

Supporting Information

Design and synthesis of an environment-sensitive 3-methylneisindoloin-1-one fluorophore for labeling of DNA-interacting protein

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General Information

NMR spectra were measured on a Bruker Advance or a Varian UNITY at 300 K. Chemical shifts (δ) are referenced to residual proton in the deuterated solvent. UV-Vis spectra were measured on a SHIMADZU UV-2450 spectrometer. Fluorescent spectra were measured on a JASCO FP-6300. ESI-MS analysis was carried out on a Bruker micrOTOF spectrometer. MALDI-TOF MS analysis was carried out on a Bruker AutoFlexIII and JEOL JMS-S3000. Fluorescence analysis of the gel by SDS-PAGE was performed by using Amersham ImageQuant 800.

Calculation of relative fluorescent quantum yields of 7 and 4b.

Relative fluorescent quantum yields of compounds were obtained from comparison with quinine sulfate (ϕ 0.51 $\lambda_{\text{ex}} = 347.5$ nm in 0.05 M H₂SO₄)^{1,2} according to the equation below³

$$\phi_x = \phi_{st} \times \left(\frac{A_{st}}{A_x}\right) \times \left(\frac{F_x}{F_{st}}\right) \times \left(\frac{n_x}{n_{st}}\right)^2$$

x = sample, st = quinine sulfate;

ϕ : relative fluorescent quantum yield

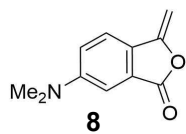
A : absorption of the sample at excited wavelength

F : Integrated fluorescence intensity

n : refractive index of solvent

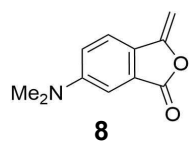
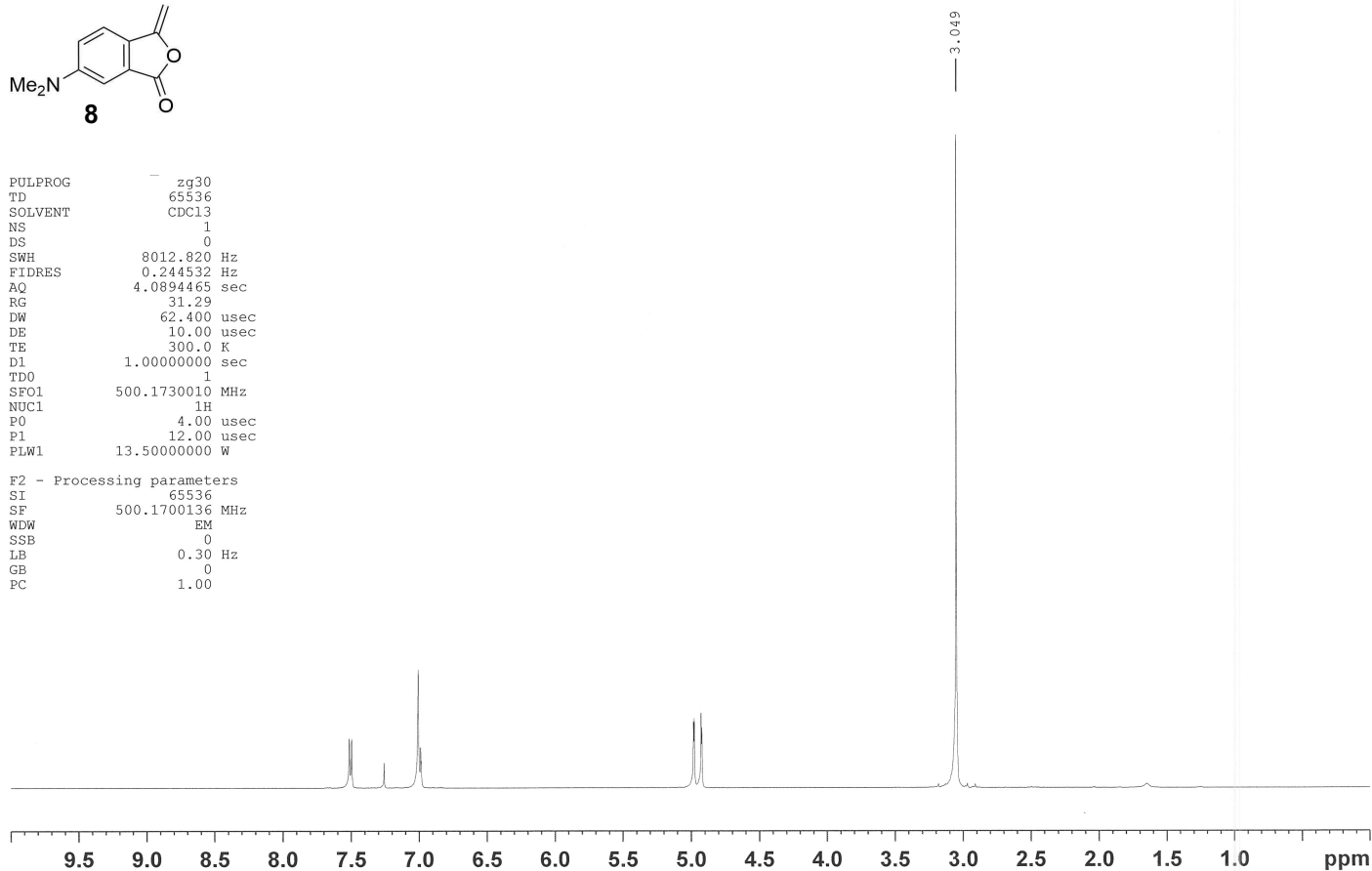
References

- 1) N, Takahashi, S. Saito, H. Hoshino, *Bunseki Kagaku*, 2003, **52**, 713-718.
- 2) J. N. Demas and G. A. Crosby, *J. Phys. Chem.*, 1071, **75**, 991-1023.
- 3) J. R. Lakowicz, (2006) *Principles of Fluorescence Spectroscopy*, 3rd ed., Springer.



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 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 31.29
 DW 62.400 usec
 DE 10.00 usec
 TE 300.0 K
 D1 1.00000000 sec
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 NUC1 1H
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 P1 12.00 usec
 PLW1 13.50000000 W

