

Fragmentations Observed in the Reactions of α -Methoxy- γ -alkoxyalkyl iodide Substrates with Super Electron Donors Derived from 4-DMAP and *N*-Methylbenzimidazole

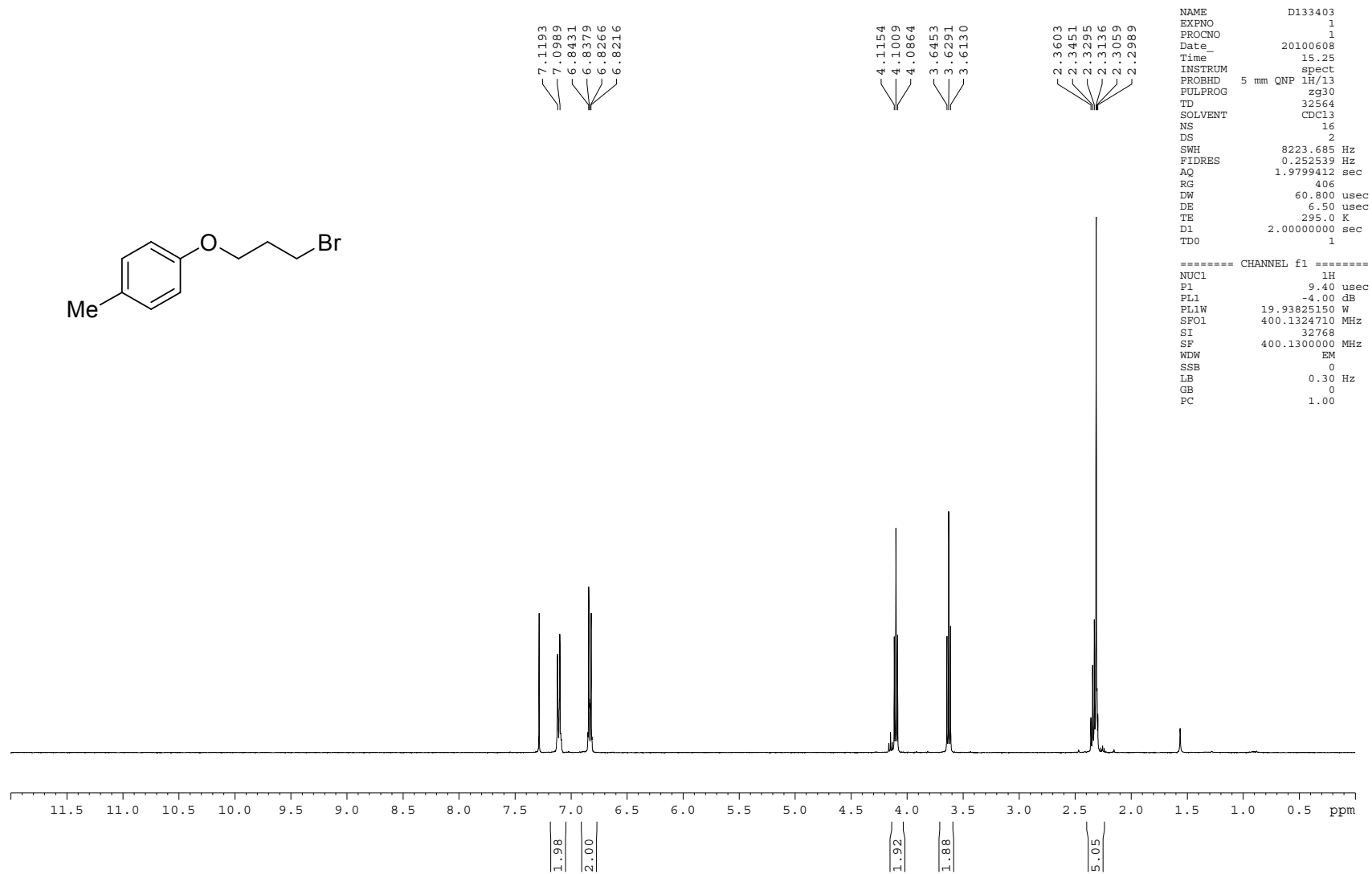
Supplementary Information.

NMR Spectra (of compounds not previously reported by us).

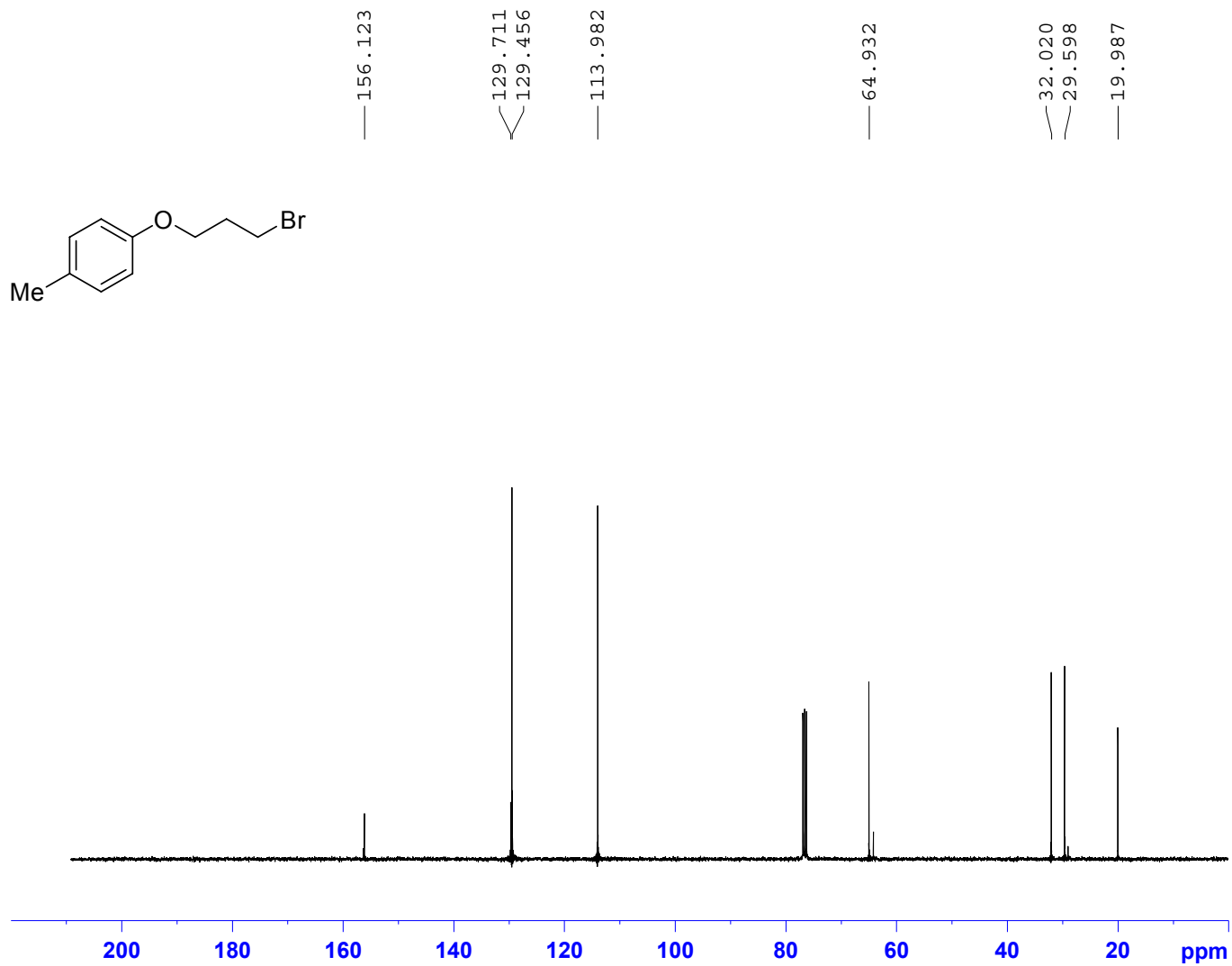
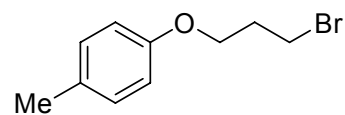
Spectrum	Compound	Page	Spectrum	Compound	Page
^1H	28e	3	^1H	28g	15
^{13}C	28e	4	^{13}C	28g	16
^1H	29e	5	^1H	29g	17
^{13}C	29e	6	^{13}C	29g	18
^1H	14e	7	^1H	14g	19
^{13}C	14e	8	^{13}C	14g	20
^1H	28f	9	^1H	28h	21
^{13}C	28f	10	^{13}C	28h	22
^1H	29f	11	^1H	29h	23
^{13}C	29f	12	^{13}C	29h	24
^1H	14f	13	^1H	14h	25
^{13}C	14f	14	^{13}C	14h	26

Spectrum	Compound	Page	Spectrum	Compound	Page
¹ H	16e	27	¹ H	30g	39
¹³ C	16e	28	¹³ C	30g	40
¹ H	16f	29	¹ H	30h	41
¹³ C	16f	30	¹³ C	30h	42
¹ H	16g	31	¹ H	precursor to 33	43
¹³ C	16g	32	¹³ C	precursor to 33	44
¹ H	16h	33	¹ H	33	45
¹³ C	16h	34	¹³ C	33	46
¹ H	30e	35	¹ H	38	47
¹³ C	30e	36	¹³ C	38	48
¹ H	30f	37	¹ H	38 + 36	49
¹³ C	30f	38	¹³ C	38 + 36	50

LB-4



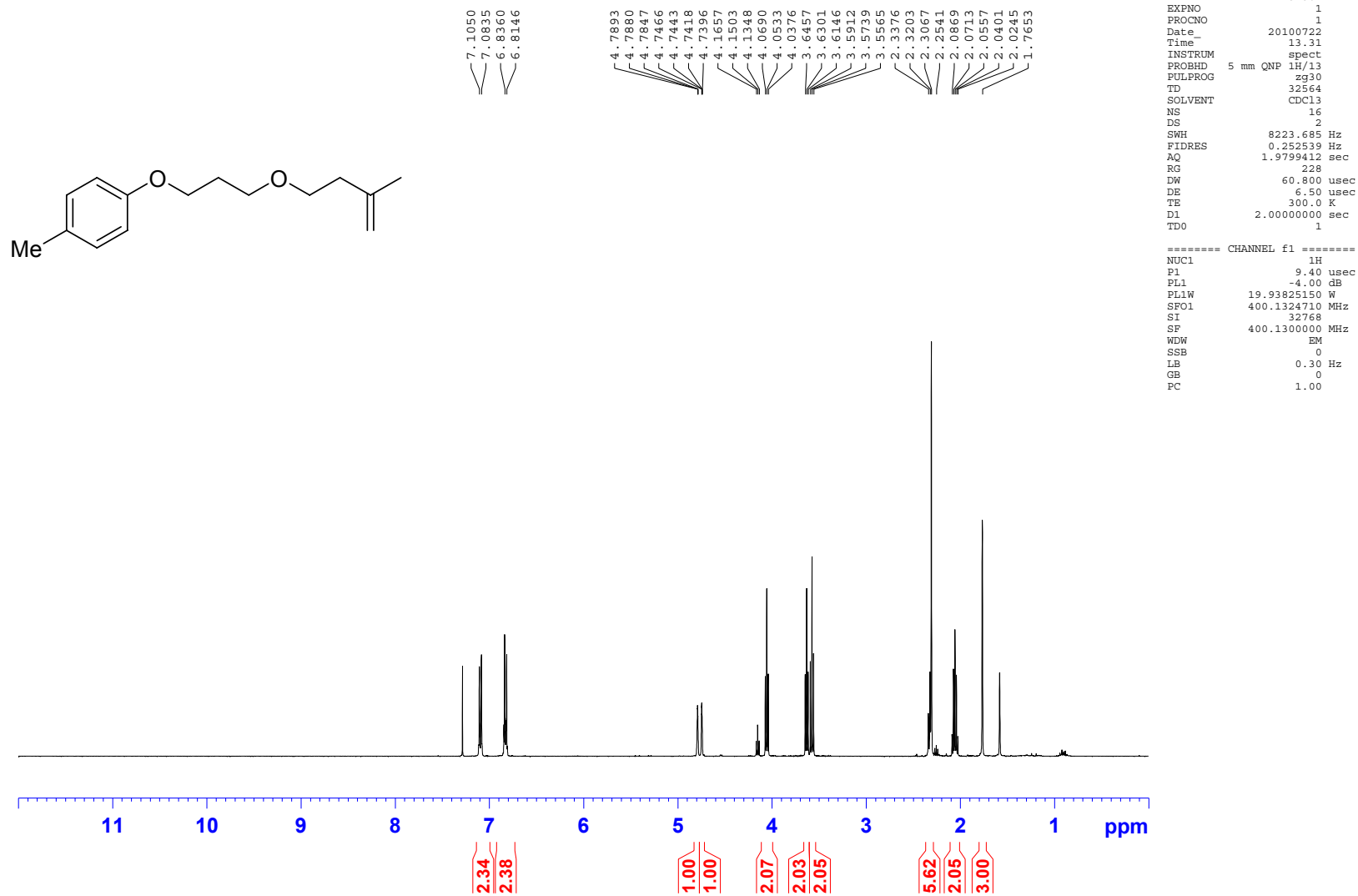
LB-4



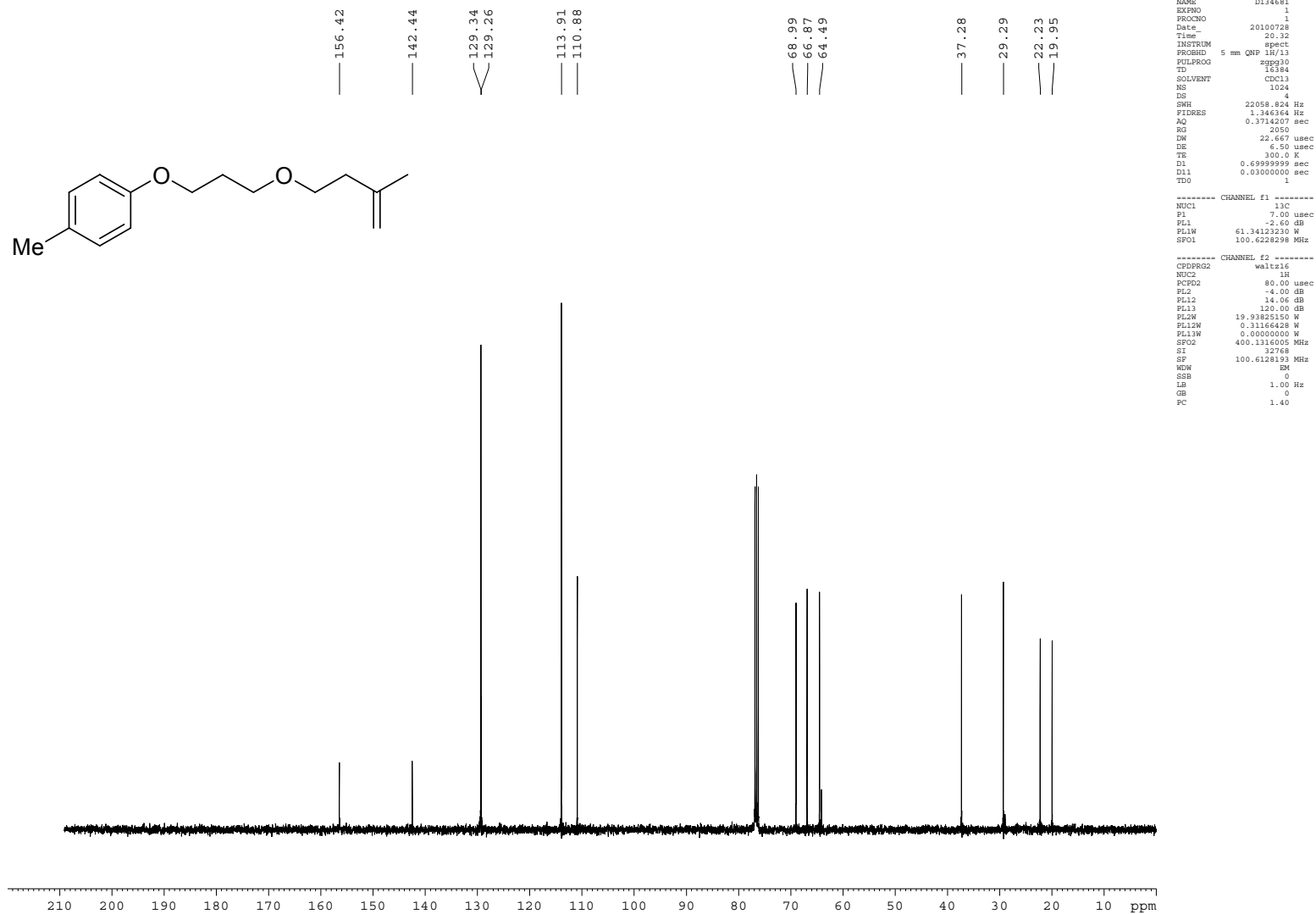
```

NAME          D134629
EXPNO         1
PROCNO        1
Date_         20100726
Time         20.39
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            16384
SOLVENT       CDCl3
NS            1024
DS            4
SWH           22058.824 Hz
FIDRES        1.346364 Hz
AQ            0.3714207 sec
RG            2050
DW            22.667 usec
DE            6.50 usec
TE            300.0 K
D1            0.69999999 sec
D11           0.03000000 sec
TDO           1
===== CHANNEL f1 =====
NUC1          13C
P1            7.00 usec
PL1           -2.60 dB
PL1W          61.34123230 W
SFO1          100.6282598 MHz
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -4.00 dB
PL12          14.06 dB
PL13          120.00 dB
PL2W          19.93825150 W
PL12W         0.31166428 W
PL13W         0.00000000 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6128193 MHz
WDW           EM
GB            0
LB            1.00 Hz
GB            0
PC            1.40
    
```

