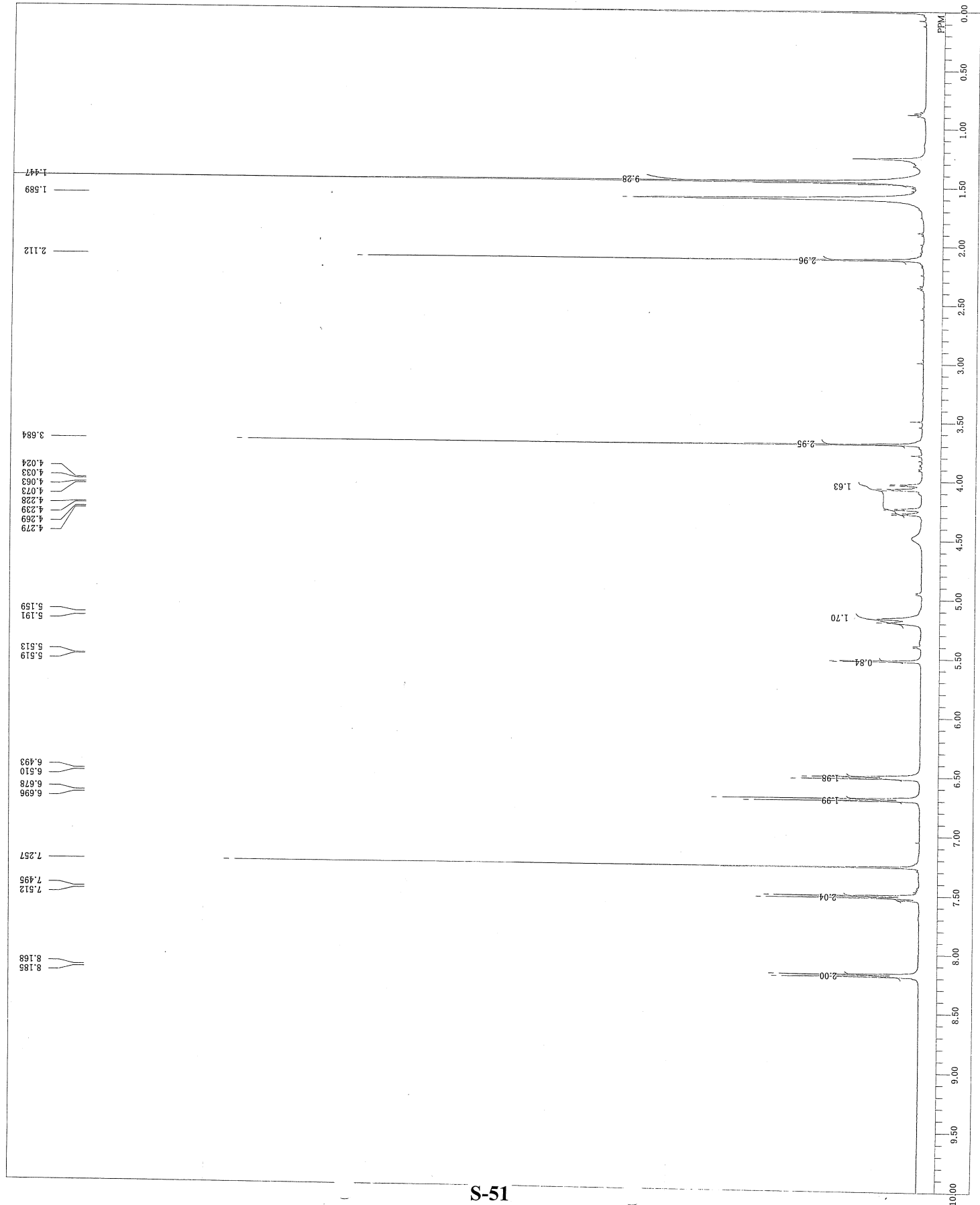


```

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

```





RII-mca204-25\_proton-1-1.jdf  
single  
2011-09-13 16:54:48  
1H  
proton.kp  
500.16 MHz  
2.41 kHz  
6.71 Hz  
16400  
9384.38 Hz  
16  
1.7459 sec  
5.0000 sec  
4.68 usec  
1H  
20.3 c  
CDCl<sub>3</sub>  
0.00 ppm  
0.12 Hz  
52  
RGAIN



File: man324-25\_Carbon-13\_als  
Date: 2011-09-13 16:59:49  
Single pulse decoupled gated NOE  
13C  
carbon, kcp  
EXMOD 125.77 MHz  
OBFRQ 7.87 KHz  
OBSET 4.21 Hz  
PULPROG zgpg30  
PC 39536.18 Hz  
SCANS 16  
ACQTM 0.8336 sec  
PD 2.0000 sec  
PW1 2.72 usec  
IRNUC 1H  
CTEMP 20.7 c  
CDCL3  
SOLVENT  
EXREF 77.00 ppm  
BF 0.12 Hz  
RGAIN 50