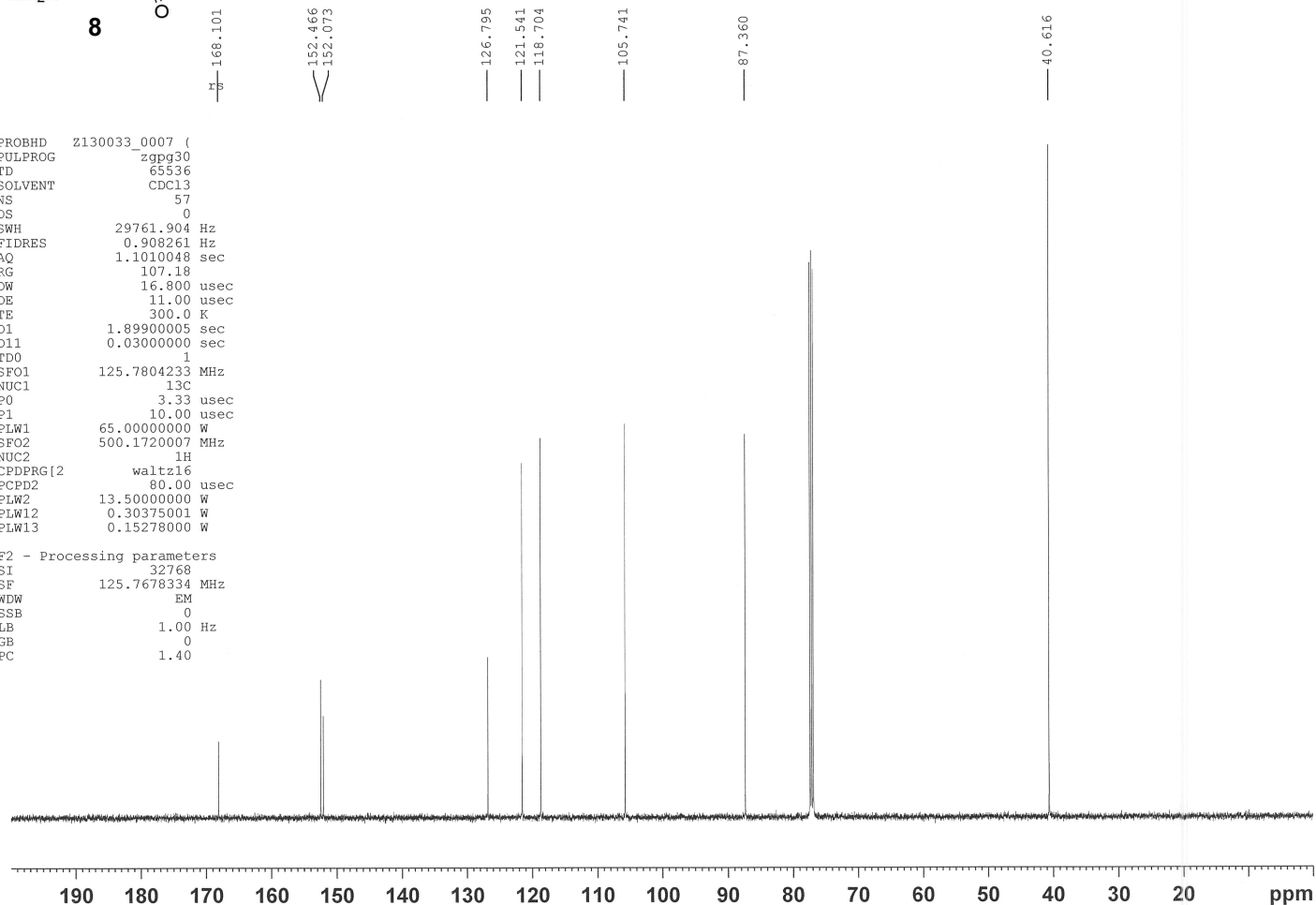
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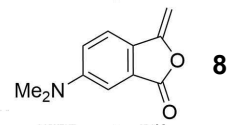
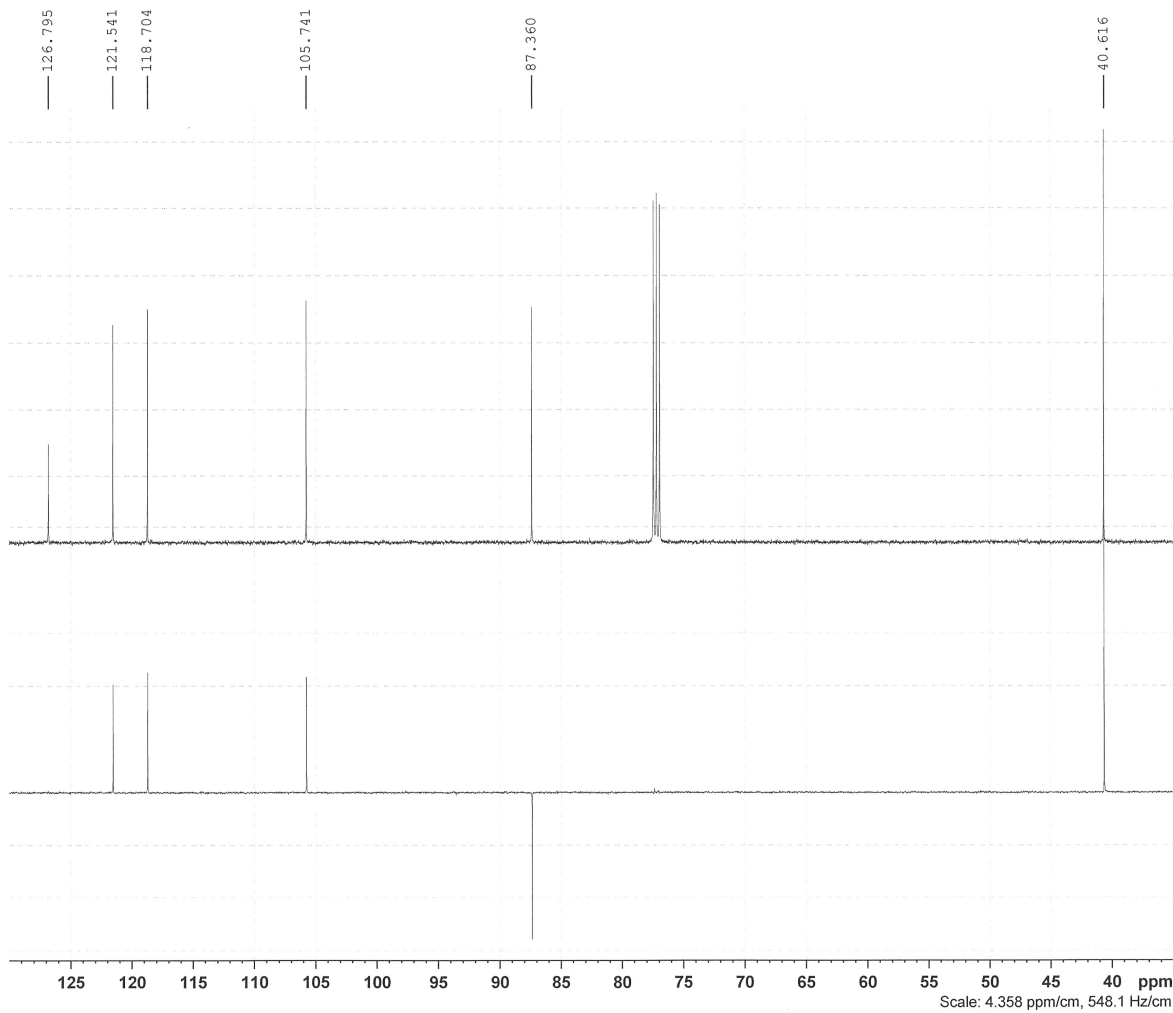


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 87.360
 40.616

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 TD 65536
 SOLVENT CDCl3
 NS 57
 DS 0
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 107.18
 DW 16.800 usec
 DE 11.00 usec
 TE 300.0 K
 D1 1.89900005 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7804233 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 65.00000000 W
 SFO2 500.1720007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 13.50000000 W
 PLW12 0.30375001 W
 PLW13 0.15278000 W

F2 - Processing parameters
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 SSB 0
 LB 1.00 Hz
 GB 0
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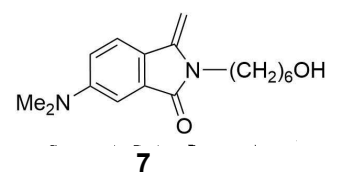
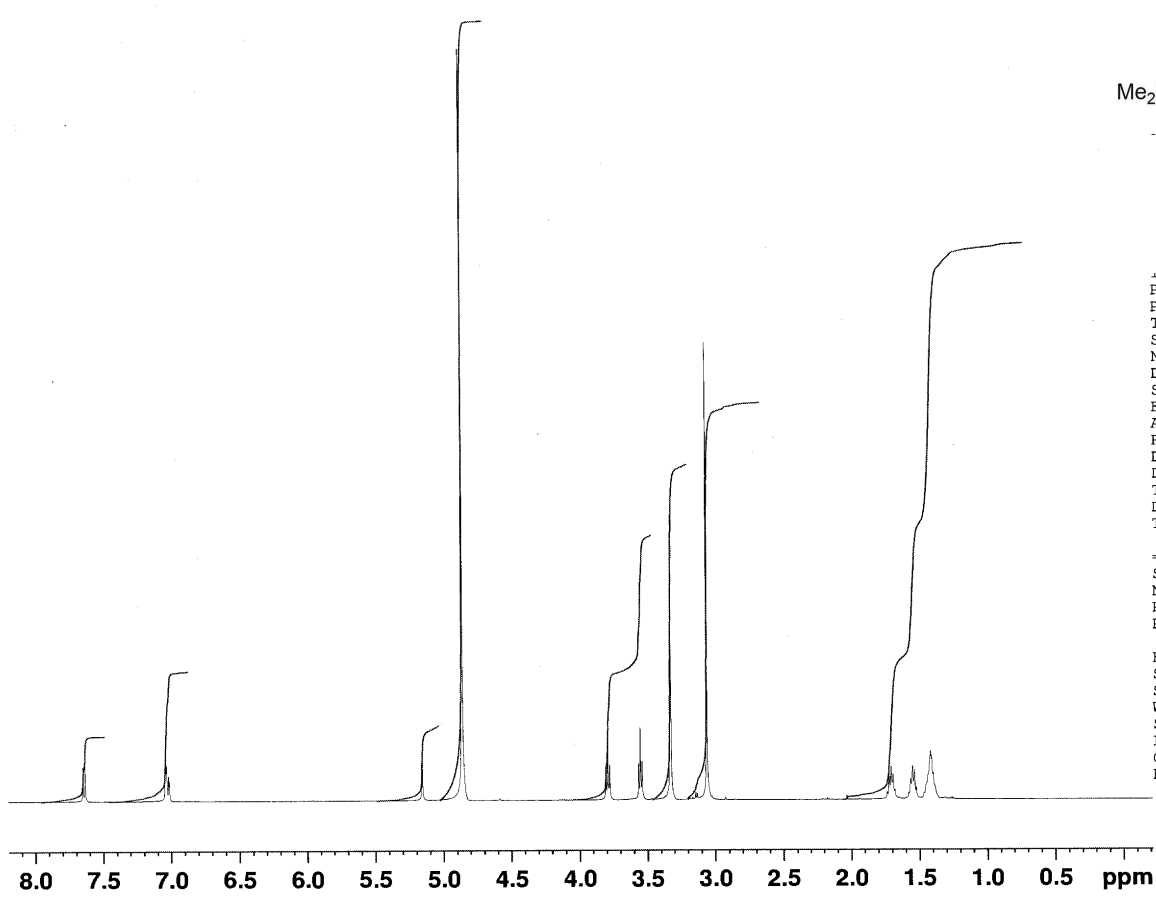
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D1        0.03000000 sec
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NUC1     13C
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P1       10.00 usec
PLW1     65.00000000 W
SF02     500.1720007 MHz
NUC2     1H
CPDPRG12 wait16
PCPD2    80.00 usec
PLW2     13.50000000 W
PLW12    0.30375001 W
PLW13    0.15278000 W
  
```