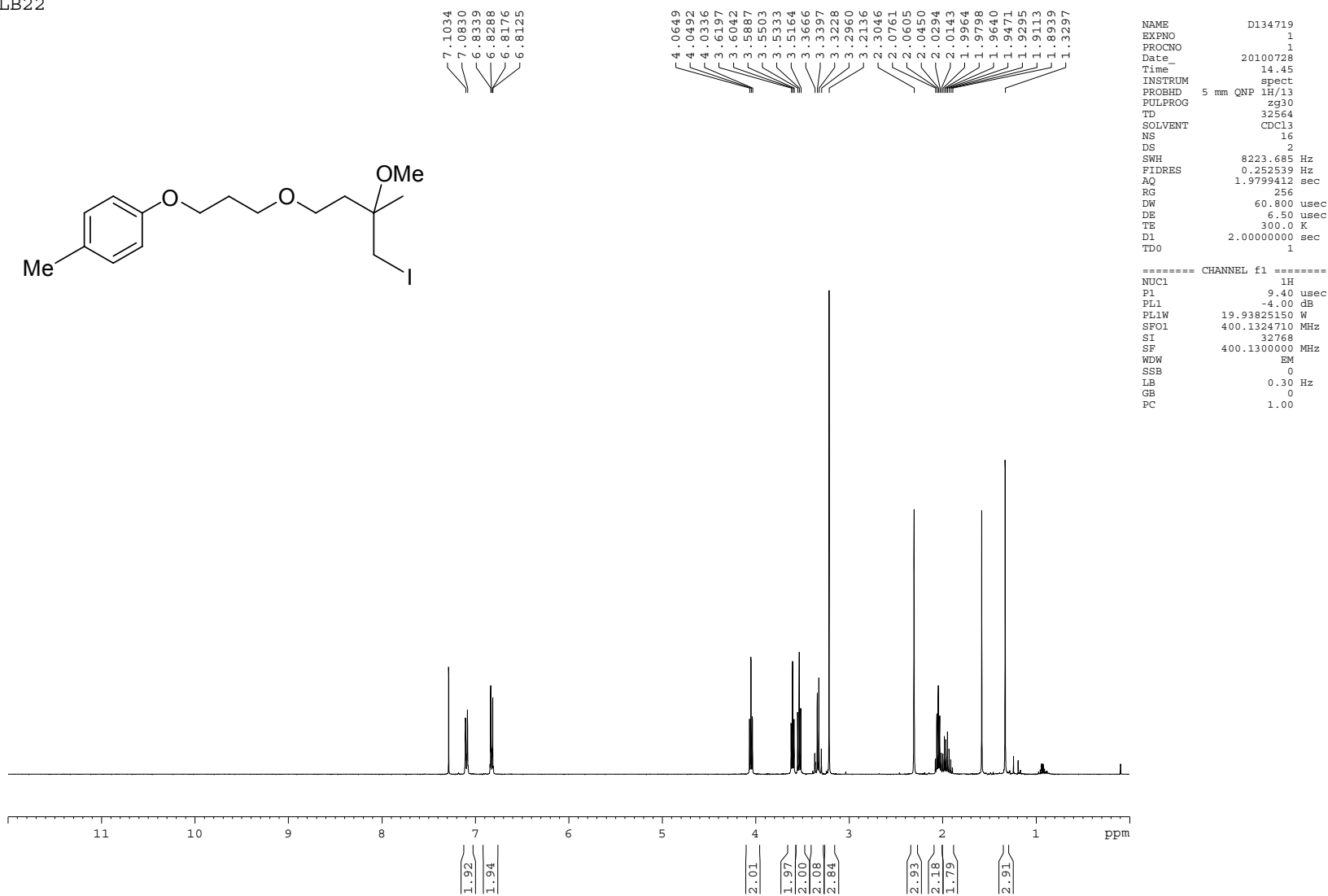
LB-21



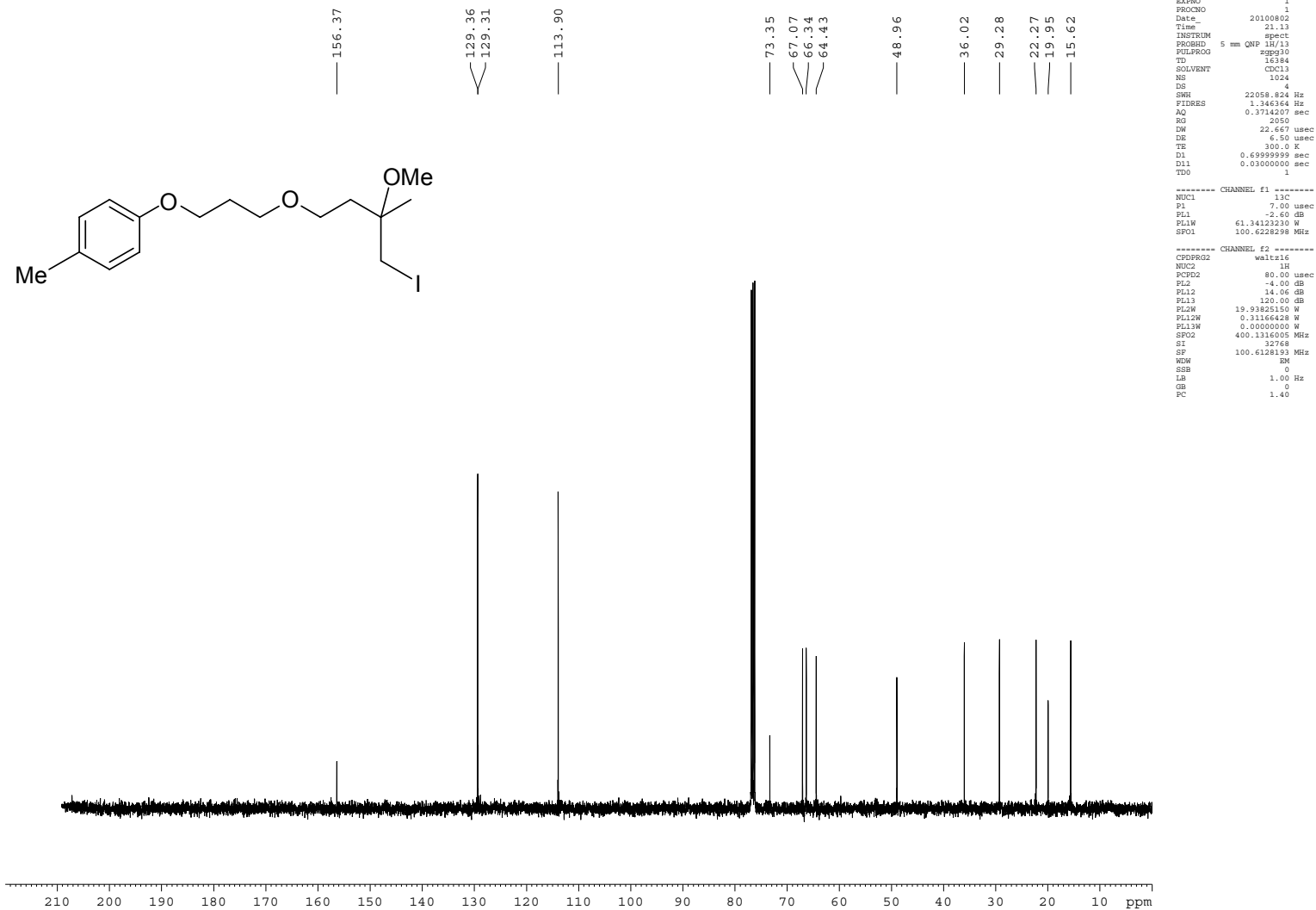
LB-21



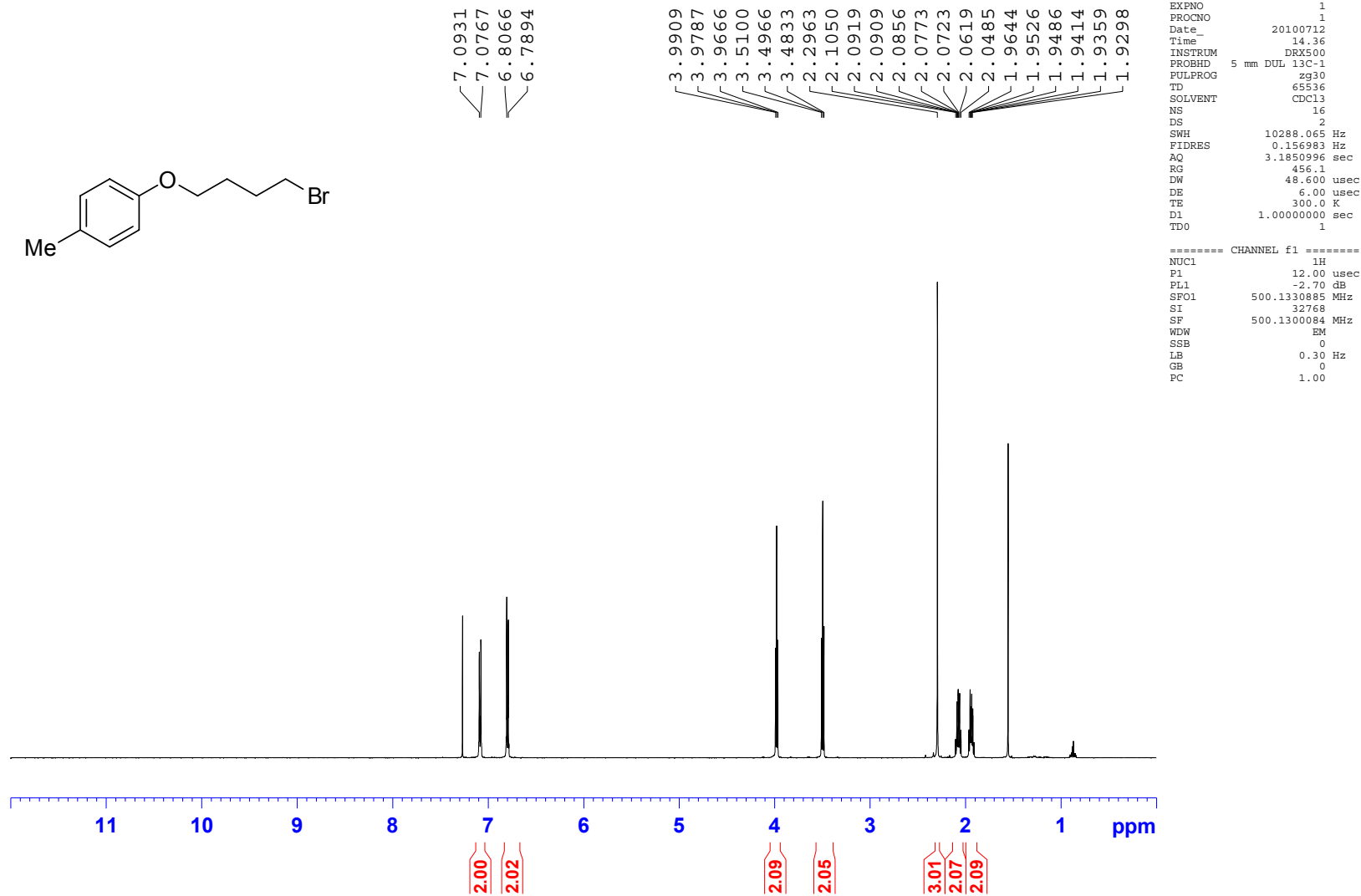
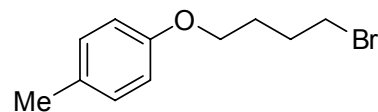
LB22



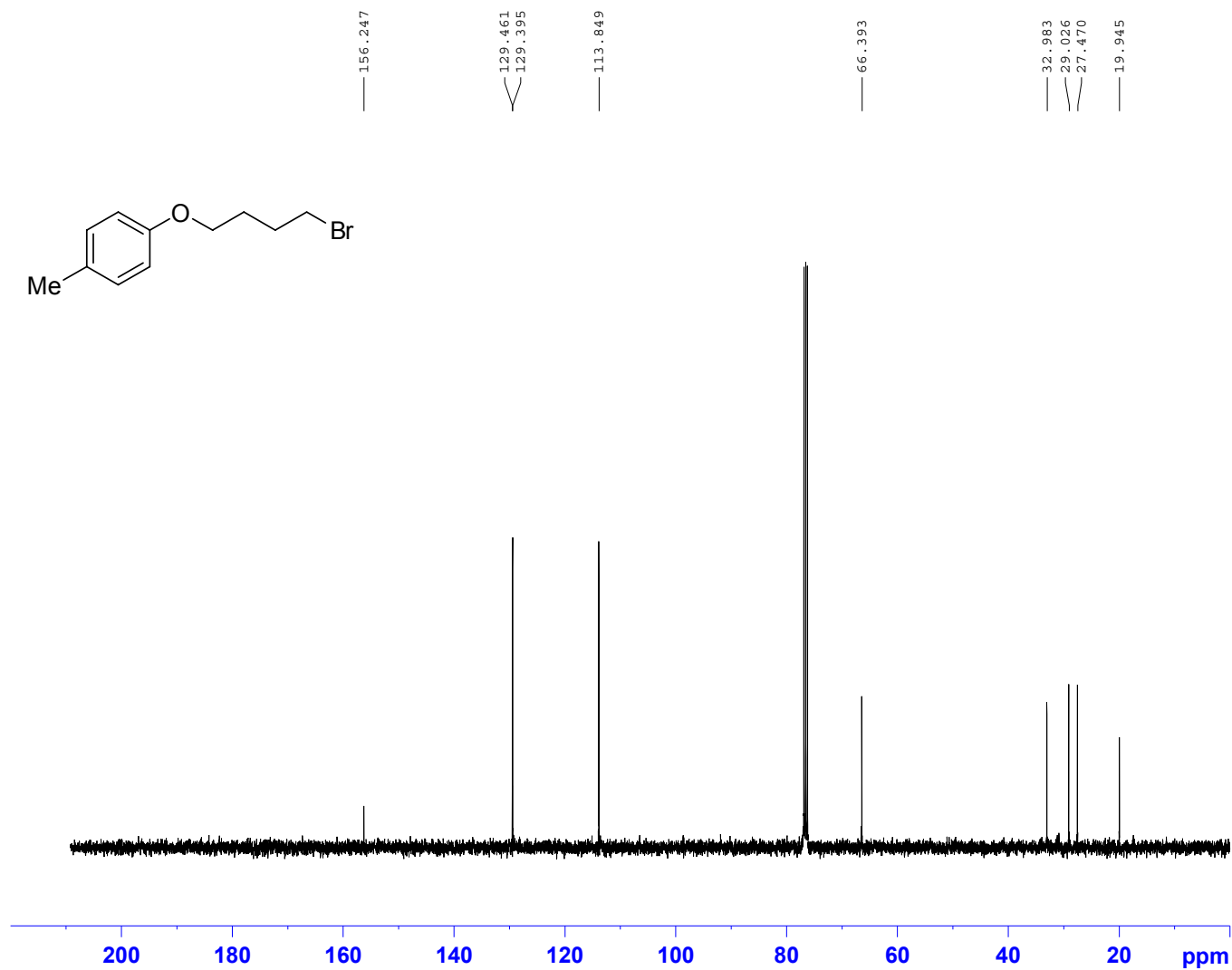
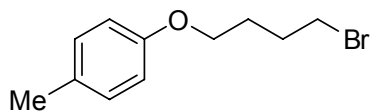
LB22



LB-16



LB-16



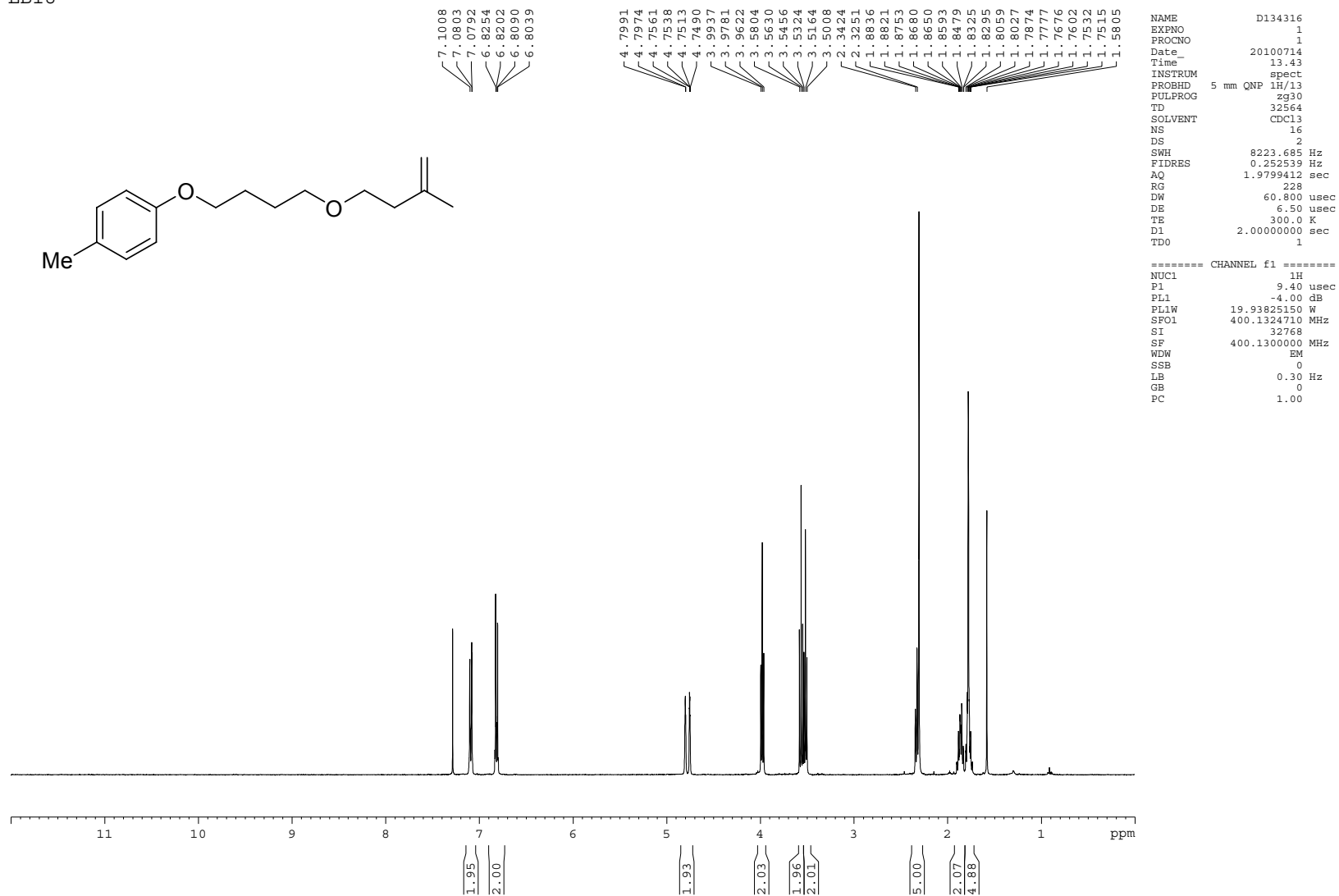
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NAME          D134678
EXPNO         1
PROCNO        1
Date_         20100728
Time         19.23
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            16384
SOLVENT       CDCl3
NS            1024
DS            4
SWH           22058.824 Hz
FIDRES        1.346364 Hz
AQ            0.3714207 sec
RG            2050
DM            22.667 usec
DE            6.50 usec
TE            300.0 K
D1            0.69999999 sec
D11           0.03000000 sec
TDO           1

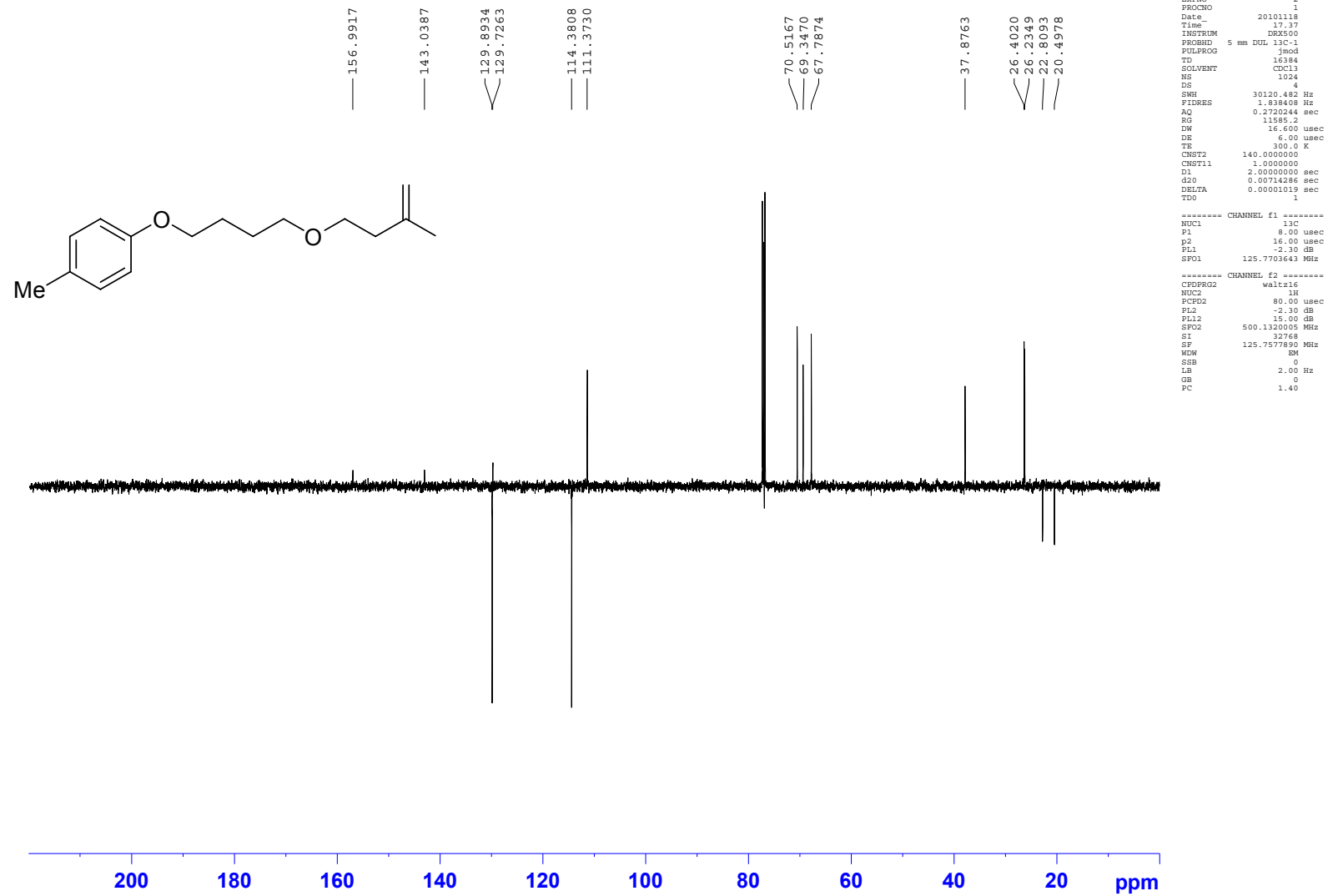
===== CHANNEL f1 =====
NUC1          13C
P1            7.00 usec
PL1           -2.60 dB
PL1W          61.34123230 W
SFO1          100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -4.00 dB
PL12          14.06 dB
PL13          120.00 dB
PL1W          19.93825150 W
PL12W         0.31164628 W
PL13W         0.00000000 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6128193 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