```

F2 - Processing parameters
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DS        0
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FIDRES    0.908261 Hz
AQ        1.1010048 sec
RG        107.18
DW        16.800 usec
DE        11.00 usec
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D1        0.03000000 sec
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SF01     125.7604233 MHz
NUC1     13C
P0       3.33 usec
P1       10.00 usec
PLW1     65.00000000 W
SF02     500.1720007 MHz
NUC2     1H
CPDPRG12 wait16
PCPD2    80.00 usec
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PLW13    0.15278000 W
  
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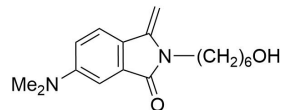
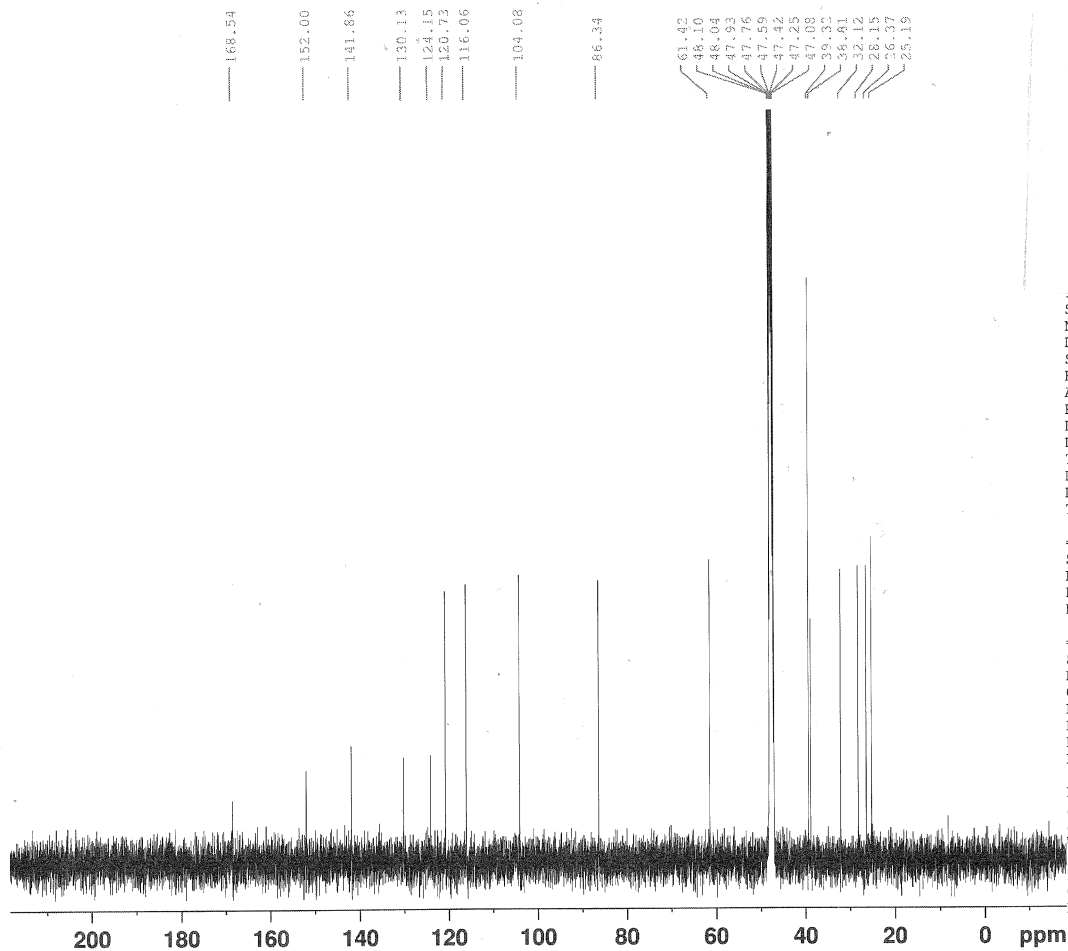


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PROBHD   5 mm CPPBBO BE
PULPROG  zg30
TD        65536
SOLVENT  MeOD
NS        16
DS        2
SWH       10000.000 Hz
FIDRES    0.152588 Hz
AQ        3.2767999 sec
RG        31.29
DW        50.000 usec
DE        10.00 usec
TE        300.1 K
DI        1.00000000 sec
TDO       1

===== CHANNEL f1 =====
SF01     500.1730888 MHz
NUC1     1H
P1       12.00 usec
PLW1     13.50000000 W

F2 - Processing parameters
SI        65536
SF        500.1700000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```

7

```

SOLVENT      MeOD
NS           129
DS           4
SWH          29761.904 Hz
FIDRES       0.454131 Hz
AQ           1.1010048 sec
RG           189.66
DW           16.800 usec
DE           11.00 usec
TE           300.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0         1
  
```

```

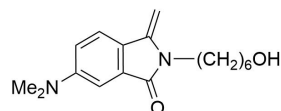
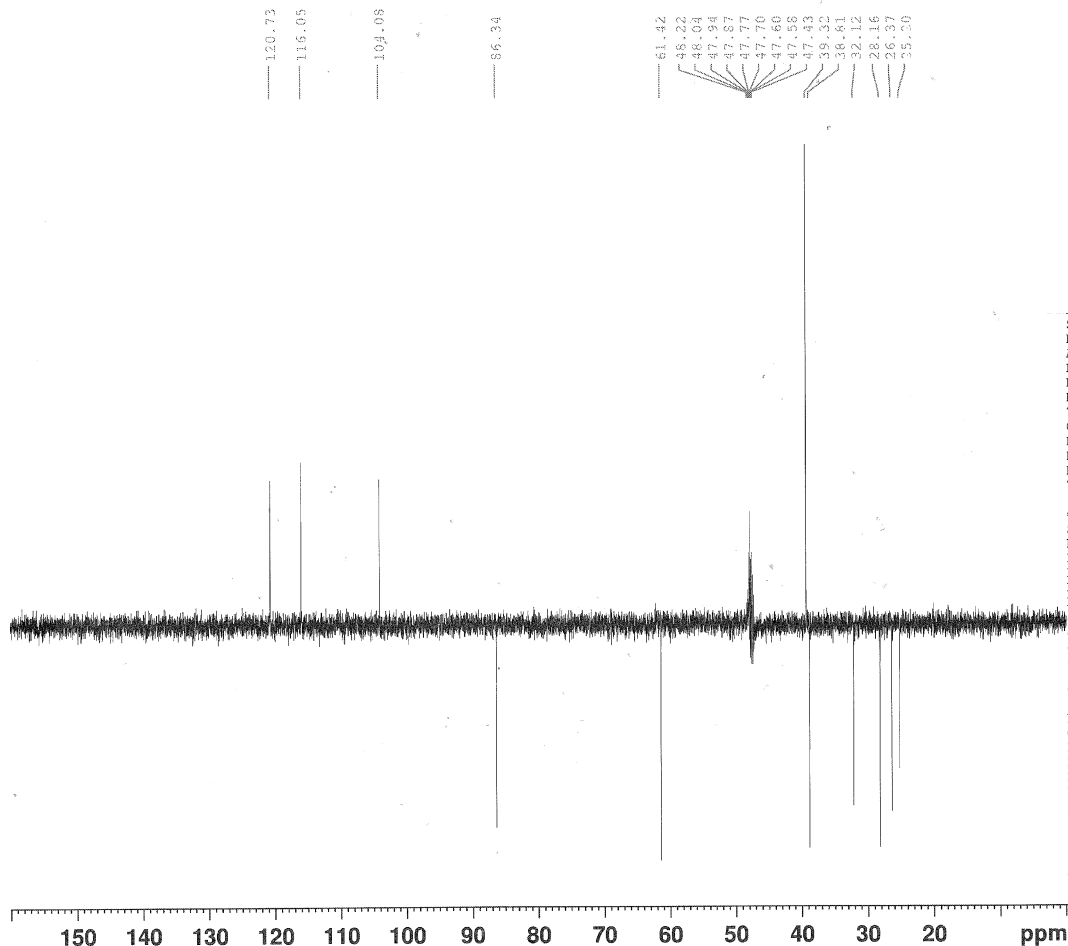
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NUC1         13C
P1           10.00 usec
PLW1         65.00000000 W
  
```

```

===== CHANNEL f2 =====
SFO2         500.1720007 MHz
NUC2         1H
CPDPRG[2]   waltz16
PCPD2        80.00 usec
PLW2         13.50000000 W
PLW12        0.30375001 W
PLW13        0.19440000 W
  
```

```

F2 - Processing parameters
SI           32768
SF           125.7678470 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```



7

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SWH          20161.291 Hz
FIDRES       0.307637 Hz
AQ           1.6252928 sec
RG           189.66
DW           24.800 usec
DE           11.00 usec
TE           300.2 K
CNST2        145.0000000
D1           2.00000000 sec
D2           0.00344828 sec
D12          0.00002000 sec
TD0         1
  
```

```

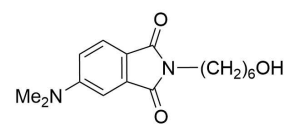
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NUC1         13C
P1           10.00 usec
P13          2000.00 usec
PLW0         0 W
PLW1         65.00000000 W
SPNAM[5]    Crp60comp.4
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SPOFFS5     0 Hz
SPW5         9.93130016 W
  
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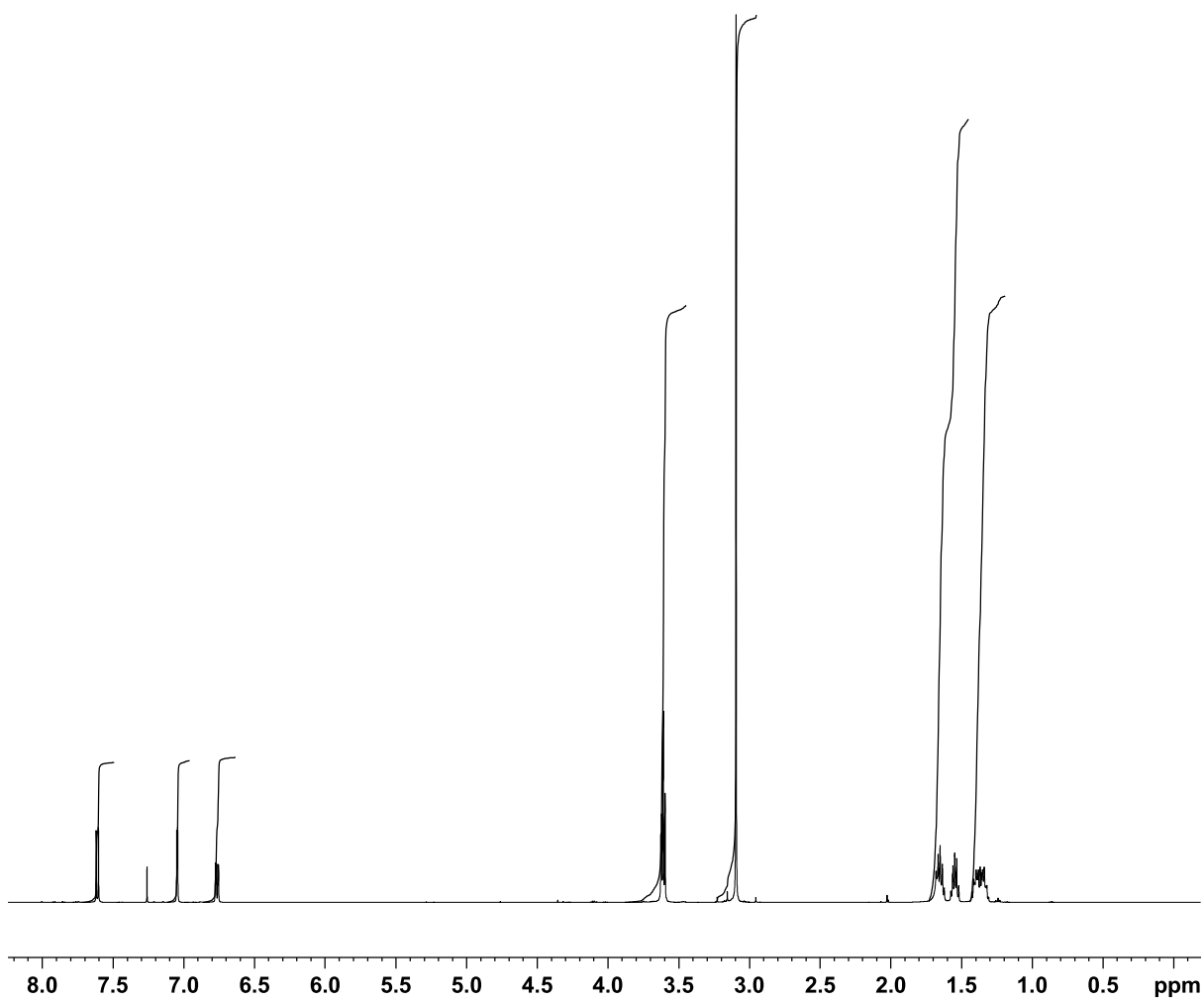
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CPDPRG[2]   waltz16
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P4           24.00 usec
PCPD2        80.00 usec
PLW2         13.50000000 W
PLW12        0.30375001 W
  