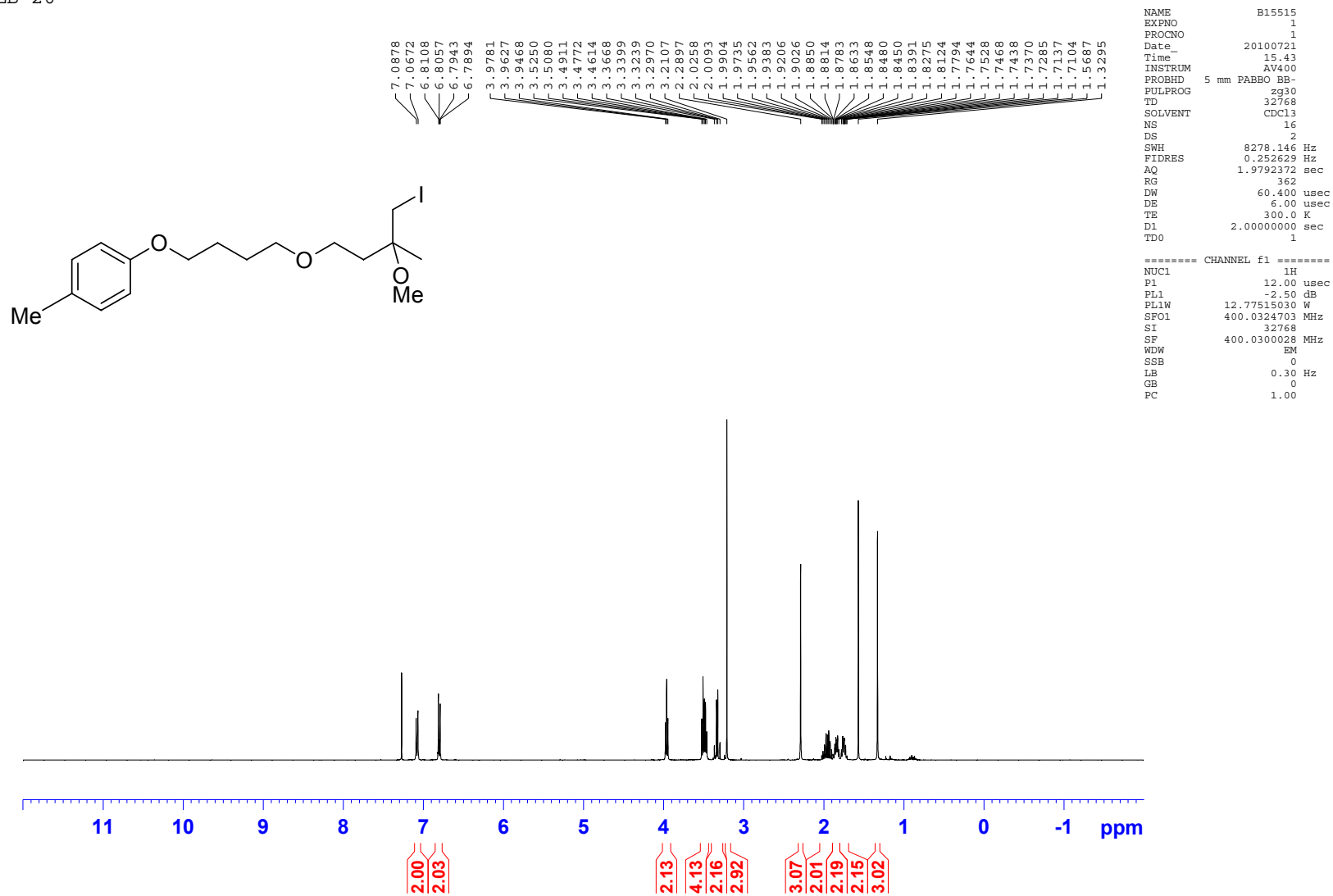
LB18



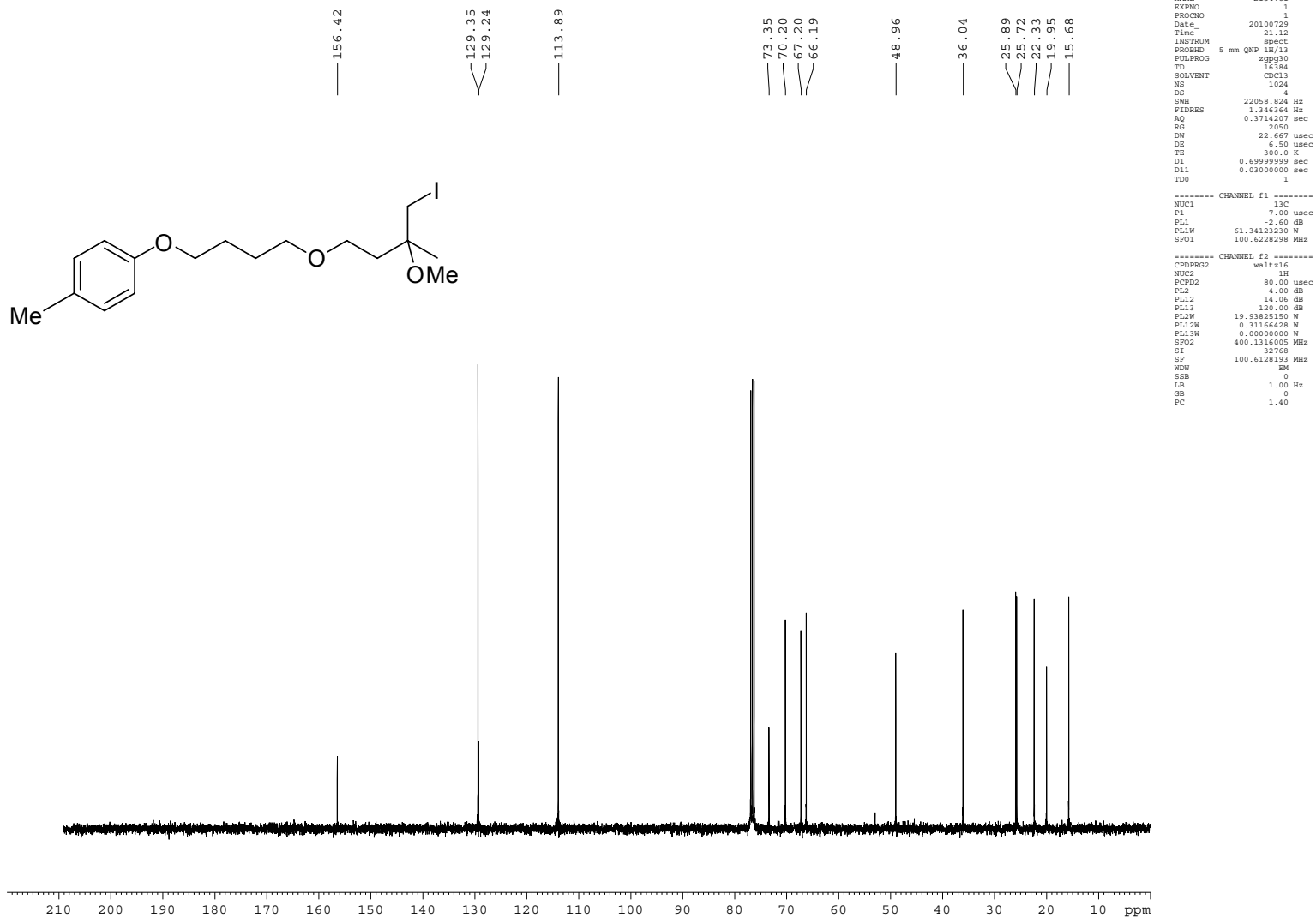
LB18



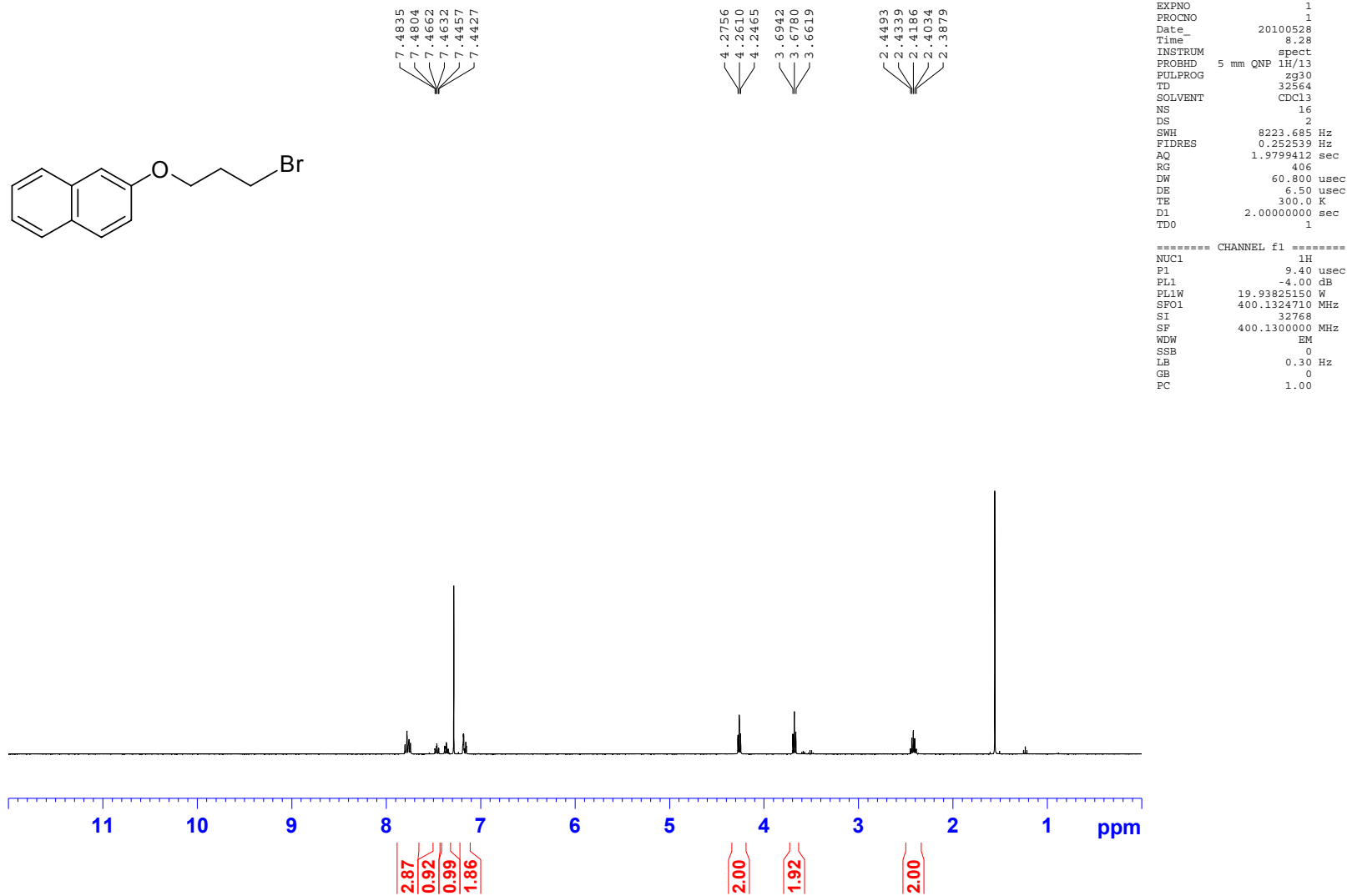
LB-20



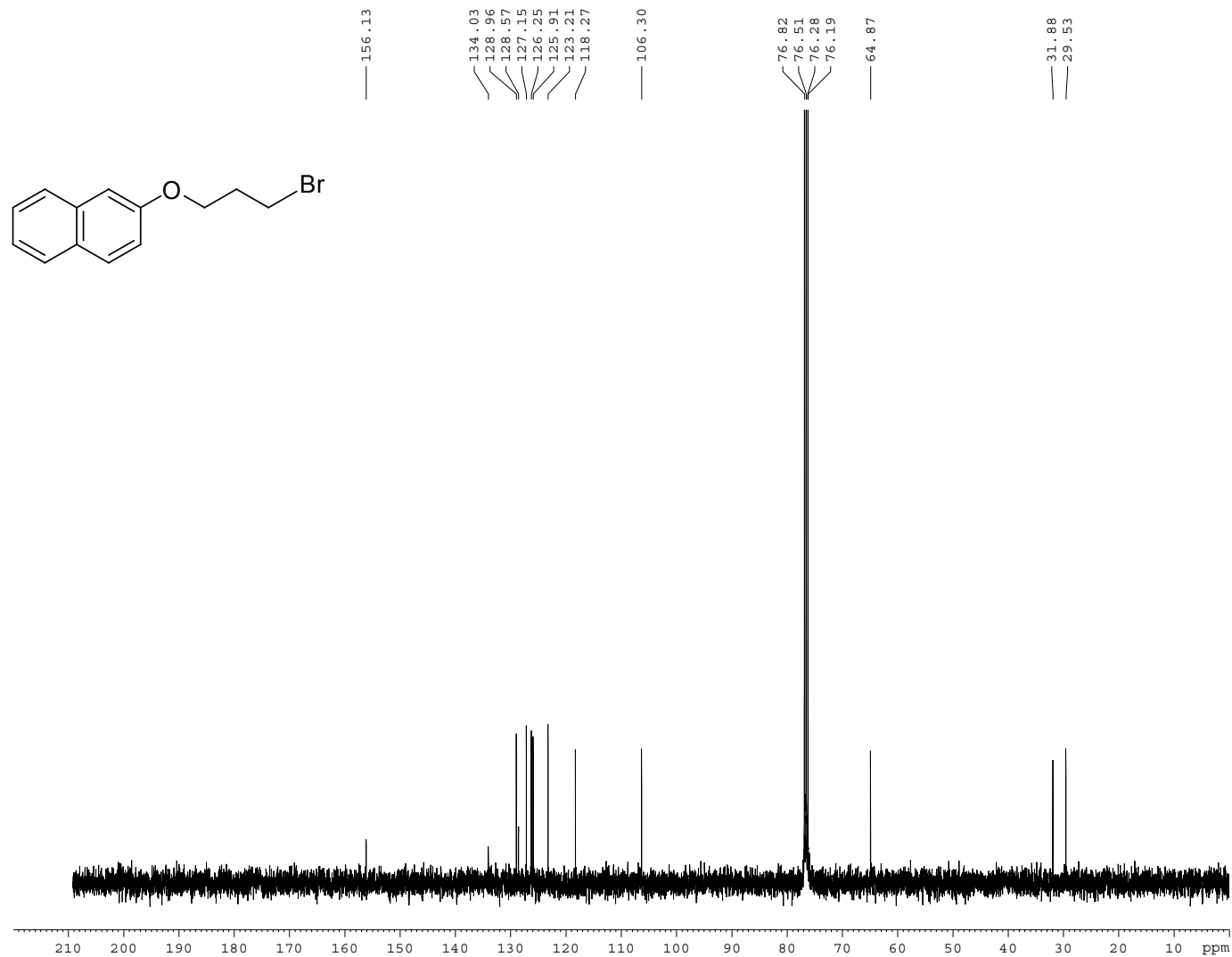
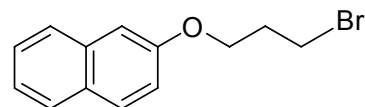
LB-20



LB7



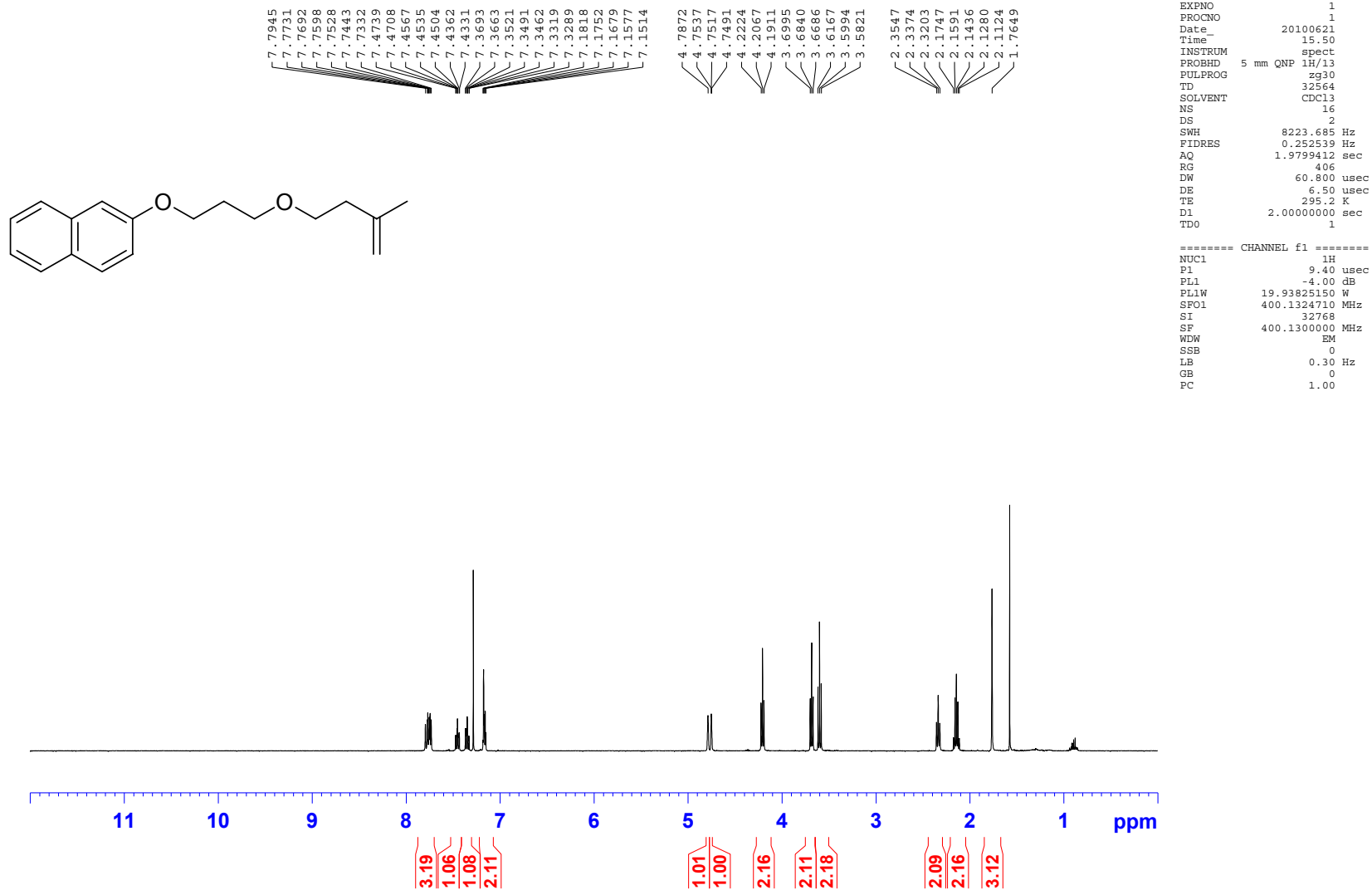
LB7



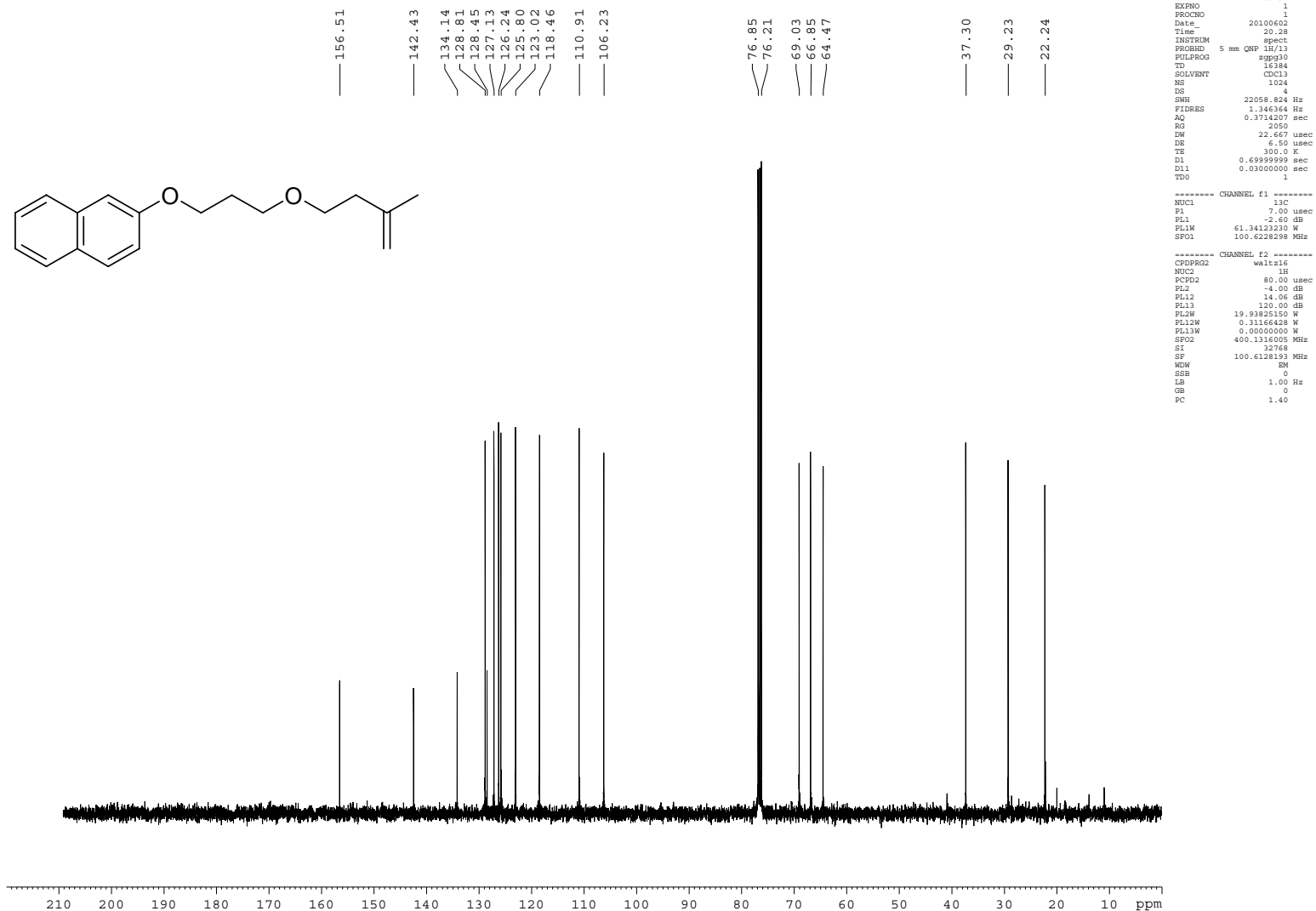
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NAME          D133785
EXPNO         1
PROCNO        1
Data_         20100625
Time          20.56
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            16384
SOLVENT       CDCl3
NS            1024
DS            4
SWH           22058.824 Hz
FIDRES        1.346364 Hz
AQ            0.3714207 sec
RG            2050
DW            22.667 usec
DE            6.50 usec
TE            300.0 K
D1            0.69999999 sec
D11           0.03000000 sec
TDO           1
----- CHANNEL f1 -----
NUC1          13C
P1            7.00 usec
PL1           -2.60 dB
PL1W          61.34123230 W
SFO1          100.628398 MHz
----- CHANNEL f2 -----
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -4.00 dB
PL12          14.06 dB
PL11          120.00 dB
PL2W          19.93825150 W
PL12W         0.31166428 W
PL11W         0.00000000 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6128193 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