```

```

F2 - Processing parameters
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```



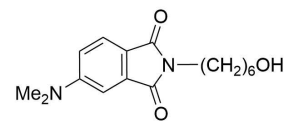
4b



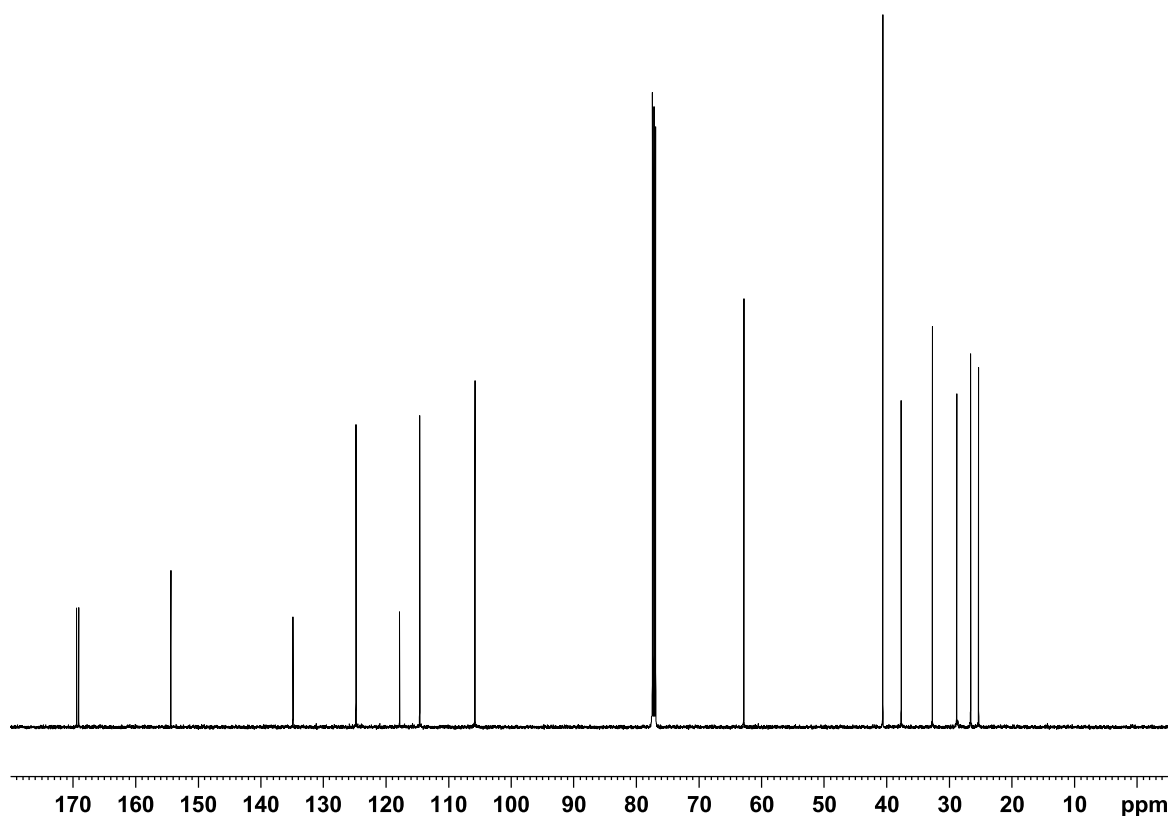
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 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 31.29
 DW 50.000 usec
 DE 13.55 usec
 TE 300.0 K
 D1 1.0000000 sec
 TD0 1
 SFO1 500.1730885 MHz
 NUC1 1H
 P0 4.00 usec
 P1 12.00 usec
 PLW 16.0000000 W
 F2 - Processing parameters
 SI 65536
 SF 500.1700121 MHz
 WDW EM
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 LB 0.30 Hz

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169.07
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134.86
124.77
117.81
114.61
105.79

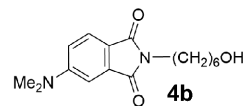
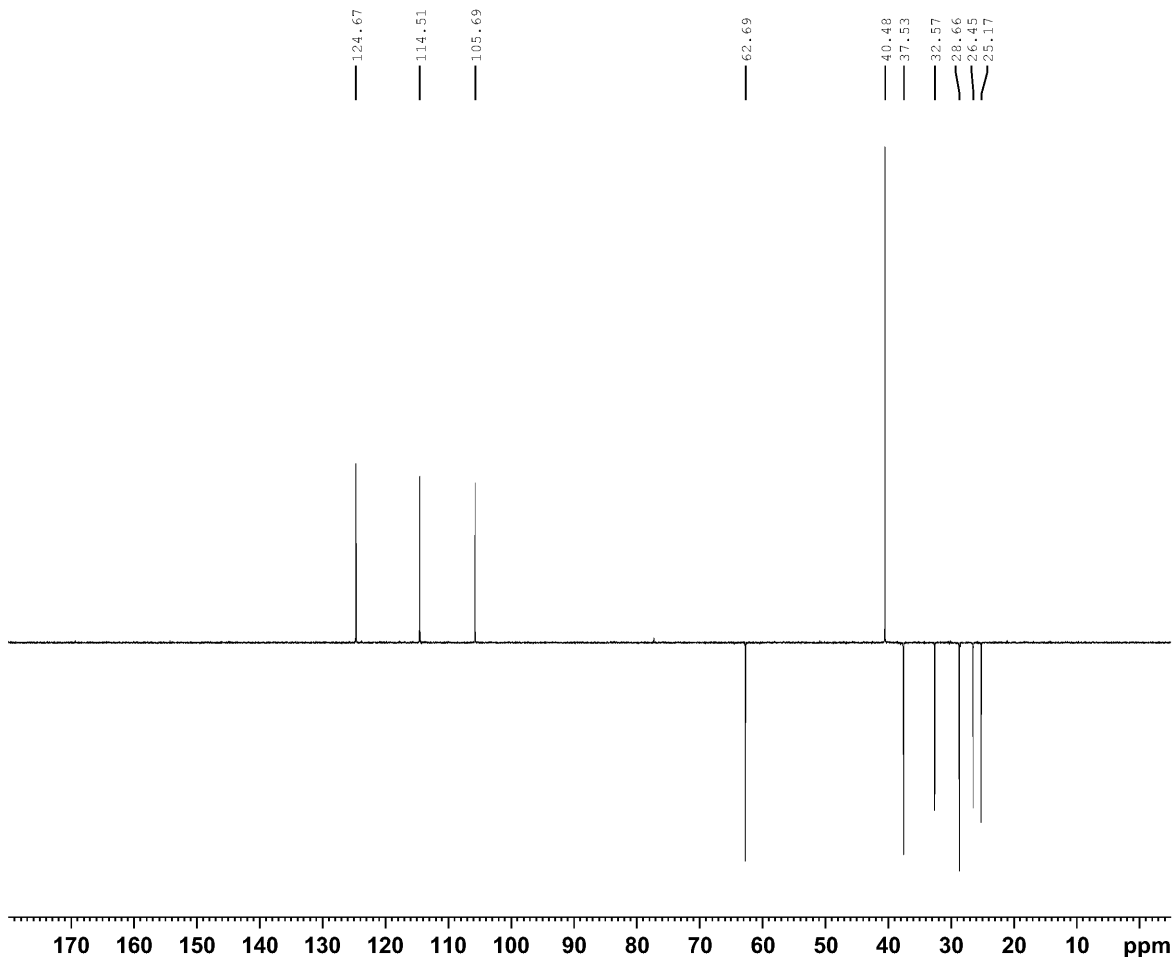
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40.58
37.63
32.67
28.76
26.55
25.27



4b

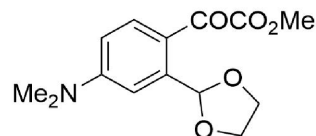
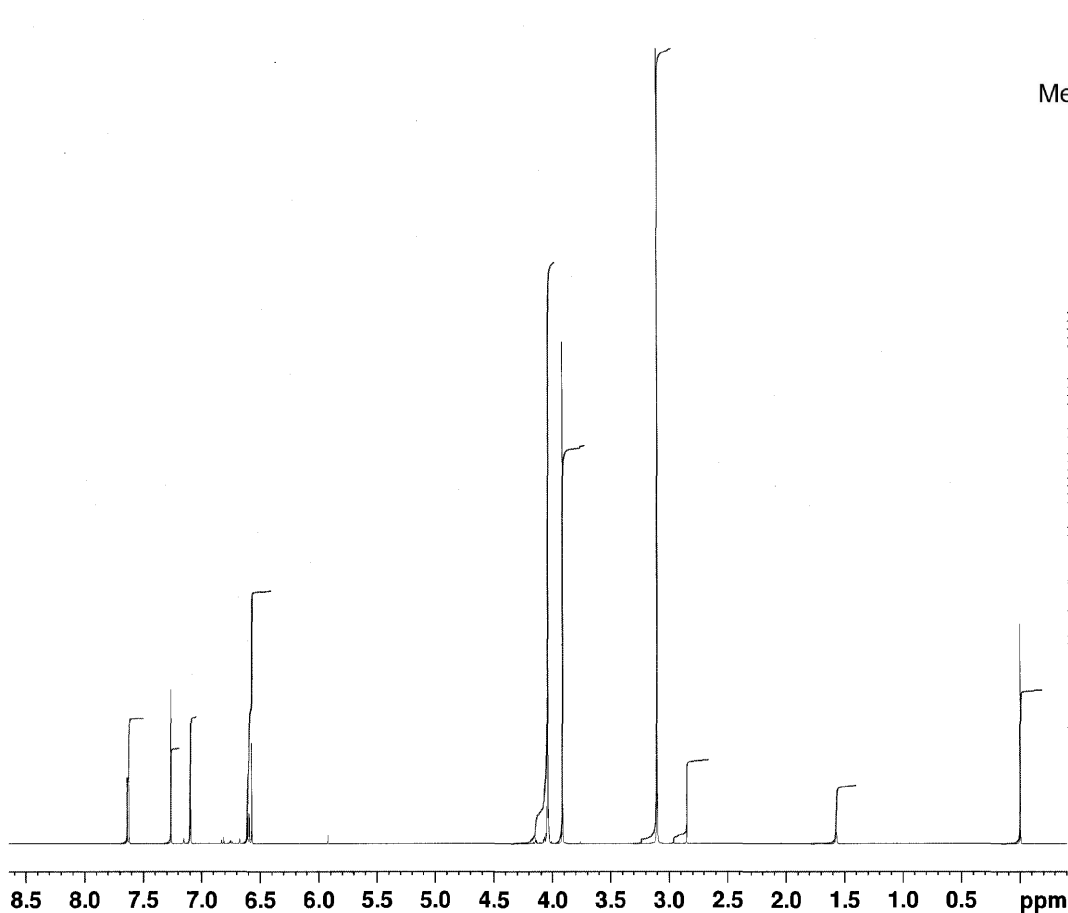


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 EXPNO 11
 PROCNO 1
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 Time 22.19 h
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 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 189.66
 DW 16.800 usec
 DE 11.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1
 SFO1 125.7804233 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW 70.0000000 W
 SFO2 500.1720007 MHz
 NUC2 1H
 CPDPRG2 waltz65
 PCPD2 80.00 usec
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 PLW3 0.3600001 W
 PLW4 0.1810800 W
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 SI 32768
 SF 125.7678345 MHz
 WDW EM



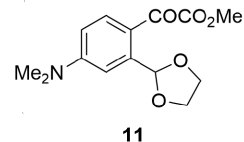
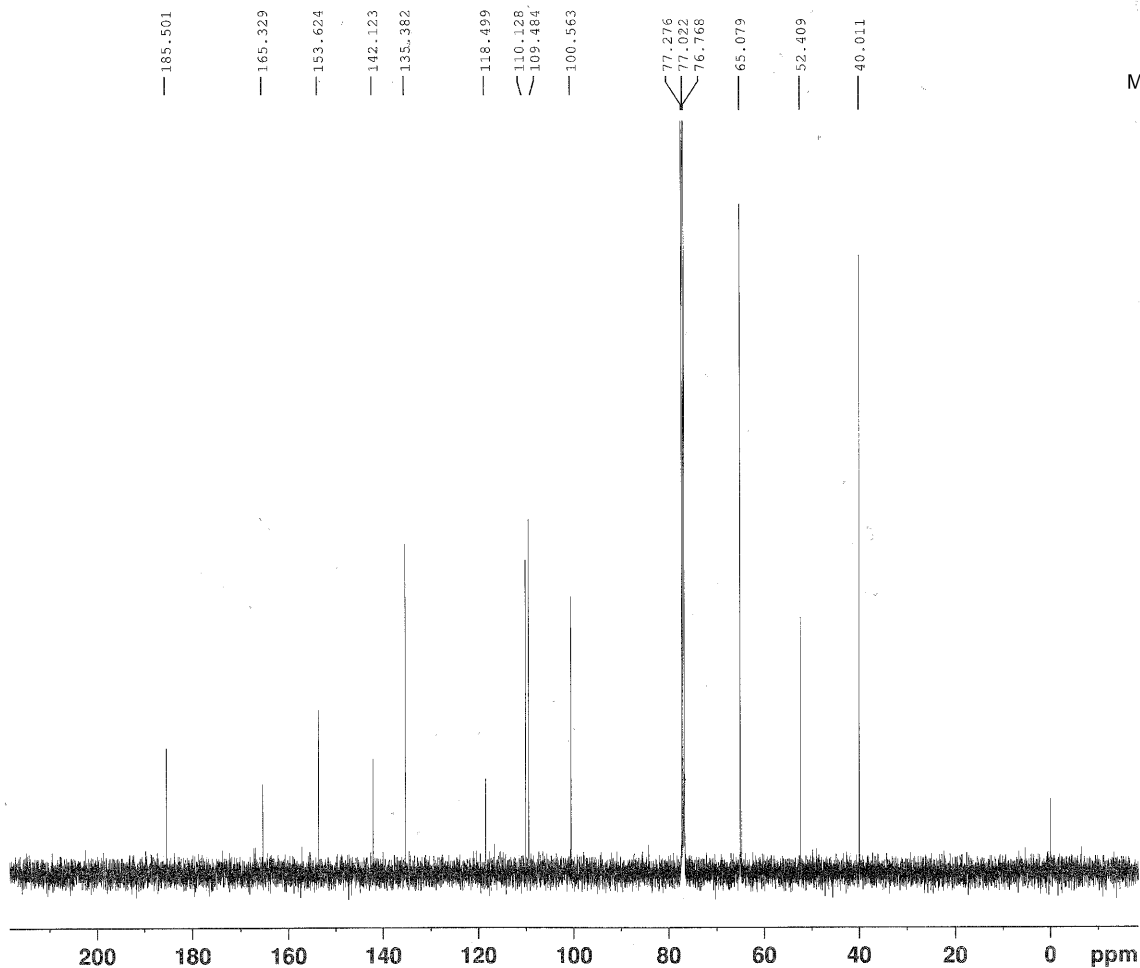
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PULPROG      dept sp135
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SOLVENT      CDCl3
NS           200
DS           8
SWH          29761.904 Hz
FIDRES       0.908261 Hz
AQ           1.1010048 sec
RG           189.66
DW           16.800 usec
DE           11.00 usec
TE           300.0 K
CNST2        145.0000000
D1           2.00000000 sec
D2           0.00344828 sec
D12          0.00002000 sec
TD0          1
SFO1         125.7779080 MHz
NUC1         13C
P1           10.00 usec
P13         2000.00 usec
PLW0         0 W
PLW1         70.0000000 W
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SPOCAL5      0.500
SPOFFS5      0 Hz
SPW5         10.69499969 W
SFO2         500.1720007 MHz
NUC2         1H
CPDPRQ[ 2]   wal tz65
P3           12.00 usec
P4           24.00 usec
PCPD2        80.00 usec
PLW2         16.0000000 W
PLW2         0.36000001 W
F2 - Processi ng parameters
SI           32768
SF           125.7678470 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```



```

-----
INSTRUM      spect
PROBHD       5 mm CPPBBO BB
PULPROG      zg30
TD           65536
SOLVENT      CDCl3
NS           16
DS           2
SWH          10000.000 Hz
FIDRES       0.152588 Hz
AQ           3.2767999 sec
RG           31.29
DW           50.000 usec
DE           10.00 usec
TE           300.1 K
D1           1.00000000 sec
TD0          1
===== CHANNEL f1 =====
SFO1         500.1730888 MHz
NUC1         1H
P1           12.00 usec
PLW1         13.50000000 W
F2 - Processing parameters
SI           65536
SF           500.1700113 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```



```

FIDRES      0.454131 Hz
AQ          1.1010048 sec
RG          107.18
DW          16.800 usec
DE          11.00 usec
TE          300.1 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0         1
  
```

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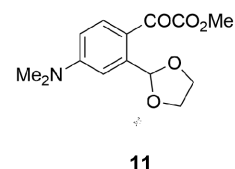
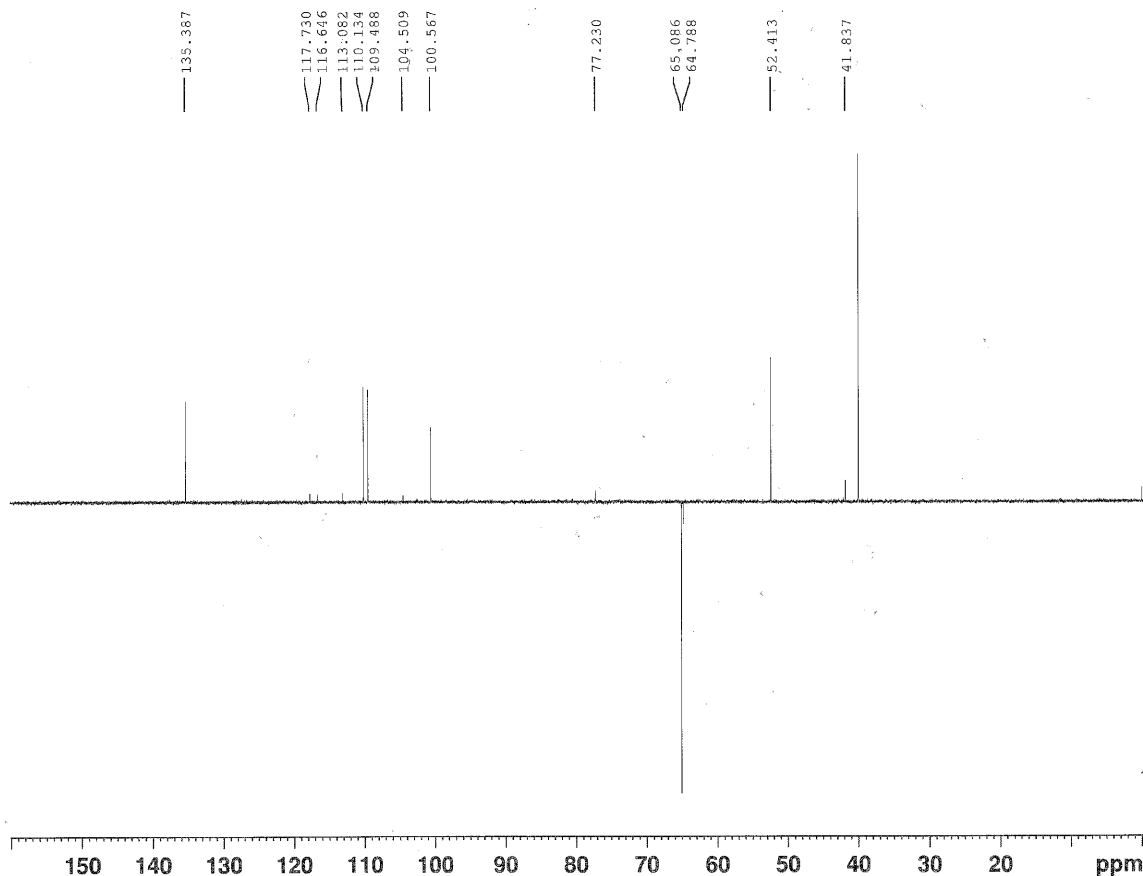
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NUC1       13C
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PLW1       65.00000000 W
  
```