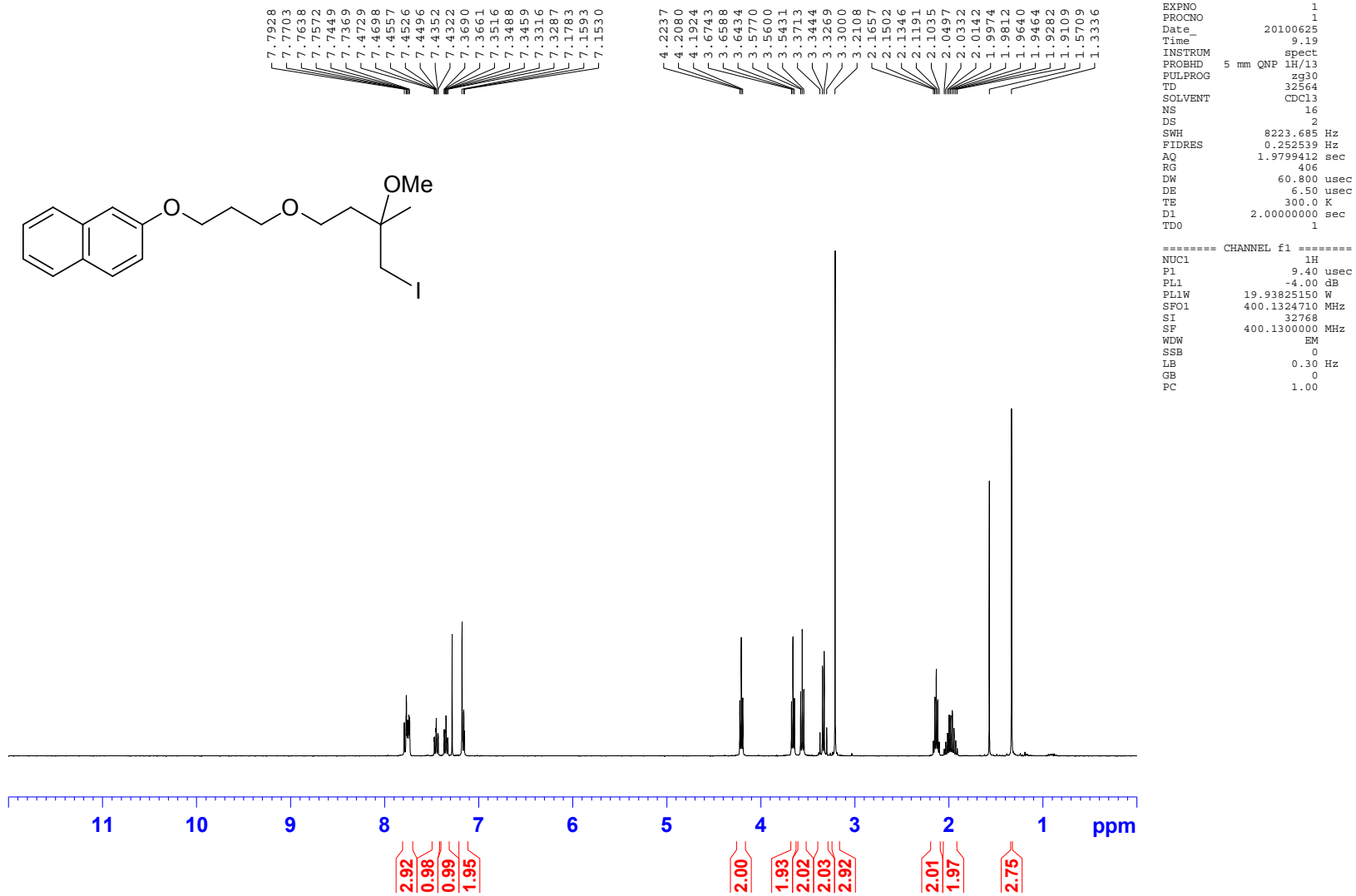
LB5



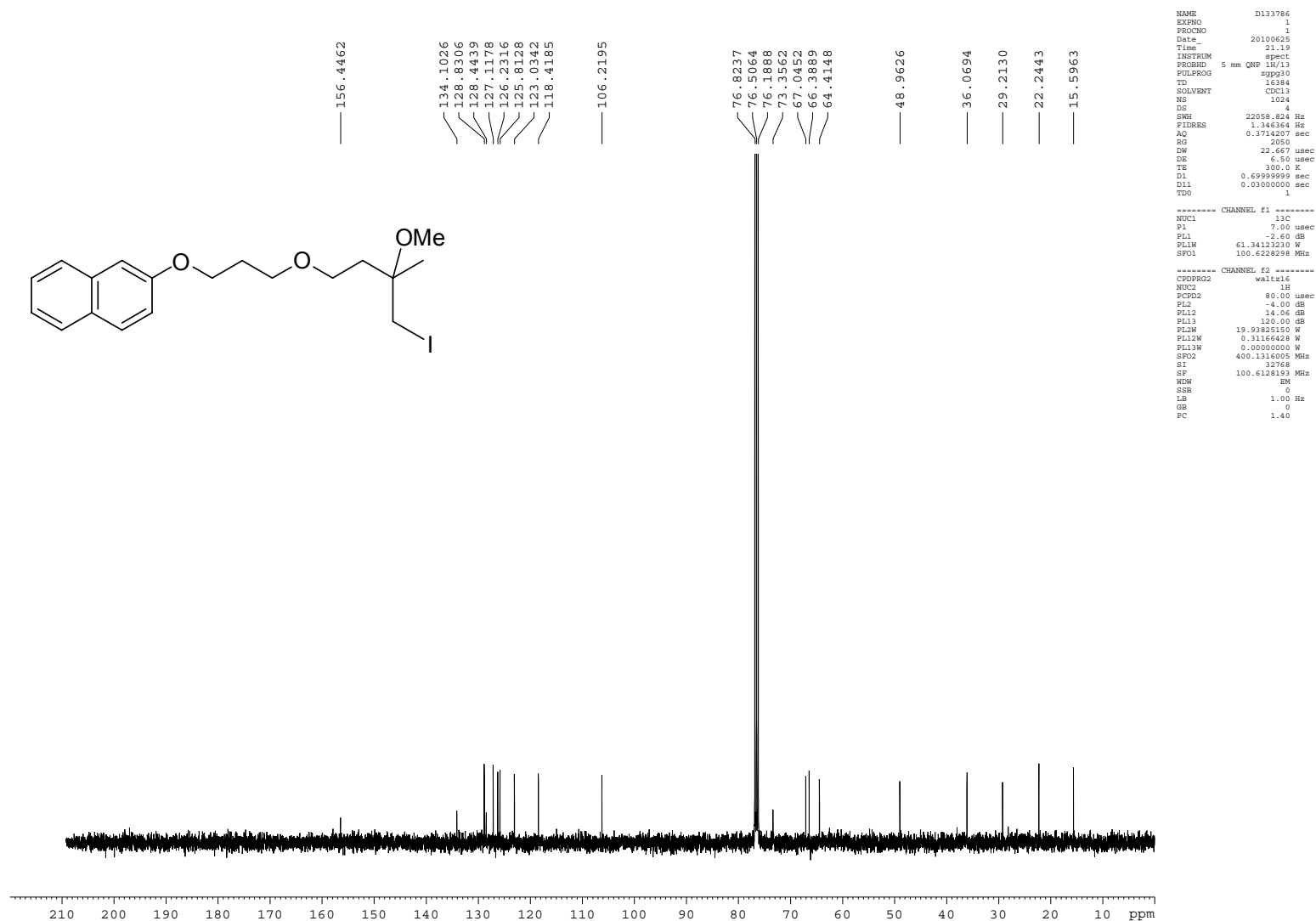
LB-5



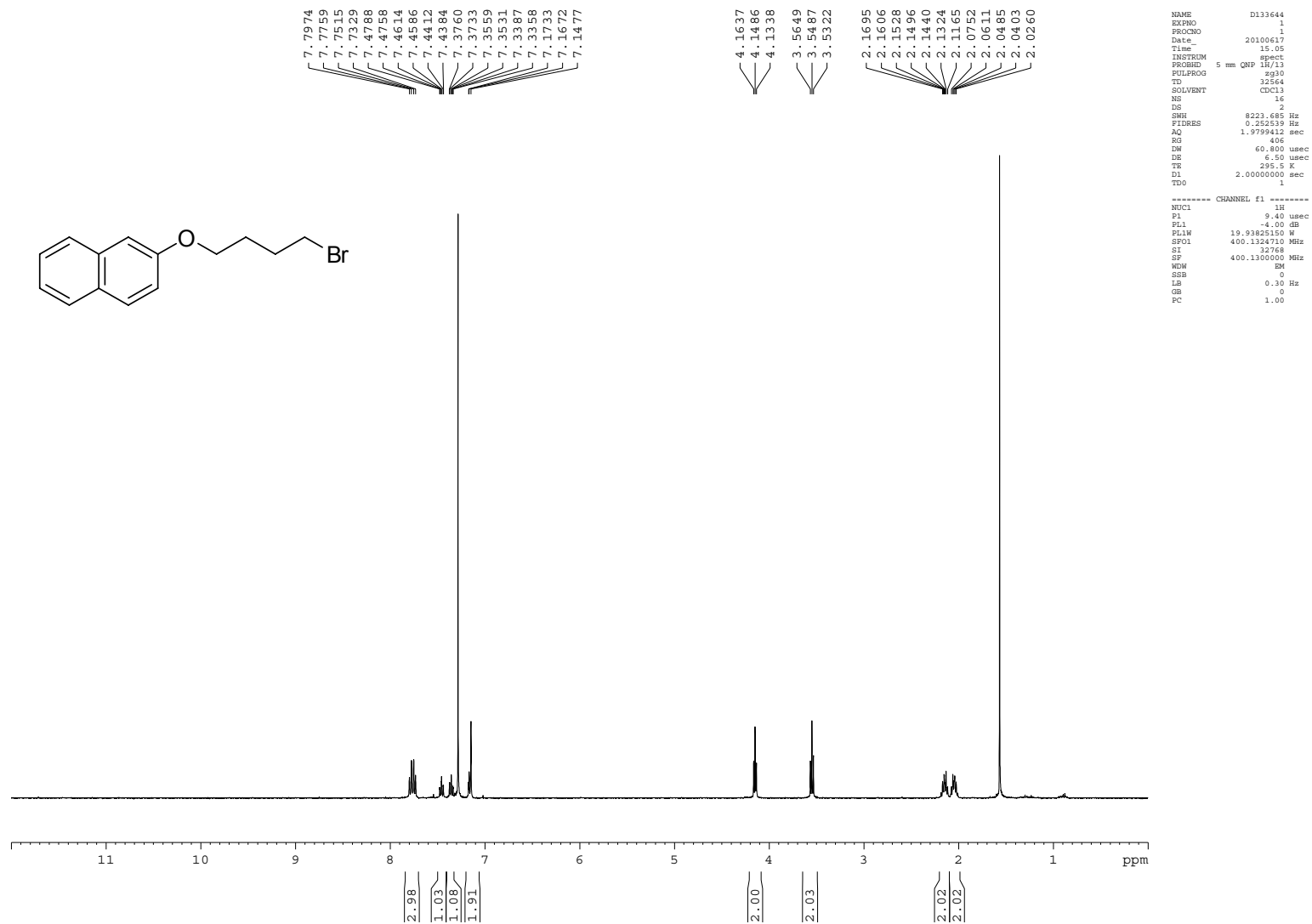
LB13



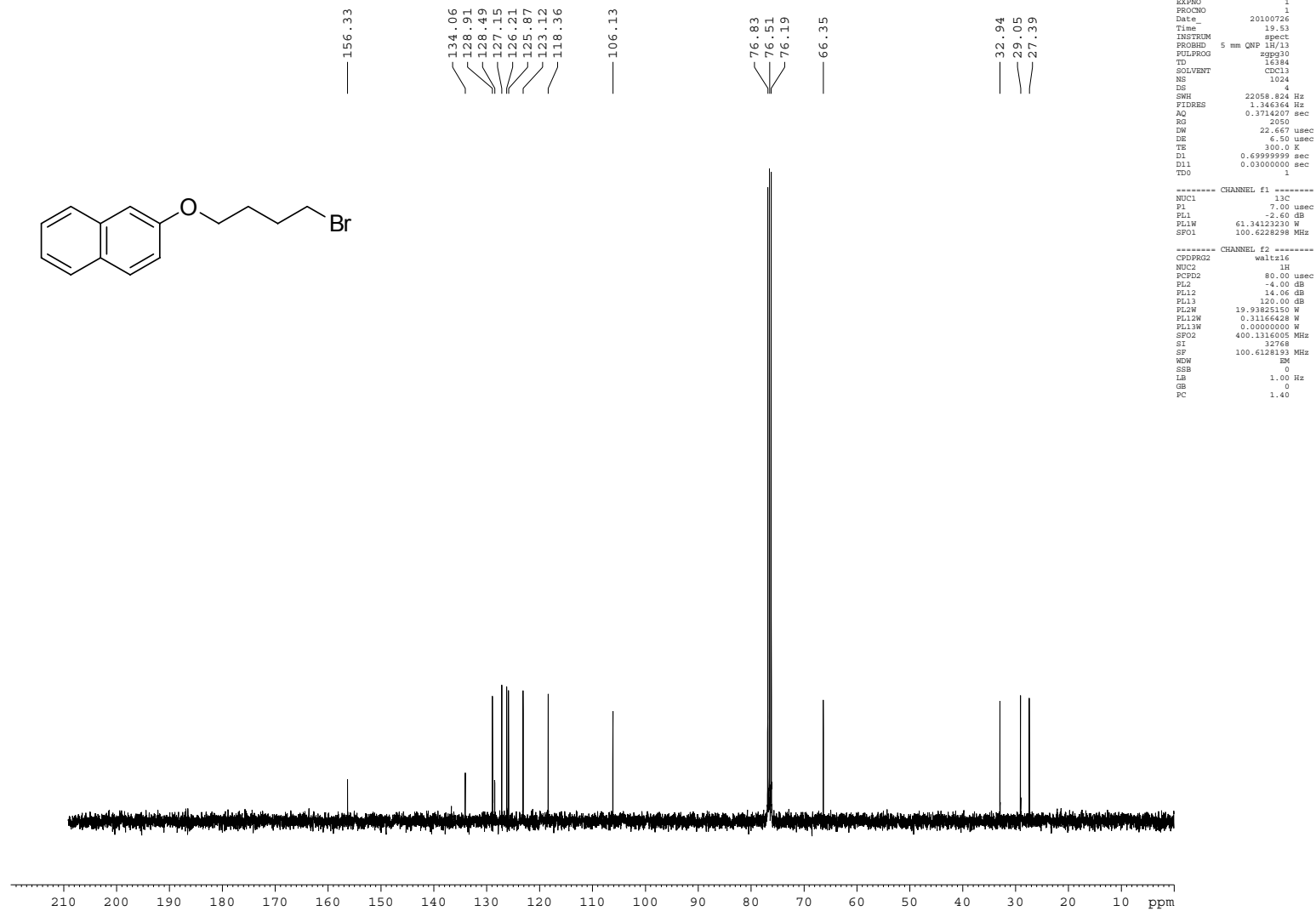
LB13



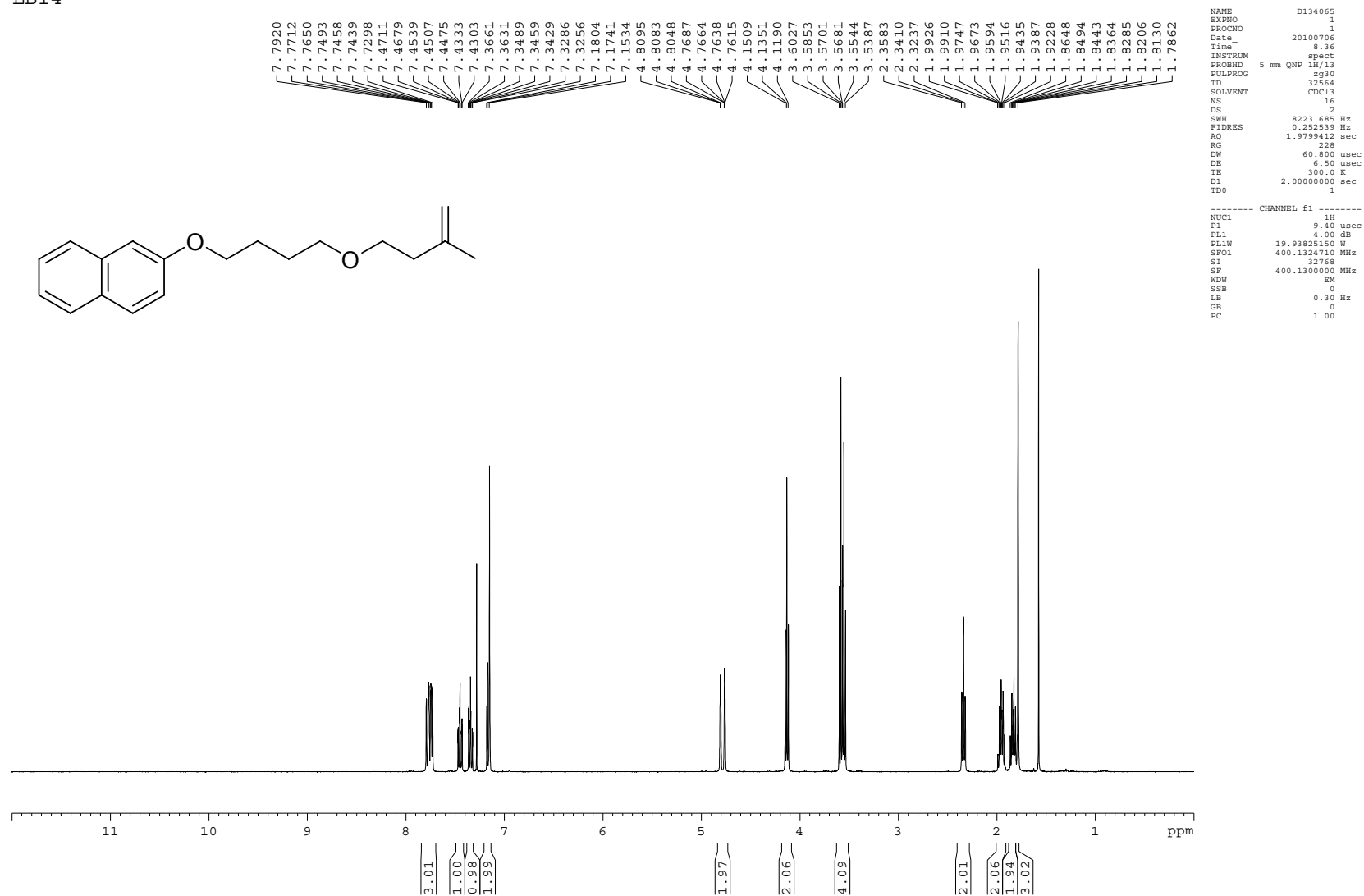
LB3



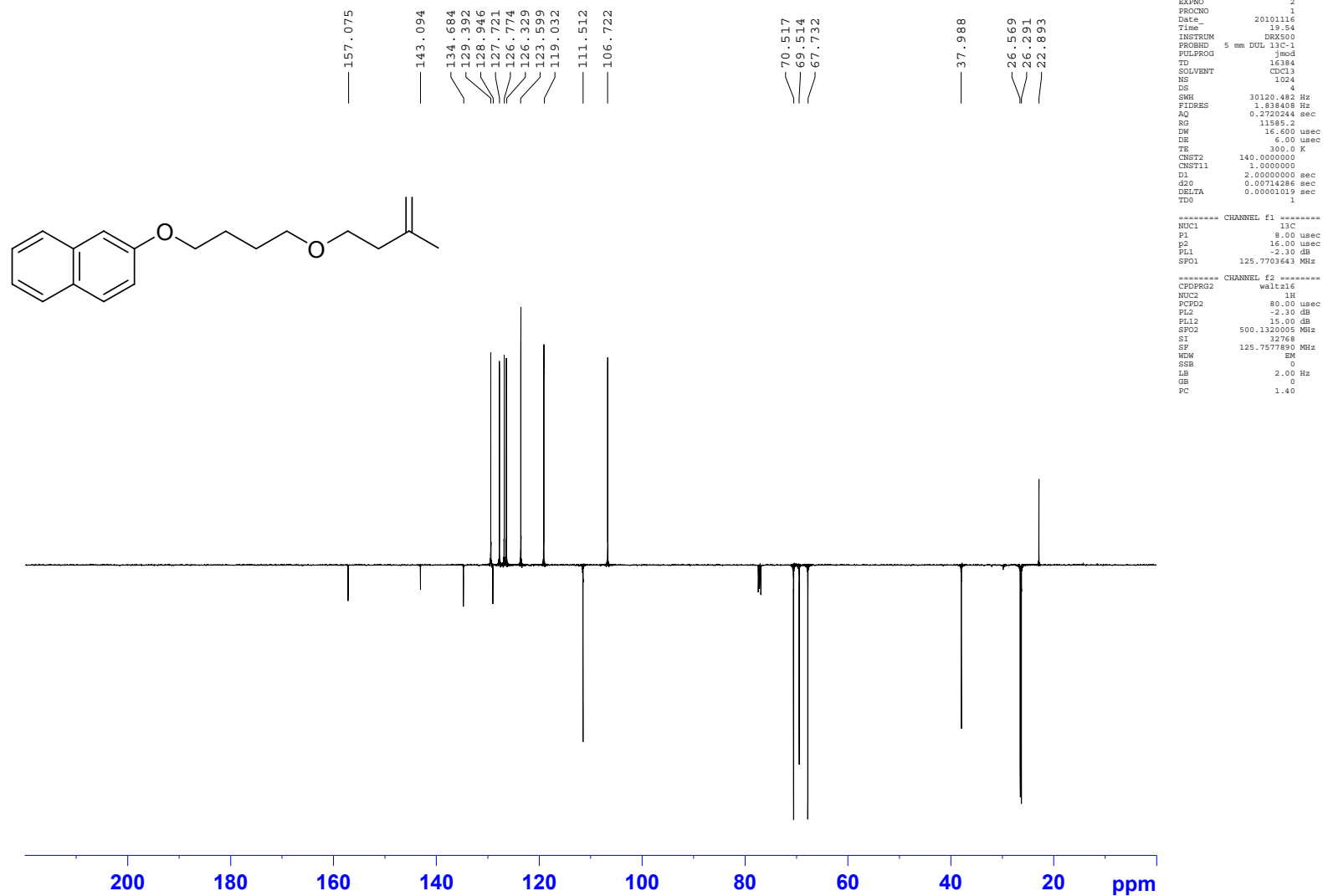
LB-11



LB14



LB14



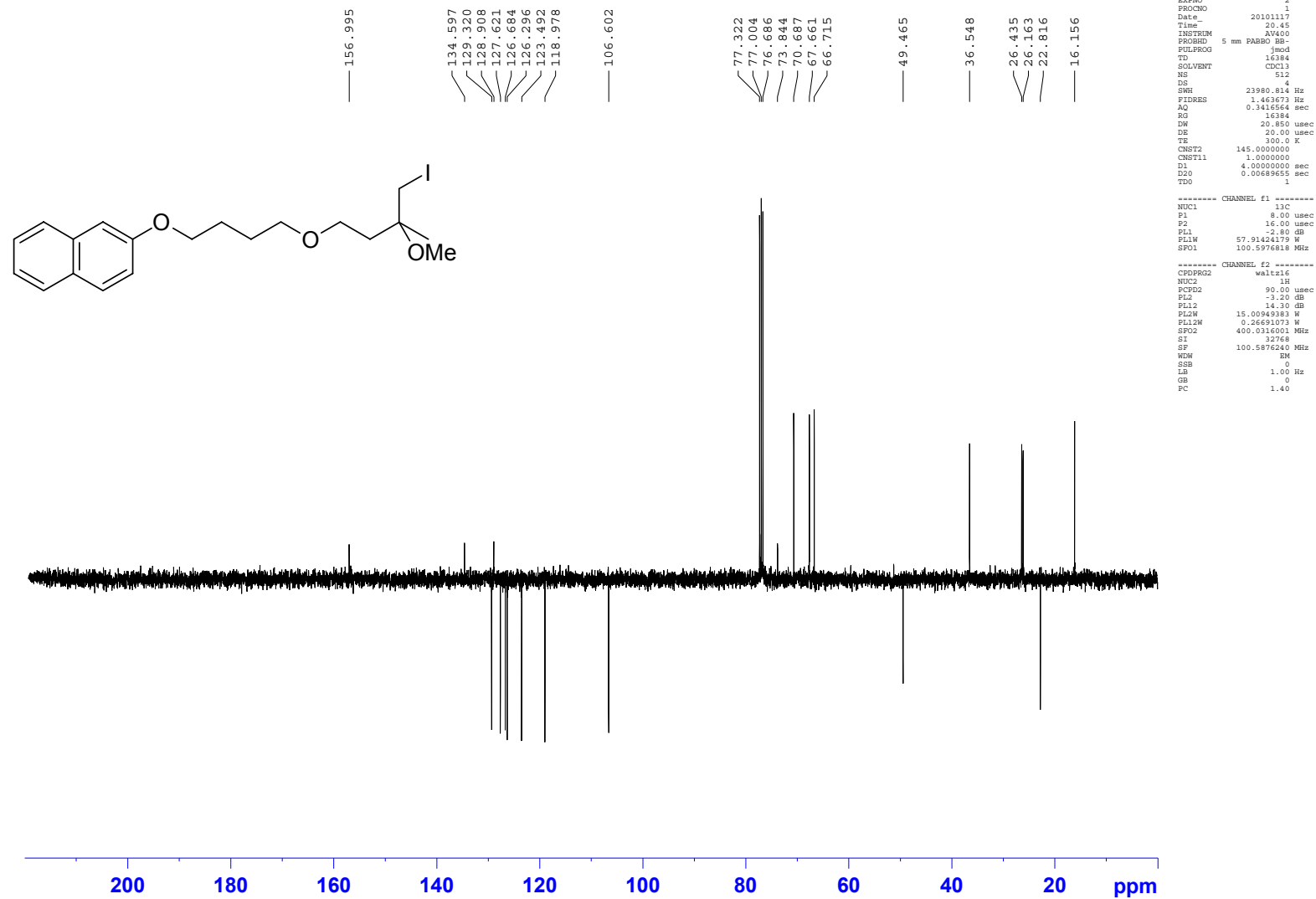
CO[C@H](C)COC(=O)OCC1=CC=CC=C2C=CC=CC=C12

```

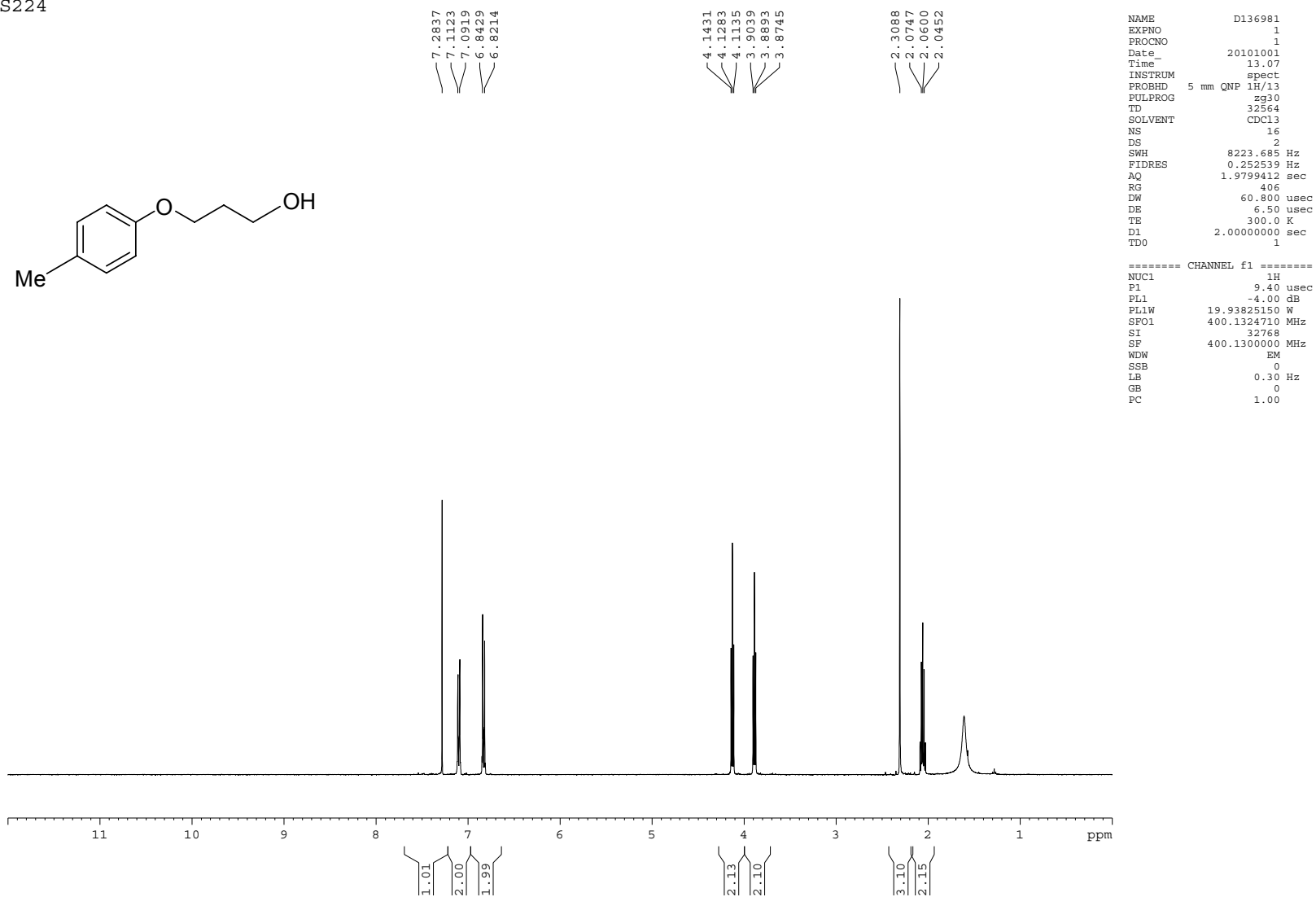
===== CHANNEL f1 =====
NUC1                1H
P1                  9.40 usec
PL1                 -4.00 dB
PL1W                19.93825150 W
SFO1                400.1324710 MHz
SI                  32768
SF                  400.1300000 MHz
WDW                  EM
SSB                  0
LB                   0.30 Hz
GB                   0
PC                   1.00