```

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SFO2       500.1720007 MHz
NUC2       1H
CPDPRG[2]  waltz16
PCPD2      80.00 usec
PLW2       13.50000000 W
PLW12      0.30375001 W
PLW13      0.19440000 W
  
```

```

F2 - Processing parameters
SI         32768
SF         125.7678470 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



```

DE          11.00 usec
TE          300.2 K
CNST2      145.0000000
D1          2.00000000 sec
D2          0.00344828 sec
D12        0.00002000 sec
TD0         1
  
```

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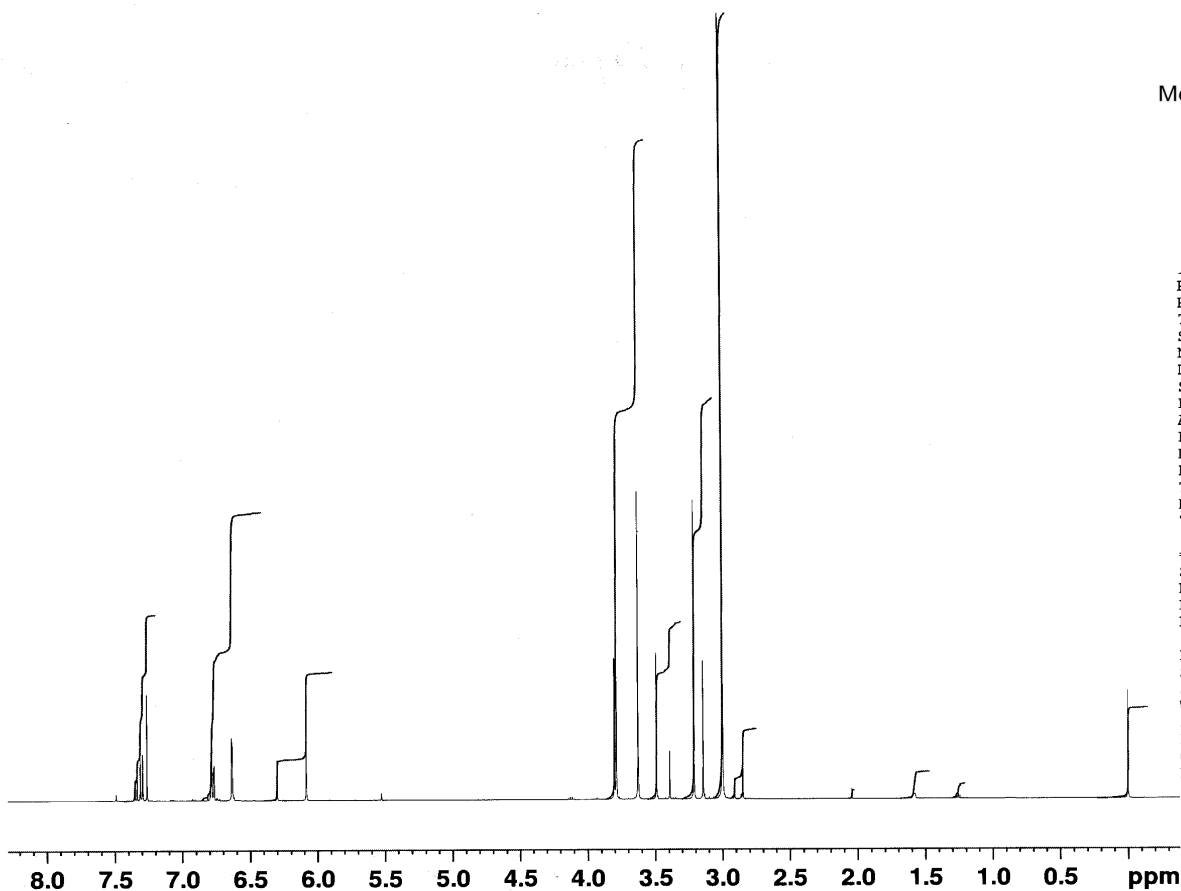
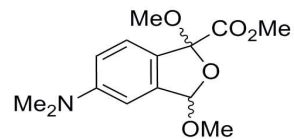
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NUC1       13C
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P13        2000.00 usec
PLW0       0 W
PLW1       65.00000000 W
SPNAM[5]   Crp60comp.4
SFOALS5    0.500
SPOFFS5    0 Hz
SPW5       9.93130016 W
  
```

```

===== CHANNEL f2 =====
SFO2       500.1715996 MHz
NUC2       1H
CPDPRG[2]  waltz16
P3         12.00 usec
P4         24.00 usec
PCPD2      80.00 usec
PLW2       13.50000000 W
PLW12      0.30375001 W
  
```

```

F2 - Processing parameters
SI         32768
SF         125.7678466 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



```

INSTRUM      spect
PROBHD       5 mm CPPBBO BB
PULPROG      zg30
TD           65536
SOLVENT      CDCl3
NS           16
DS           2
SWH          10000.000 Hz
FIDRES       0.152588 Hz
AQ           3.2767999 sec
RG           31.29
DW           50.000 usec
DE           10.00 usec
TE           300.1 K
D1           1.00000000 sec
TDO         1
  
```

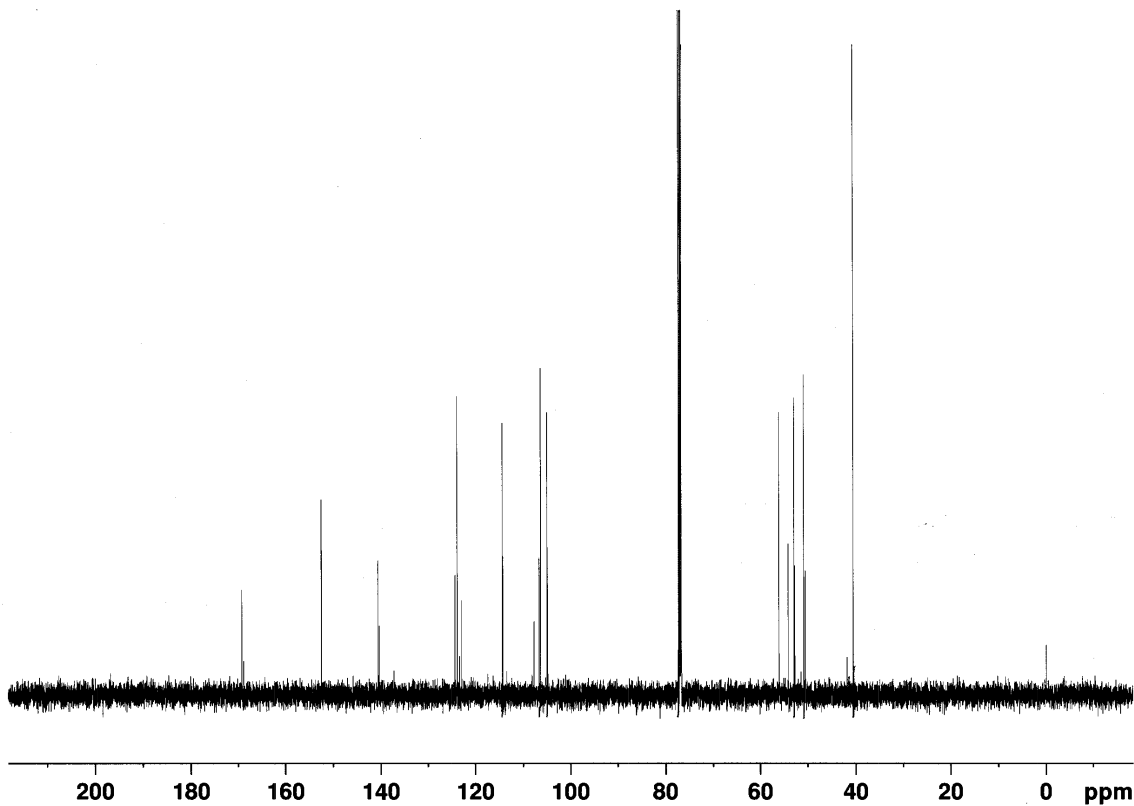
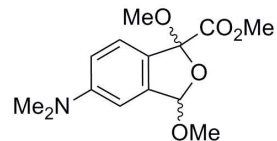
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===== CHANNEL f1 =====
SFO1         500.1730888 MHz
NUC1         1H
P1           12.00 usec
PLW1         13.50000000 W
  
```