```

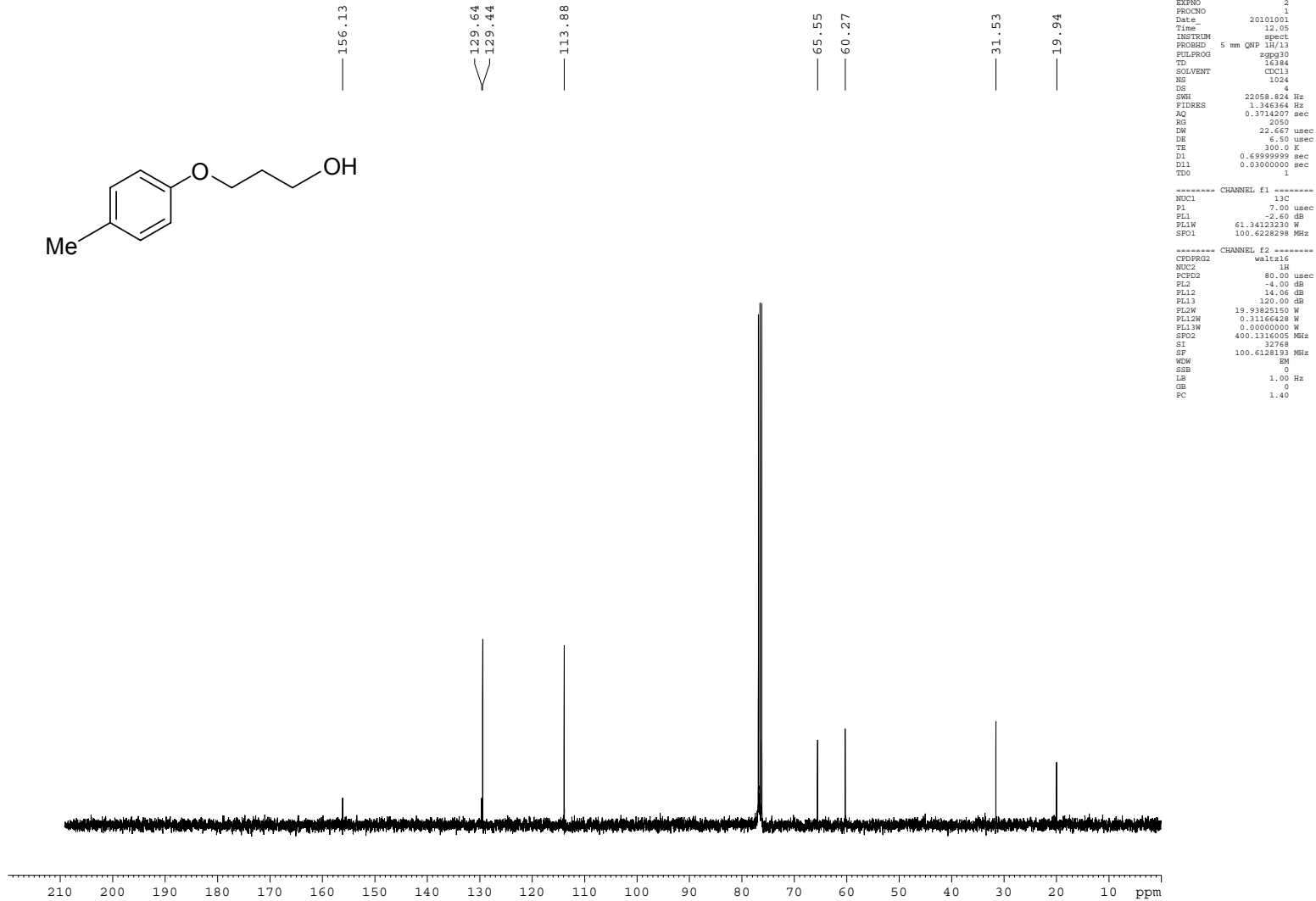
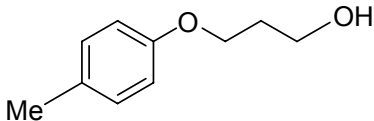
LB17



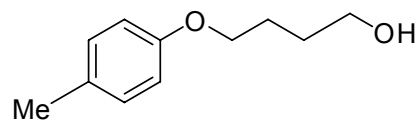
RS224



RS224



RS218



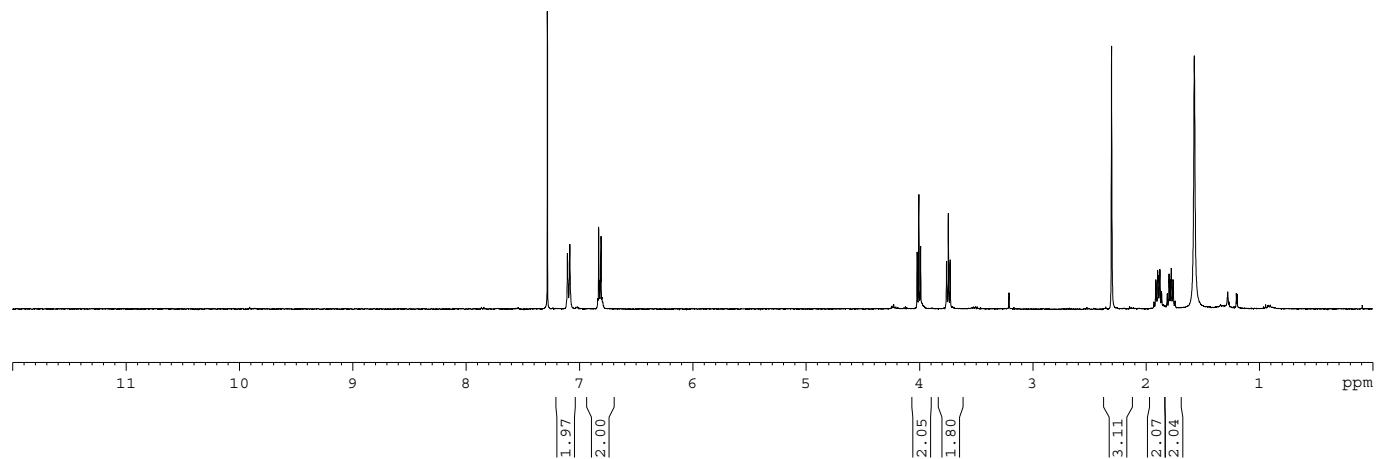
7.1067
7.0858
6.8316
6.8265
6.8153
6.8102

4.0212
4.0060
3.9906
3.7616
3.7458
3.7302

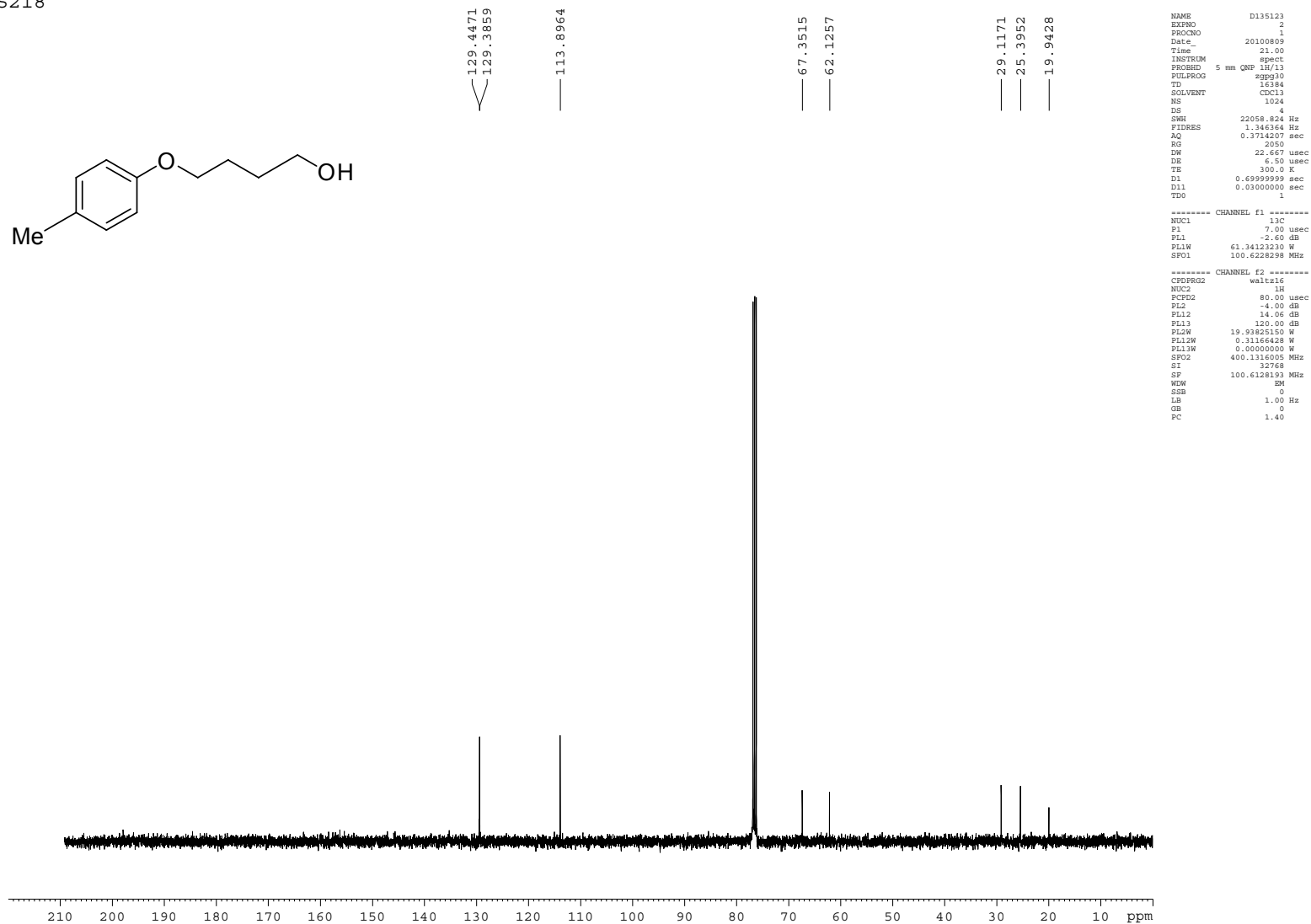
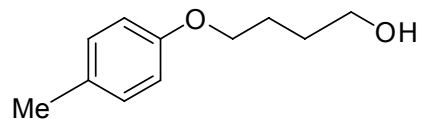
2.3056
1.9144
1.8989
1.8933
1.8788
1.7986
1.7844
1.7790
1.7633

```
NAME          D136736
EXPNO         1
PROCNO        1
Date_         20100923
Time_         18.25
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zg30
TD            32564
SOLVENT       CDCl3
NS            16
DS            2
SWH           8223.685 Hz
FIDRES        0.252539 Hz
AQ            1.9799412 sec
RG            406
DW            60.800 usec
DE            6.50 usec
TE            300.0 K
D1            2.00000000 sec
TD0           1
```

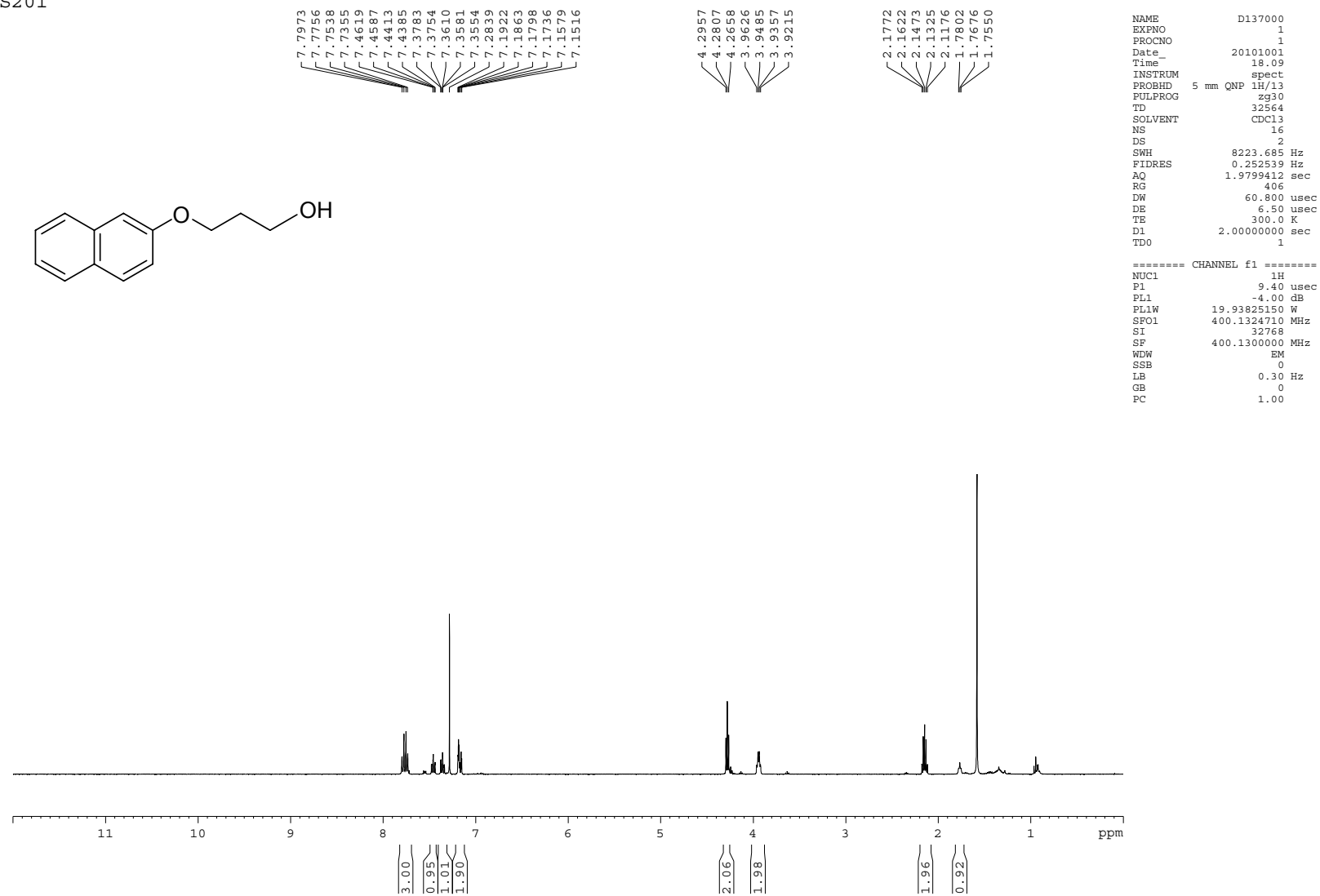
```
===== CHANNEL f1 =====
NUC1          1H
P1            9.40 usec
PL1           -4.00 dB
PL1W          19.93825150 W
SFO1          400.1324710 MHz
SI            32768
SF            400.1300000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```



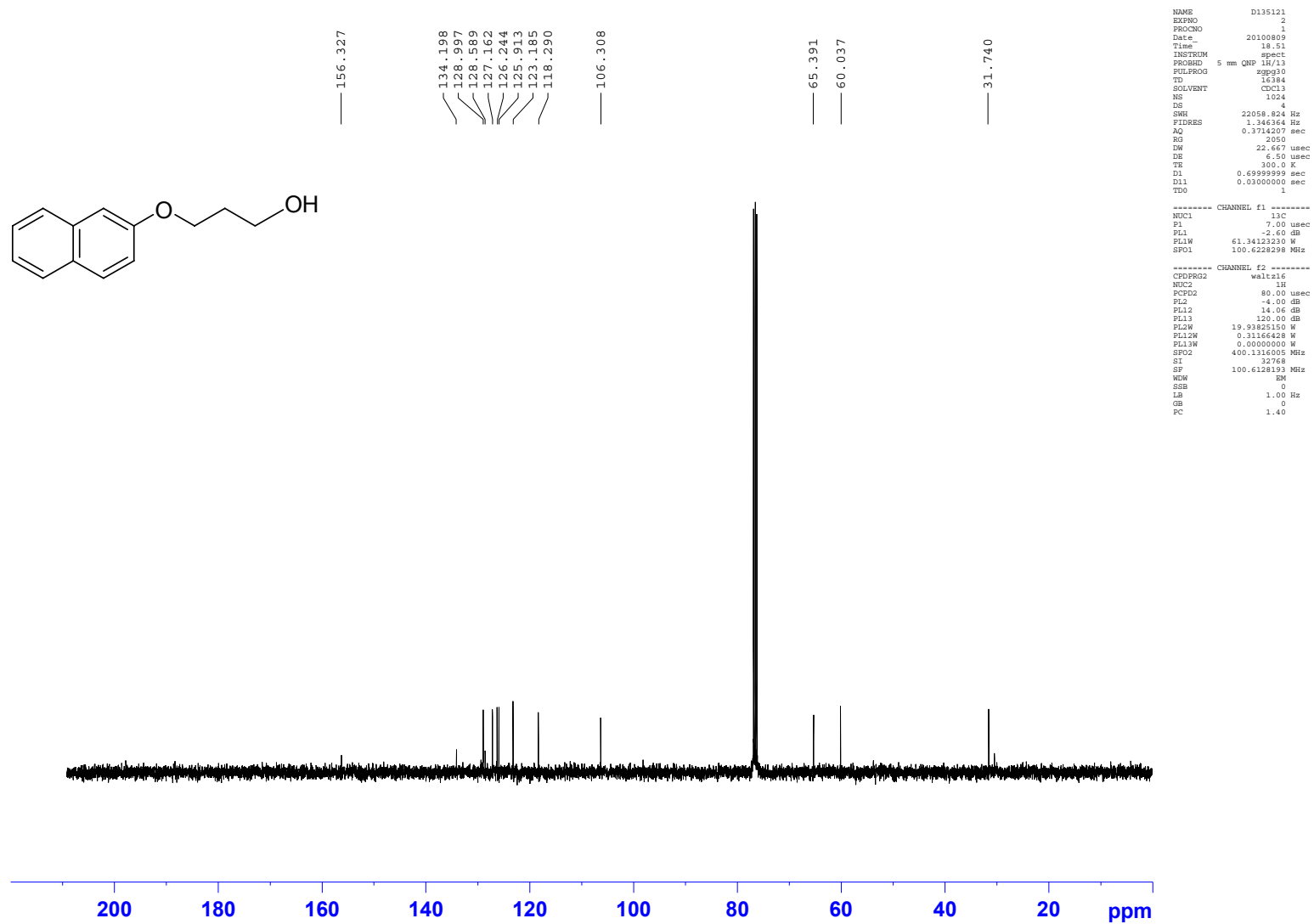
RS218



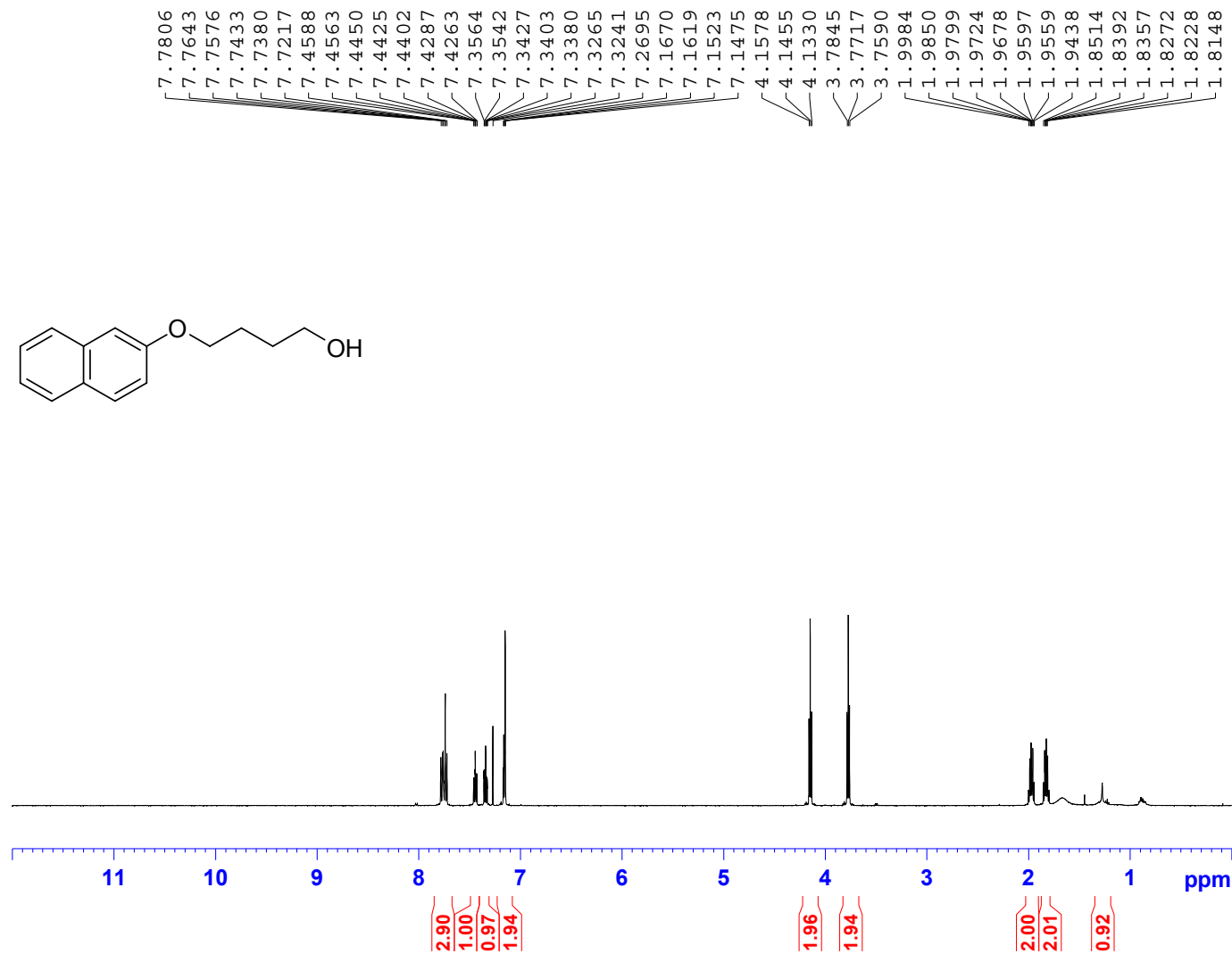
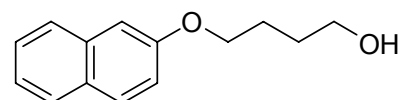
RS201



RS201



RS213

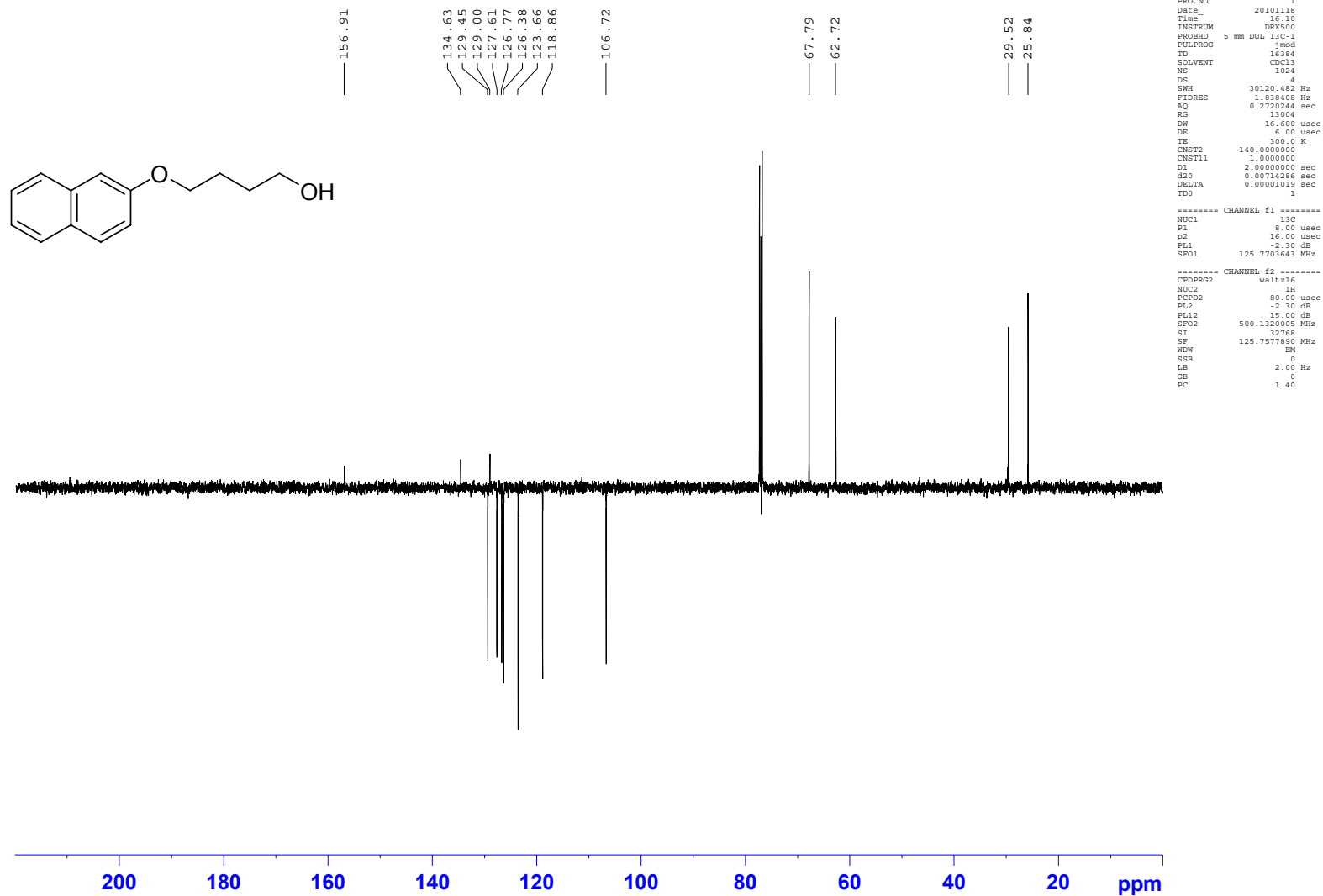


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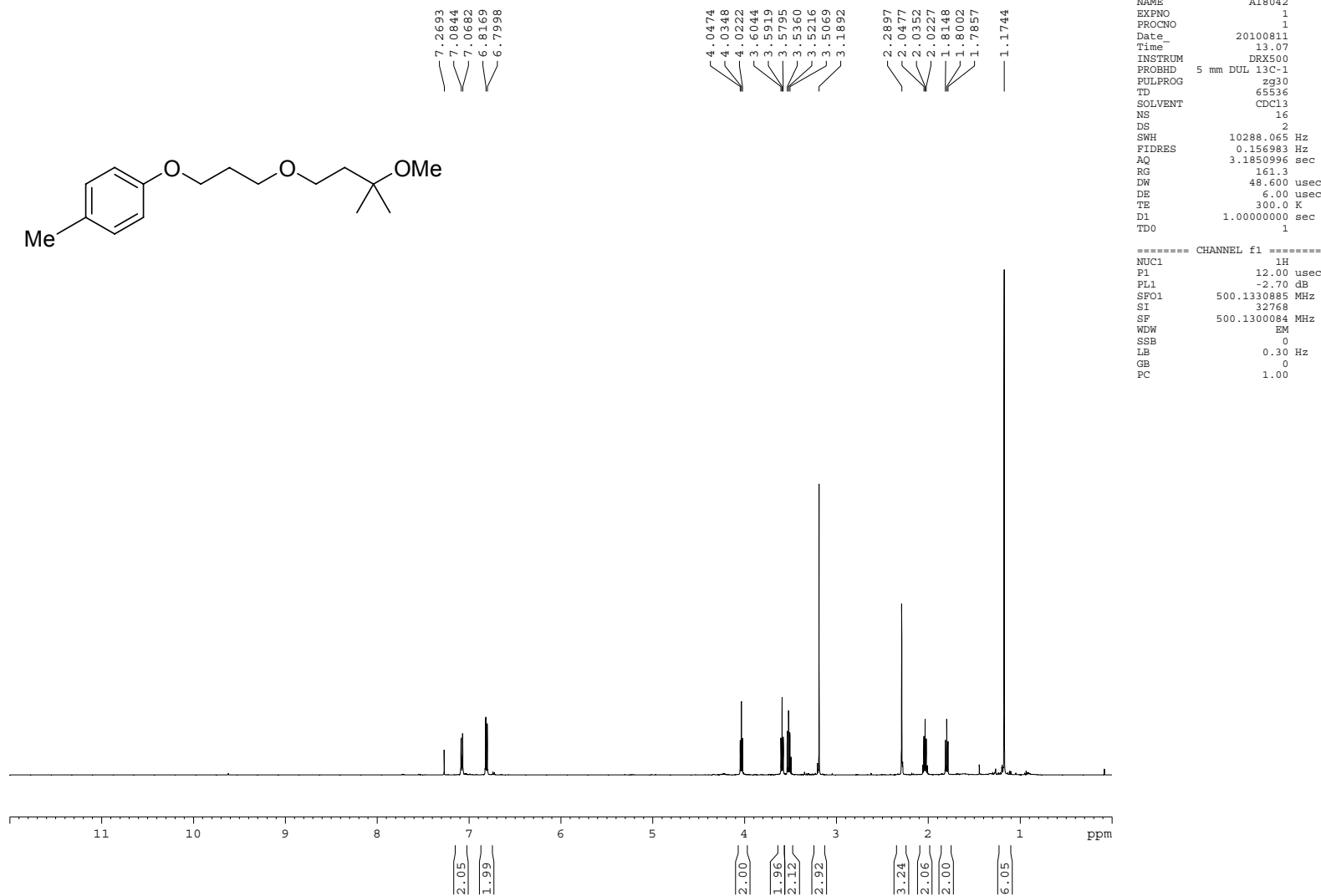
NAME           A19626
EXPNO          1
PROCNO         1
Date_          20101118
Time_          15.30
INSTRUM        DRX500
PROBHD         5 mm DUL 13C-1
PULPROG        zg30
TD             65536
SOLVENT        CDCl3
NS             16
DS             2
SWH            10288.065 Hz
FIDRES         0.156983 Hz
AQ            3.1850996 sec
RG            574.7
DW            48.600 usec
DE            6.00 usec
TE            300.0 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1           1H
P1            12.00 usec
PL1           -2.70 dB
SFO1          500.1330885 MHz
SI            32768
SF            500.1300084 MHz
WDW            EM
SSB            0
LB            0.30 Hz
GB            0
PC            1.00
    
```

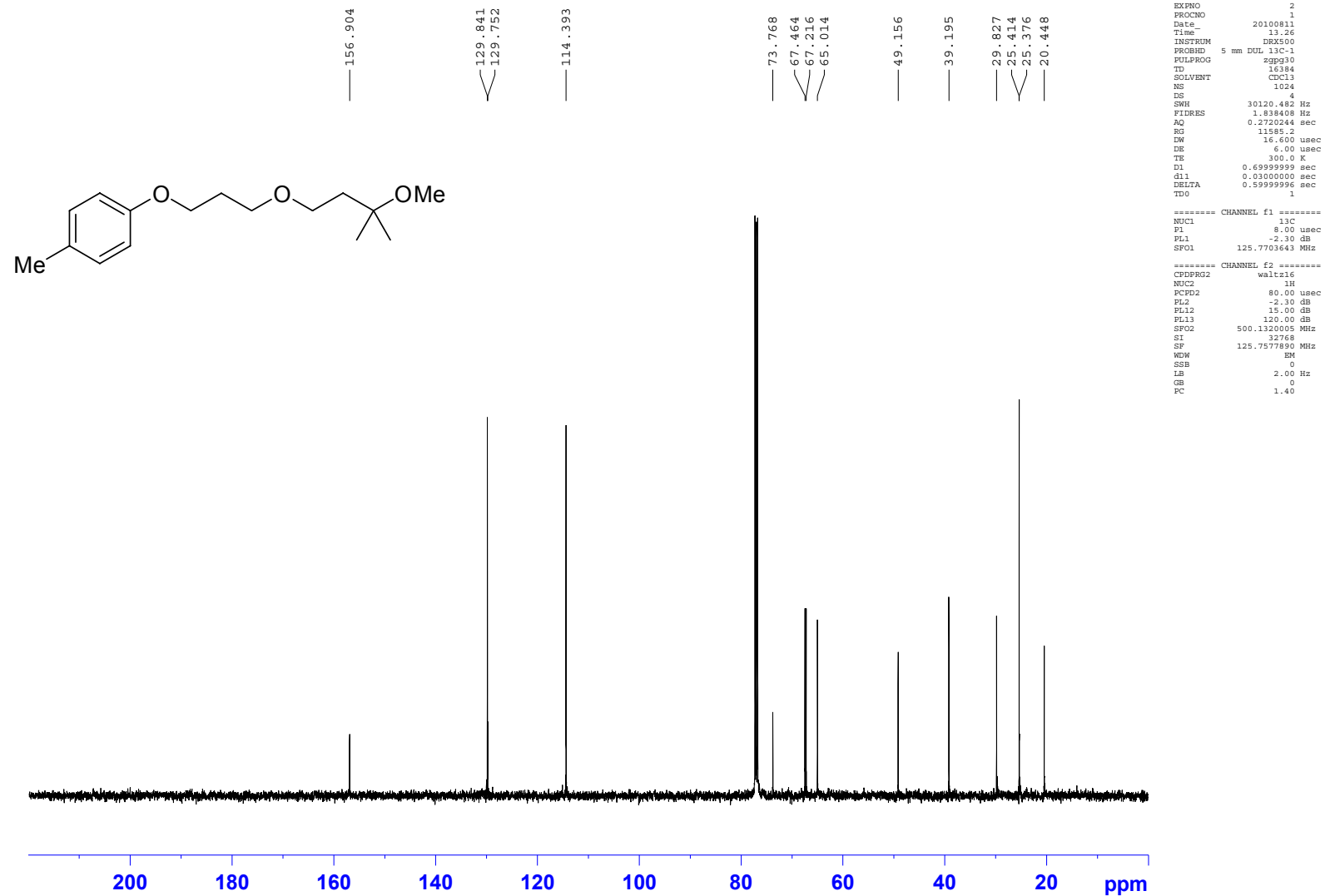
RS213



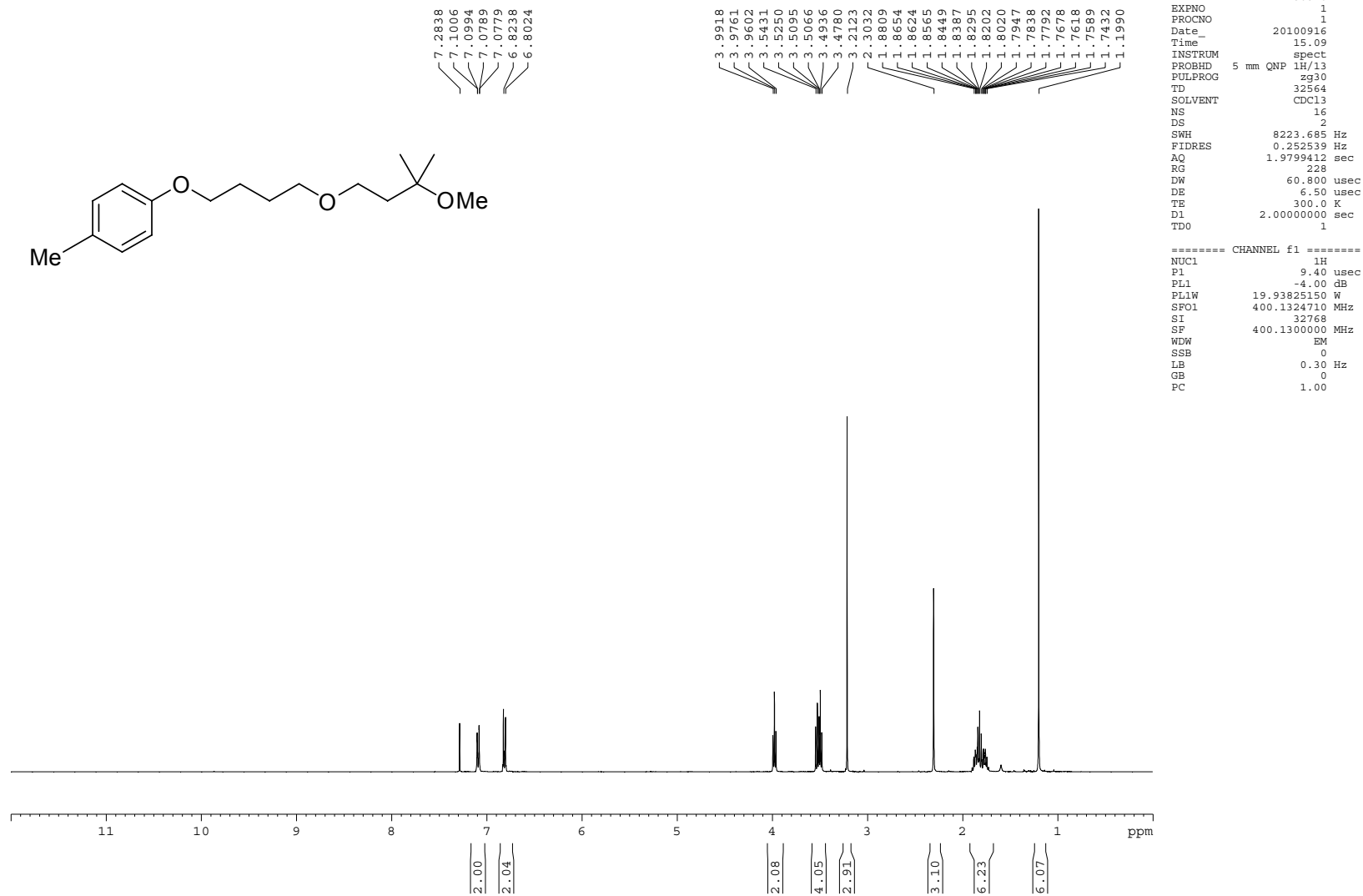
RS231



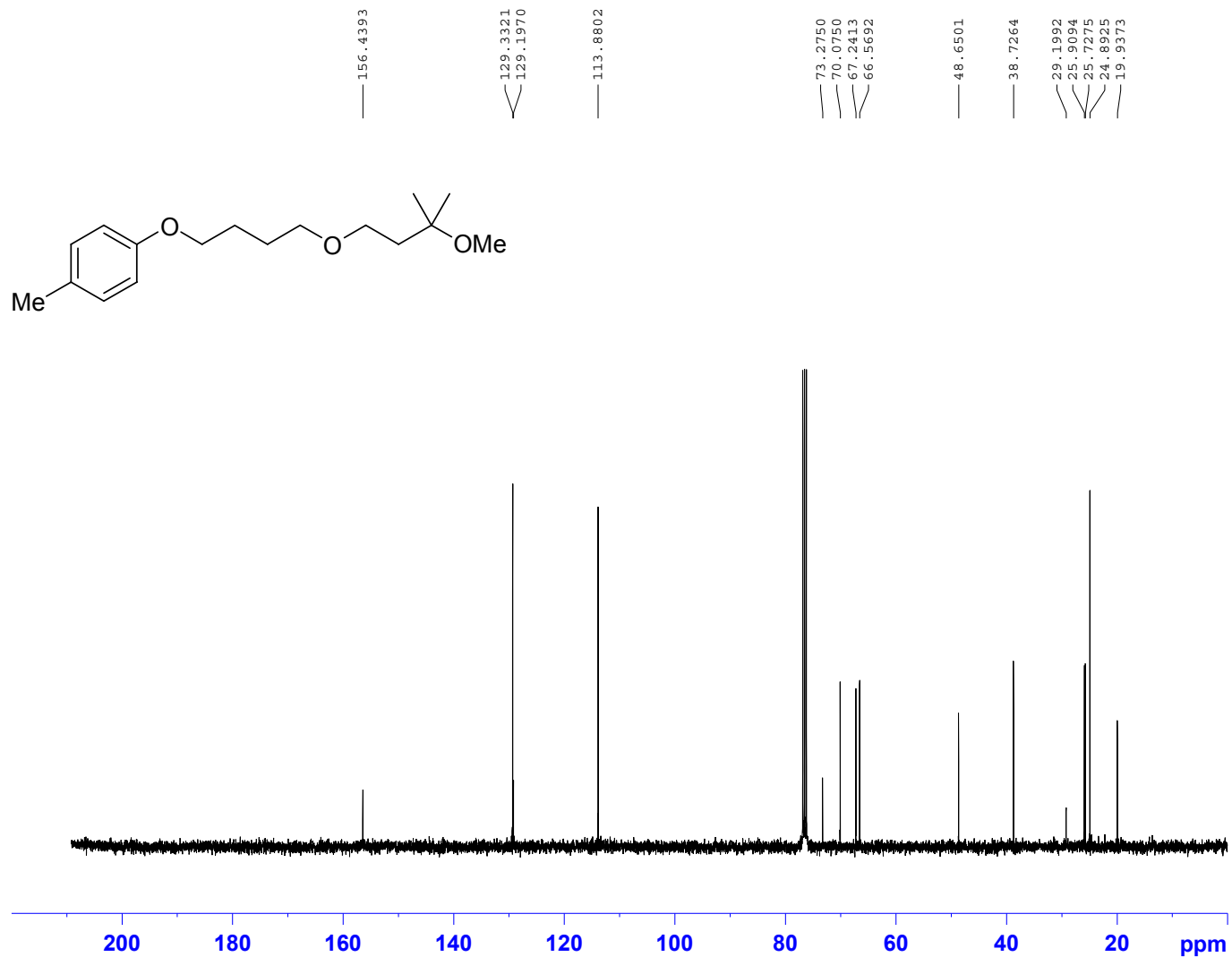
RS231 Fraction 1



RS241



RS230 F1



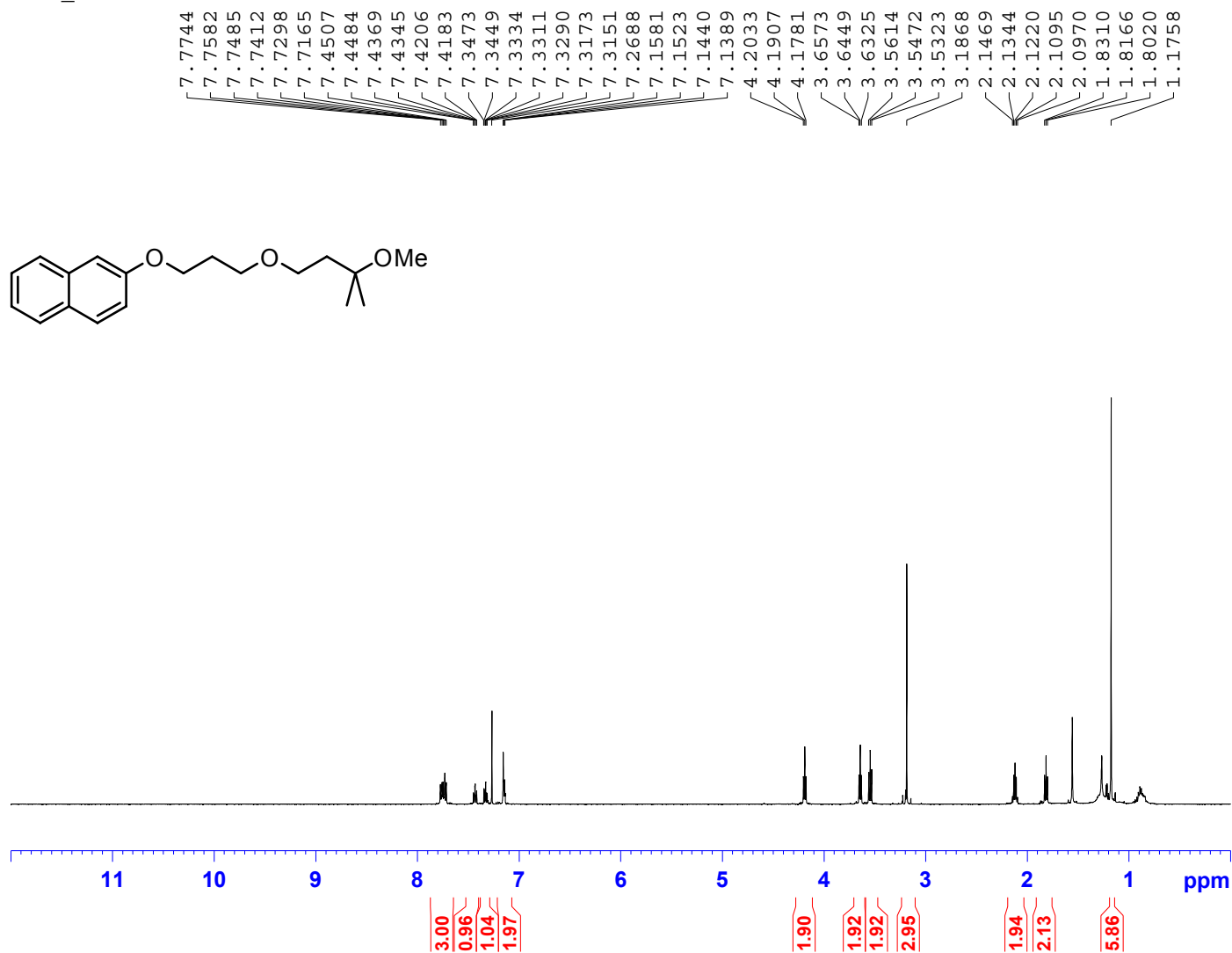
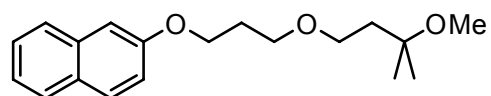
```

NAME          DI35122
EXPNO         2
PROCNO        1
Date_         20100809
Time          19.15
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            16384
SOLVENT       CDCl3
NS            1024
DS            4
SHE          22058.824 Hz
FIDRES        1.346364 Hz
AQ            0.3714207 sec
RG            2050
DW            22.667 usec
DE            6.50 usec
TE            300.0 K
D1            0.69999999 sec
D11           0.03000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1           13C
P1             7.00 usec
PL1            -2.60 dB
PL1W          61.34123230 W
SFO1          100.6228298 MHz

===== CHANNEL f2 =====
CFOPRG2       waltz16
NUC2           1H
PCPD2         80.00 usec
PL2            -4.00 dB
PL12          14.06 dB
PL13          120.00 dB
PLW          19.93825150 W
PL12W         0.31166428 W
PL13W         0.00000000 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6128193 MHz
WDW           EM
SSB            0
LB            1.00 Hz
GB            0
PC            1.40
    
```

RS232_F1

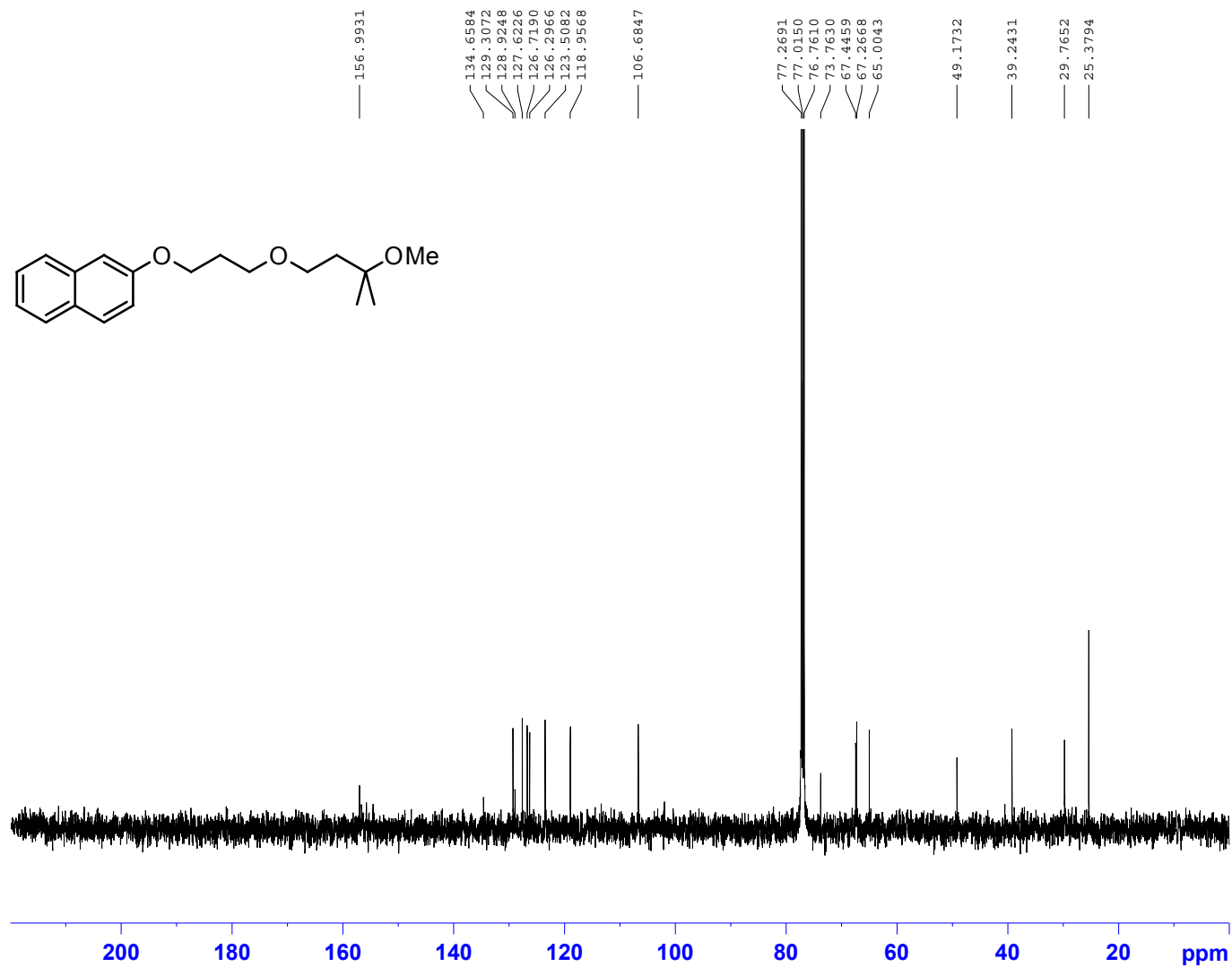


```

NAME          A20014
EXPNO         1
PROCNO        1
Date_         20101213
Time          15.27
INSTRUM       DEX500
PROBHD        5 mm DUL 13C-1
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           10288.065 Hz
FIDRES        0.156983 Hz
AQ            3.1850996 sec
RG            724.1
DW            48.600 usec
DE            6.00 usec
TE            300.0 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1           1H
P1            12.00 usec
PL1           -2.70 dB
SFO1          500.1330885 MHz
SI            32768
SF            500.1300084 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```

RS232_F1



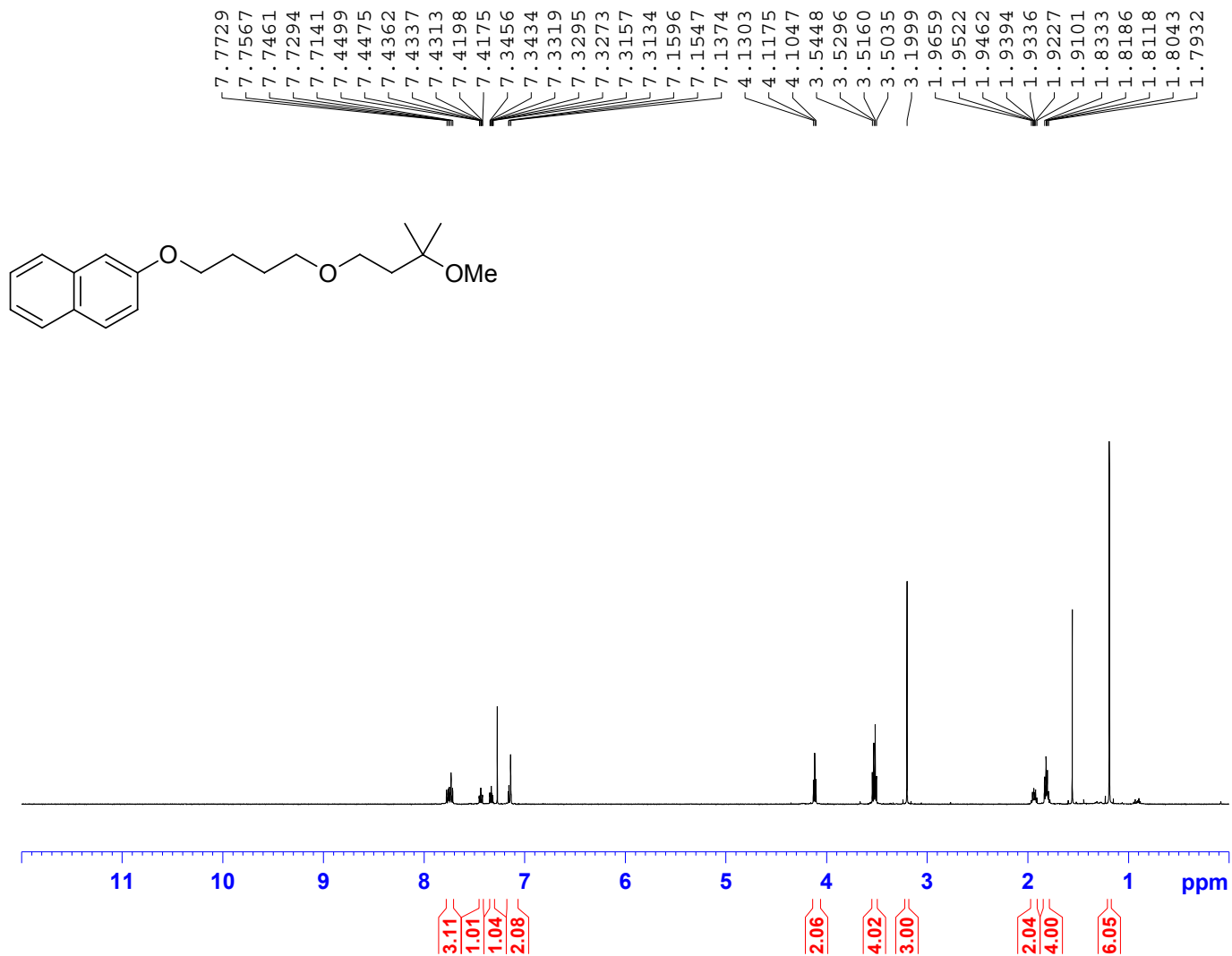
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NAME          A20014
EXPNO         2
PROCNO        1
Date_         20101213
Time          15.46
INSTRUM       DRX500
PROBHD        5 mm DUL 13C-1
PULPROG       zgpg30
TD            16384
SOLVENT       CDCl3
NS            1024
DS            4
SWH           30120.482 Hz
FIDRES        1.838408 Hz
AQ            0.2720244 sec
RG            8192
DM            16.600 usec
DE            6.00 usec
TE            300.0 K
D1            0.69999999 sec
d11           0.03000000 sec
DELTA         0.59999996 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            8.00 usec
PL1           -2.30 dB
SFO1          125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -2.30 dB
PL12          15.00 dB
PL13          120.00 dB
SFO2          500.1320005 MHz
SI            32768
SF            125.7577890 MHz
WDW           EM
SSB           0
LB            2.00 Hz
GB            0
PC            1.40
  
```

RS217 Fraction 1

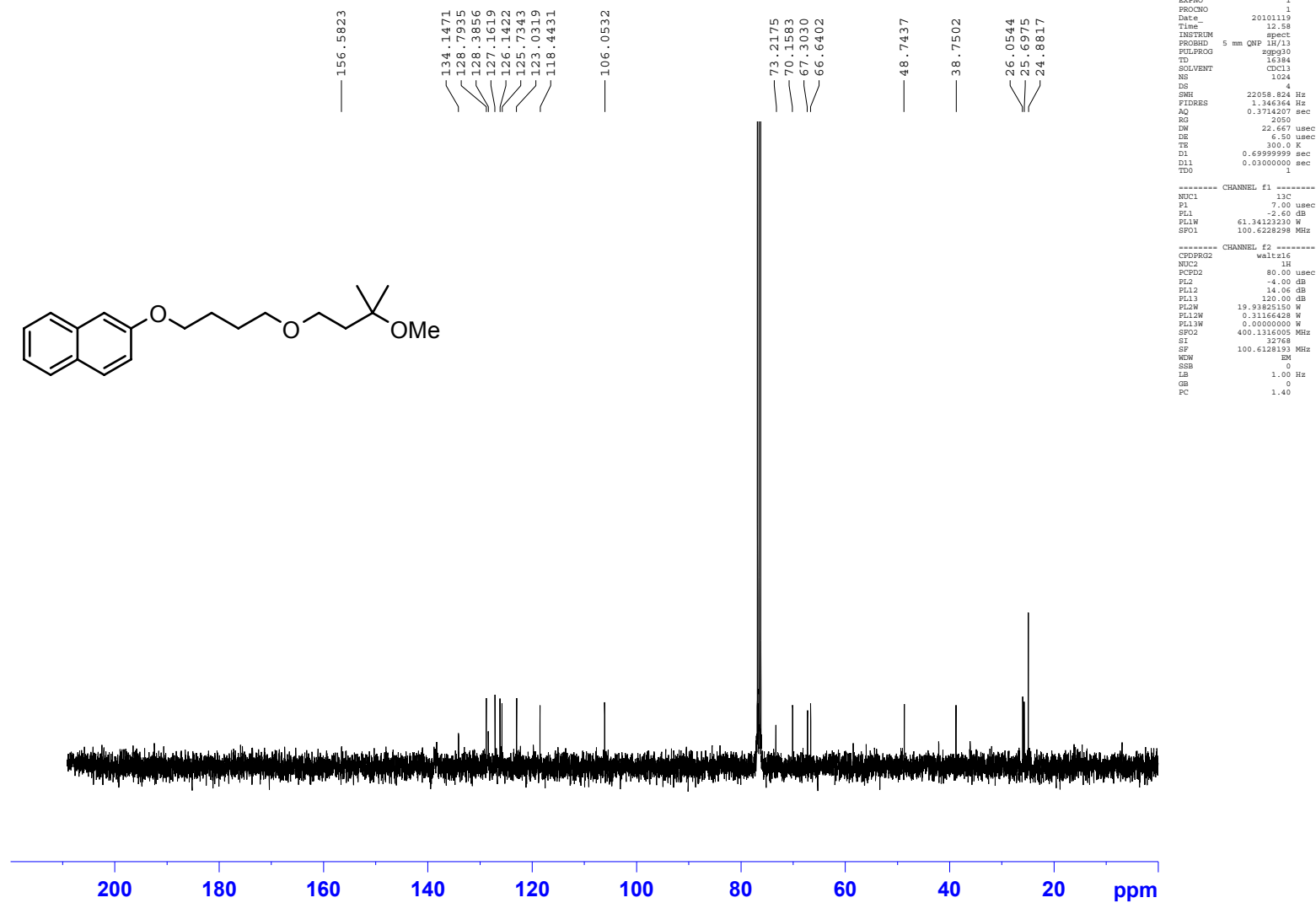


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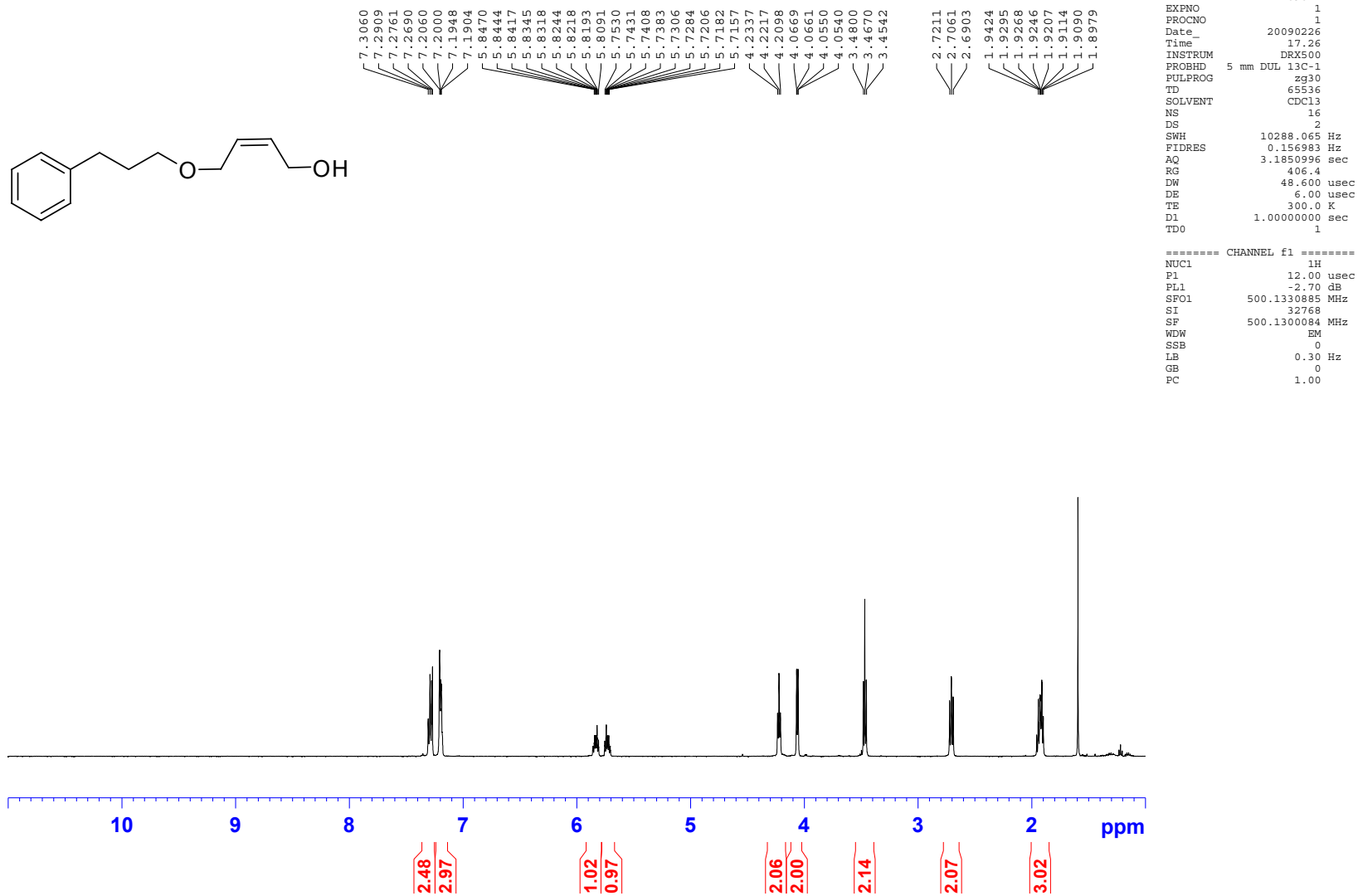
NAME          Al9653
EXPNO         1
PROCNO        1
Date_         20101119
Time          12.01
INSTRUM       DRX500
PROBHD        5 mm DUL 13C-1
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           10288.065 Hz
FIDRES        0.156983 Hz
AQ            3.1850996 sec
RG            912.3
DW            48.600 usec
DE            6.00 usec
TE            300.0 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            12.00 usec
PL1           -2.70 dB
SFO1          500.1330885 MHz
SI            32768
SF            500.1300084 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```

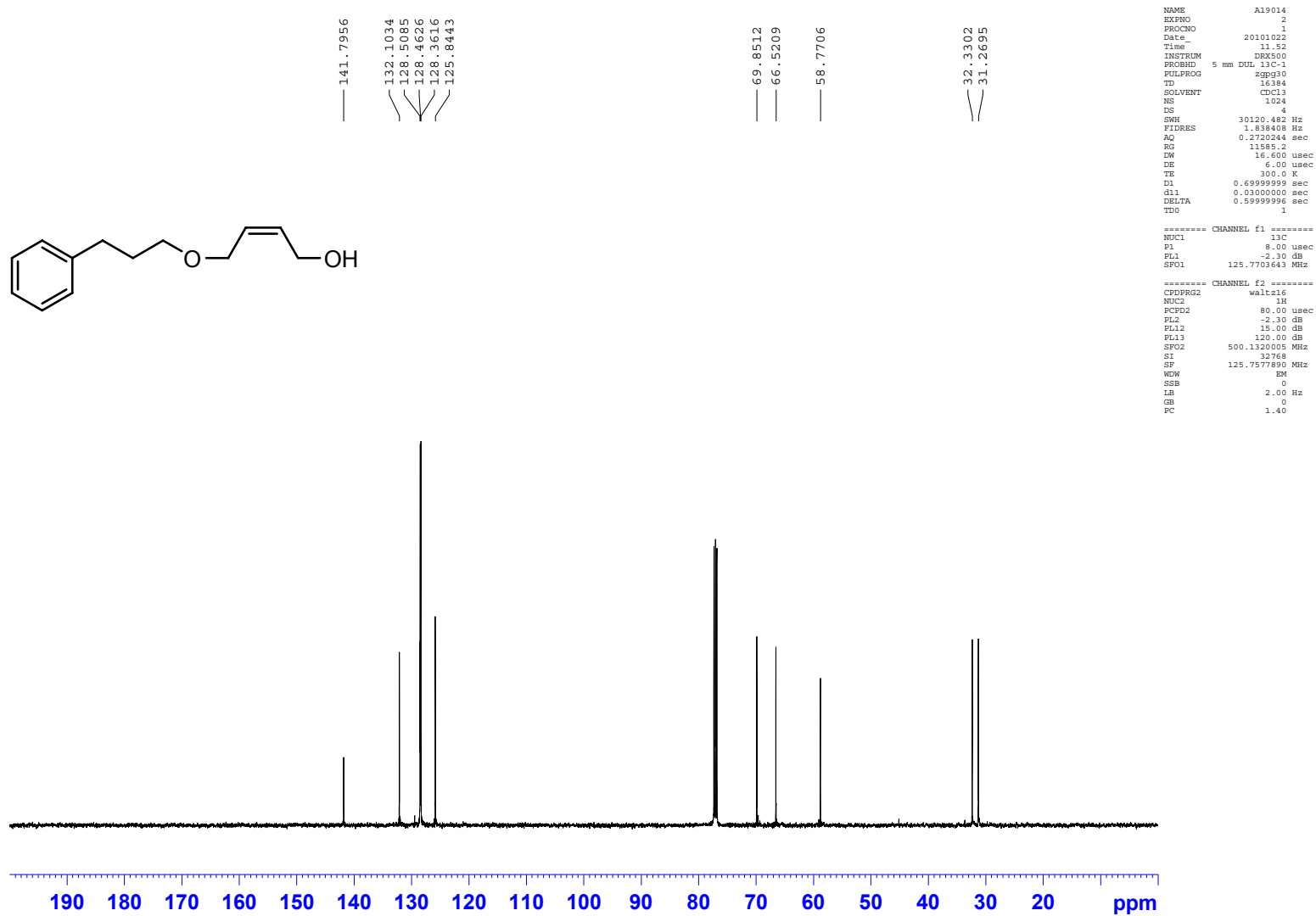
RS217



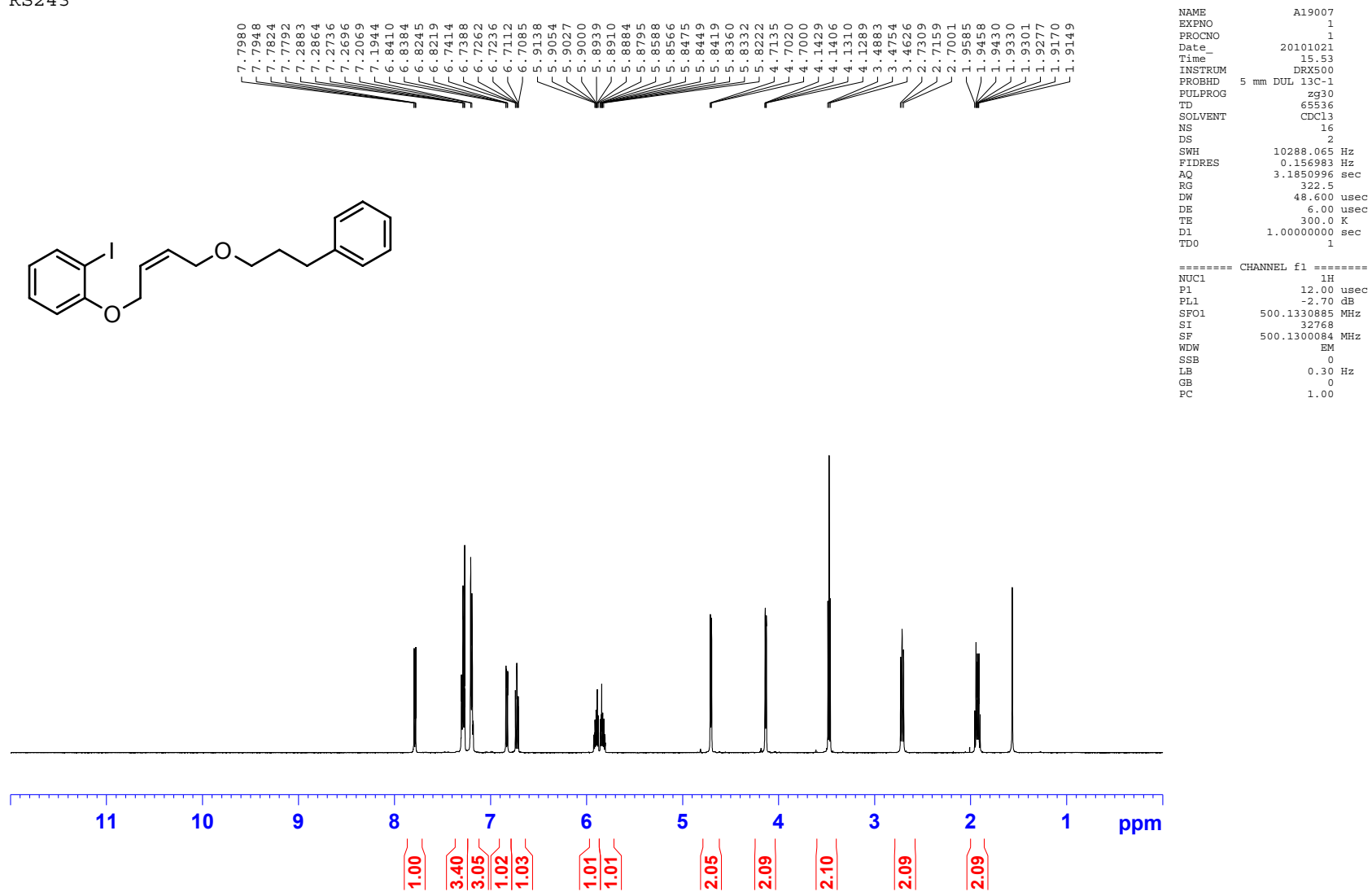
RS242



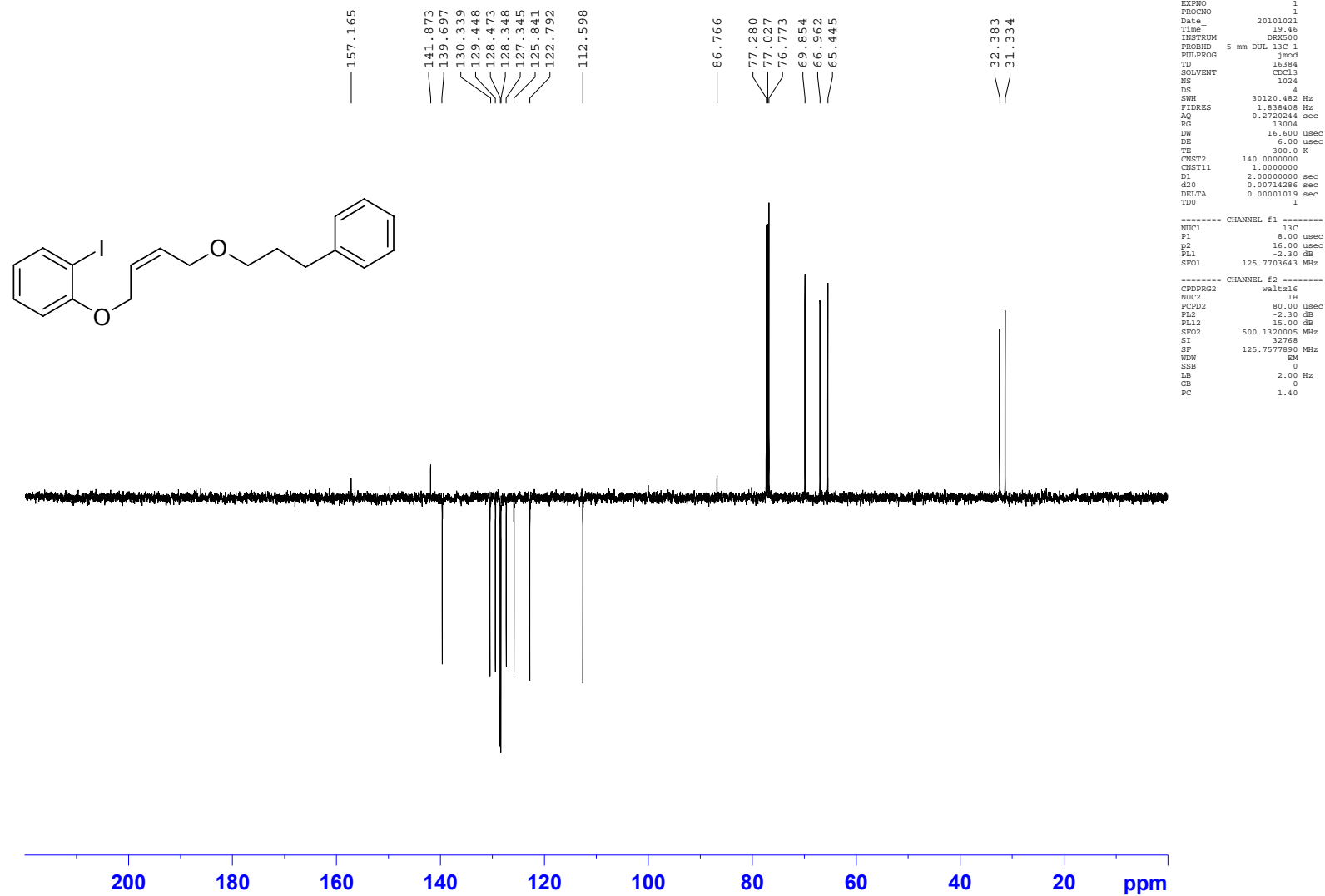
RS242



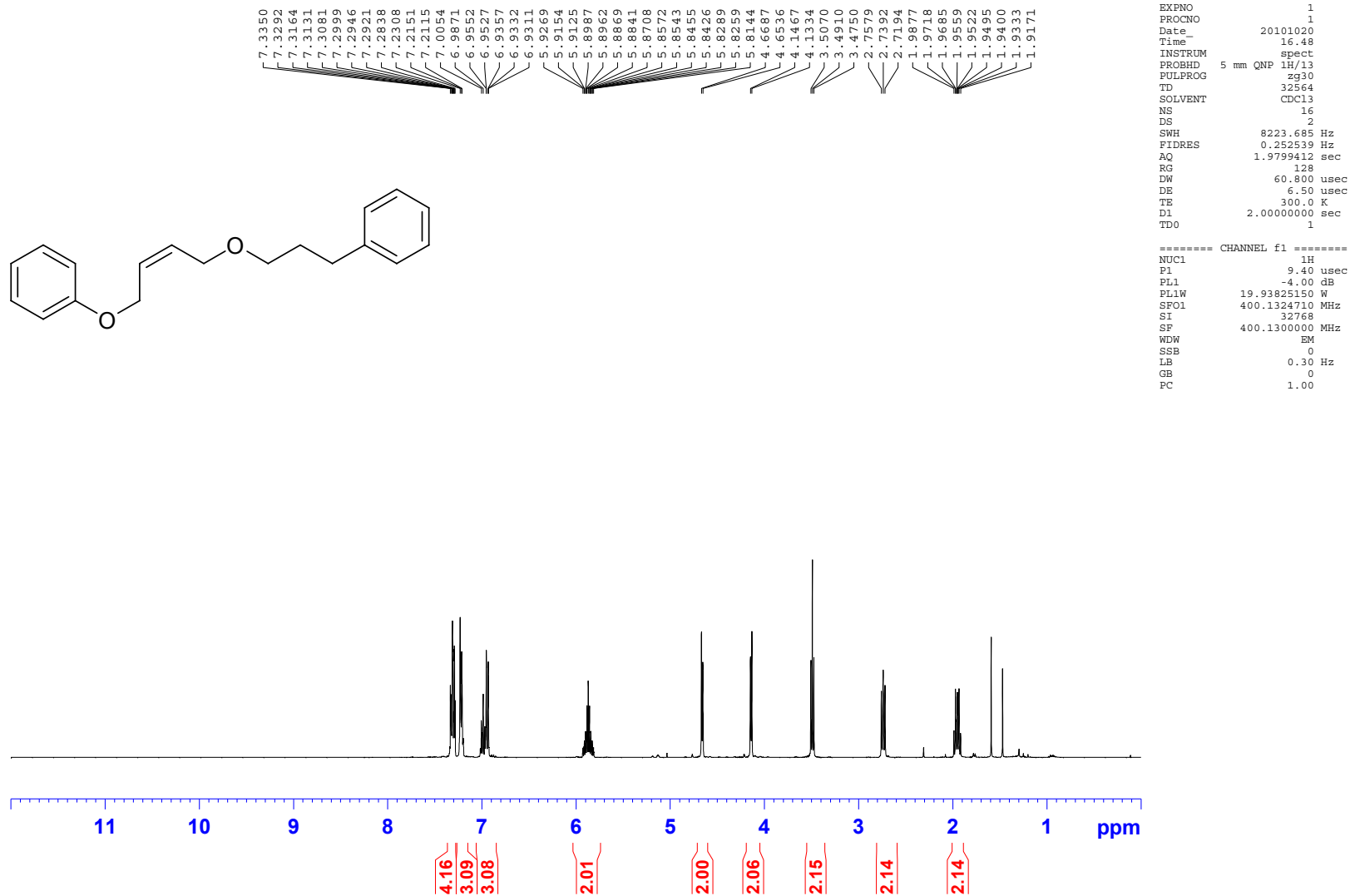
RS243



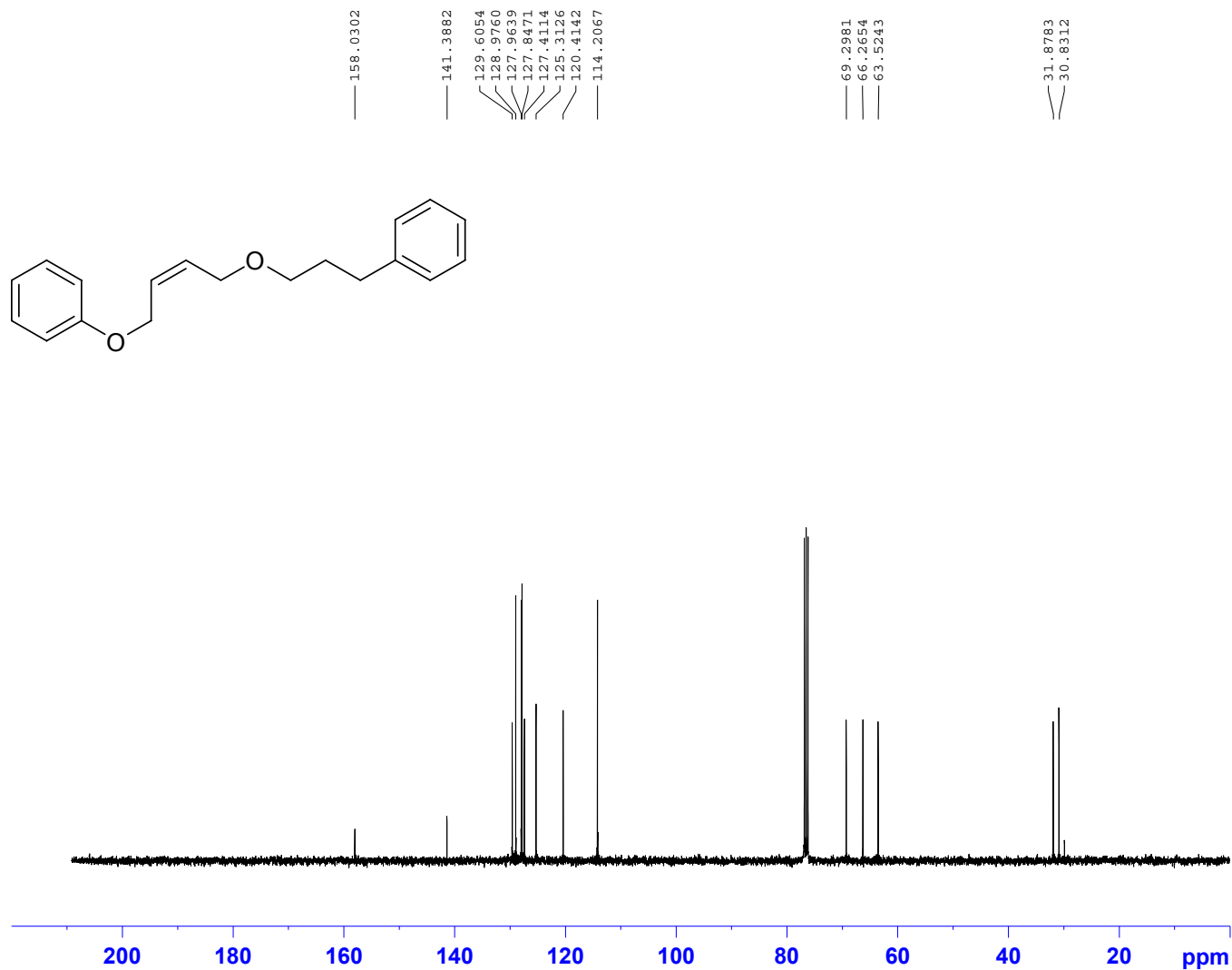
RS243



RS248



RS248



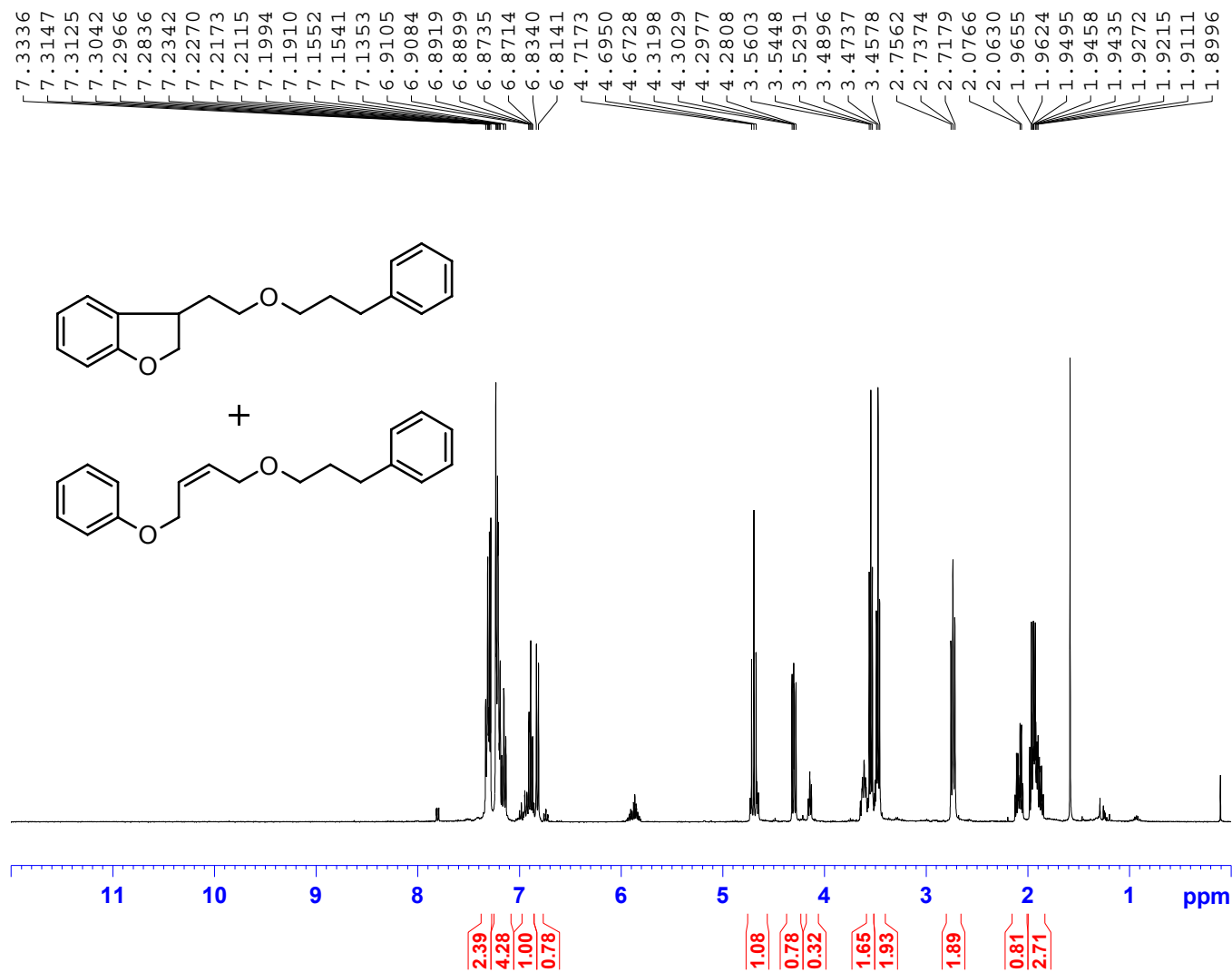
```

NAME          D137413
EXPNO         2
PROCNO        1
Date_         20101020
Time          19.23
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            65384
SOLVENT       CDCl3
NS            1024
DS            4
SWH           22058.824 Hz
FIDRES        1.346364 Hz
AQ            0.3714207 sec
RG            2050
DW            22.667 usec
DE            6.50 usec
TE            300.0 K
D1            0.69999999 sec
D11           0.03000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1          13C
P1            7.00 usec
PL1           -2.60 dB
PL1W          61.34122230 W
SFO1          100.6282898 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -4.00 dB
PL12          14.06 dB
PL13          120.00 dB
PL2W          19.93825150 W
PL12W         0.31166428 W
PL13W         0.00000000 W
SFO2          400.1316005 MHz
SI            12768
SF            100.6128193 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

RS249-1

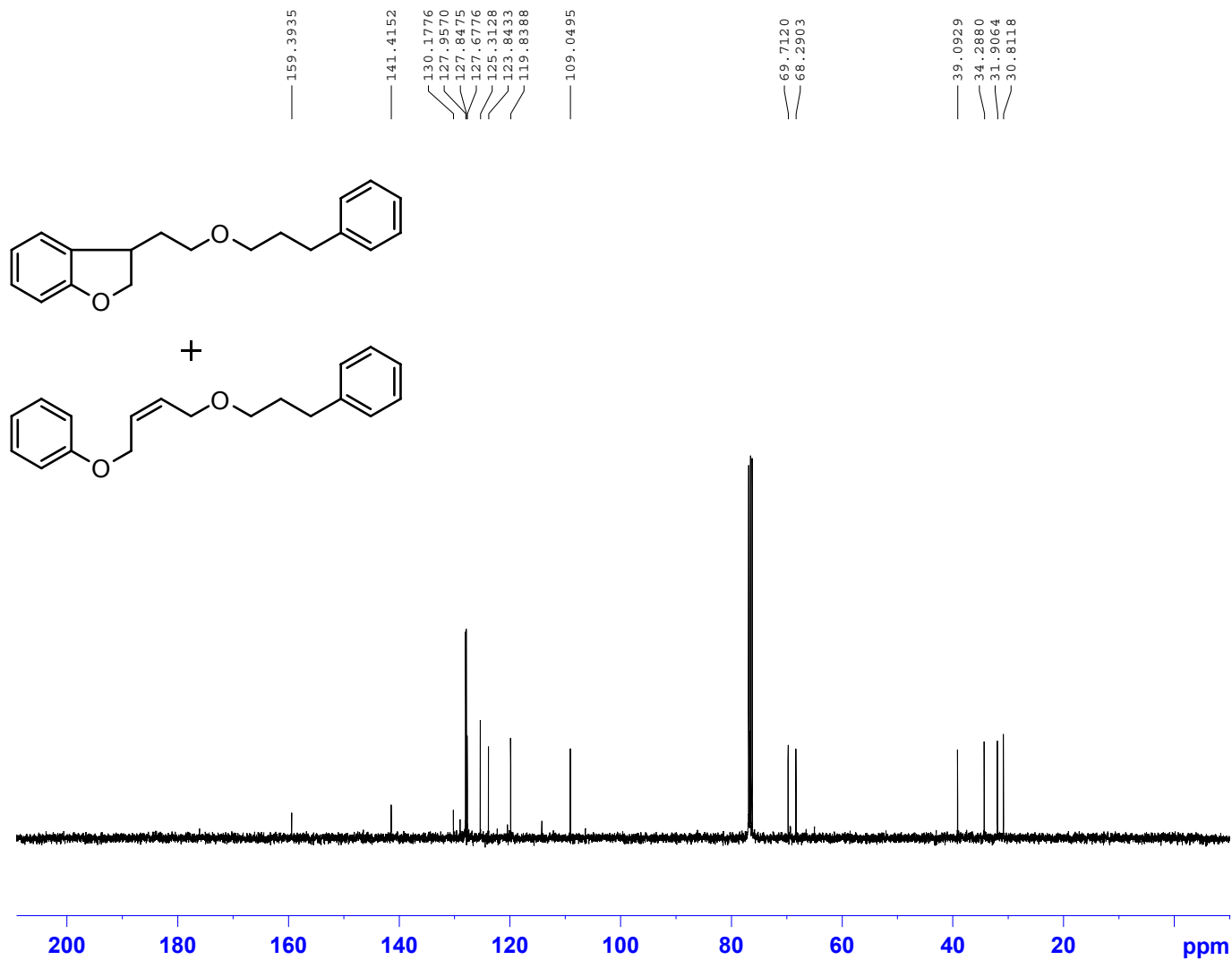


```

NAME          D137414
EXPNO         1
PROCNO        1
Date_         20101020
Time          16.53
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zg30
TD            32564
SOLVENT       CDCl3
NS            16
DS            2
SWH           8223.685 Hz
FIDRES        0.252539 Hz
AQ            1.9799412 sec
RG            181
DW            60.800 usec
DE            6.50 usec
TE            300.0 K
D1            2.00000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1          1H
P1            9.40 usec
PL1           -4.00 dB
PL1W          19.93825150 W
SFO1          400.1324710 MHz
SI            32768
SF            400.1300000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

RS249-1



```

NAME          D137414
EXPNO         2
PROCNO        1
Date_         20101020
Time         17.13
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            16384
SOLVENT       CDCl3
NS            1024
DS            4
SWH           22058.824 Hz
FIDRES        1.346364 Hz
AQ            0.1714207 sec
RG            2050
DW            22.667 usec
DE            6.50 usec
TE            300.0 K
D1            0.69999999 sec
D11           0.03000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1           13C
P1            7.00 usec
PL1           -2.60 dB
PL1W          61.3412330 W
SFO1          100.628398 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2          80.00 usec
PL2           -4.00 dB
PL12          14.06 dB
PL13          120.00 dB
PL2W          19.93825150 W
PL12W          0.31166428 W
PL13W          0.00000000 W
SFO2          400.1316005 MHz
SI            32768
SF           100.6128193 MHz
WDW           EM
SSB            0
LB            1.00 Hz
GB            0
PC            1.40
    
```