```

F2 - Processing parameters
SI           65536
SF           500.1700108 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```

169.288
 168.857
 152.541
 140.682
 140.416
 124.333
 123.906
 123.373
 122.831
 114.337
 114.272
 107.758
 106.674
 106.329
 104.972
 104.906
 56.130
 54.181
 52.953
 52.808
 52.731
 50.880
 50.561
 41.867
 40.583



```

MUS          107.14
DW           16.800 usec
DE           11.00 usec
TE           300.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TDO         1
  
```

```

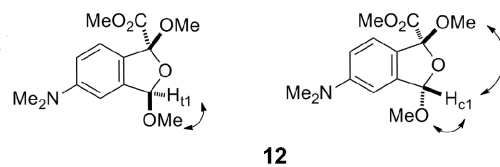
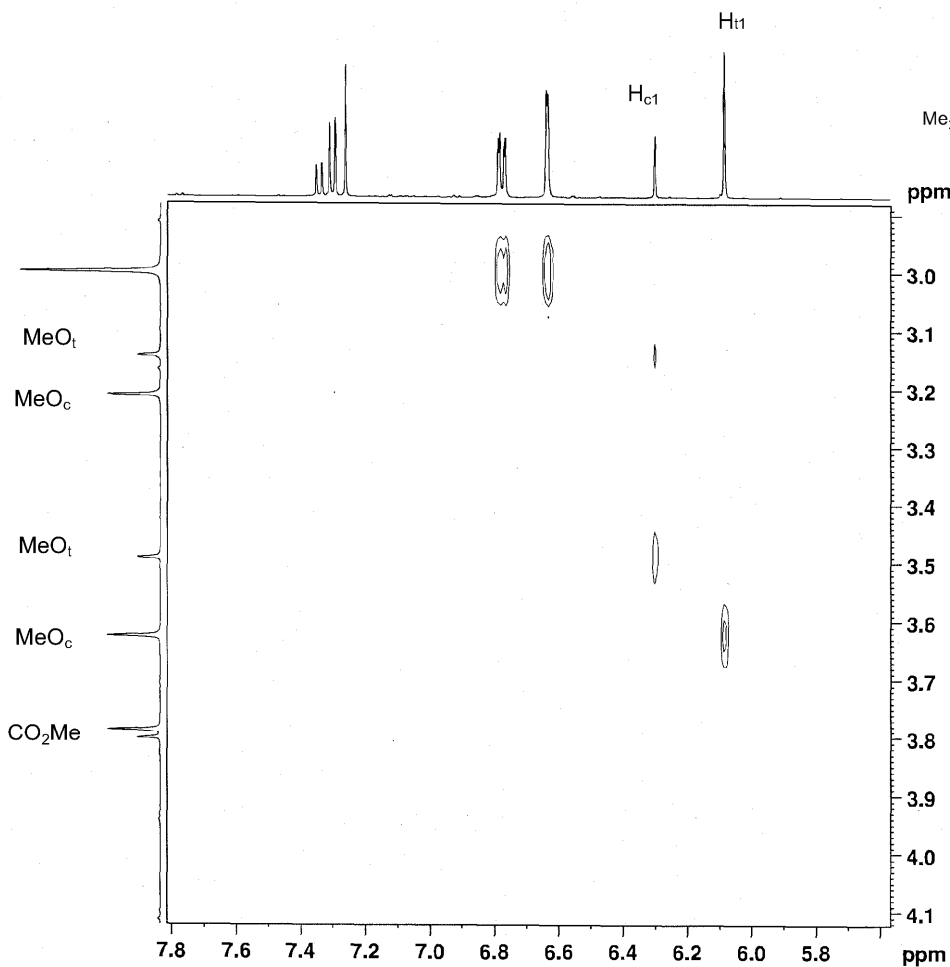
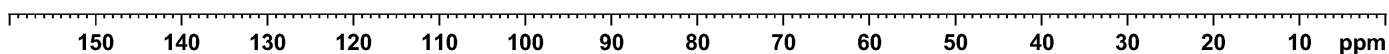
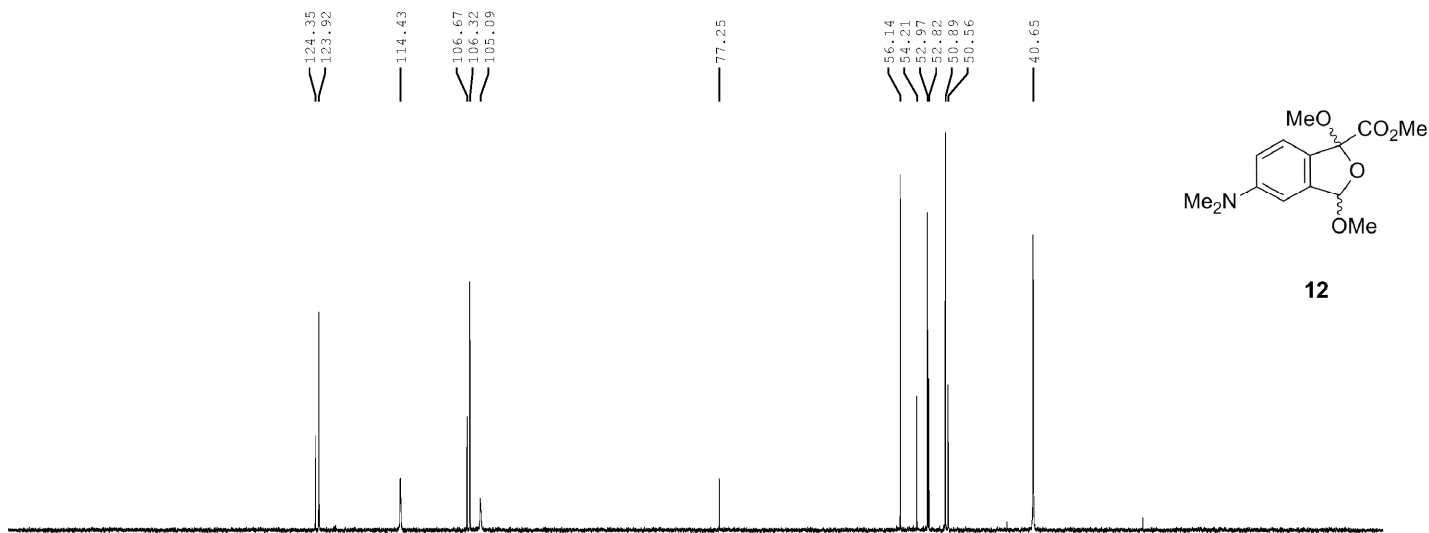
===== CHANNEL f1 =====
SFO1         125.7804227 MHz
NUC1         13C
P1           10.00 usec
PLW1         65.00000000 W
  
```

```

===== CHANNEL f2 =====
SFO2         500.1720007 MHz
NUC2         1H
CPDPRG[2]   waltz16
PCPD2        80.00 usec
PLW2         13.50000000 W
PLW12        0.30375001 W
PLW13        0.19440000 W
  
```

```

F2 - Processing parameters
SI           32768
SF           125.7678470 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```



```

SOLVENT      CDCl3
NS           4
DS           32
SWH          4237.288 Hz
FIDRES       2.068988 Hz
AQ           0.2416640 sec
RG           17.03
DW           118.000 usec
DE           10.00 usec
TE           300.1 K
D0           0.00010232 sec
D1           1.96313586 sec
D8           0.30000001 sec
D11          0.03300000 sec
D12          0.00002000 sec
D16          0.00010000 sec
IN0          0.00023600 sec

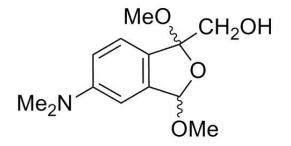
----- CHANNEL f1 -----
SF01         500.1718560 MHz
NUC1         1H
P1           12.00 usec
P2           24.00 usec
P17          2500.00 usec
PLW1         13.50000000 W
PLW2         2.87570000 W

----- GRADIENT CHANNEL -----
GPNAM[1]     SPSQ10.00
GP2         40.00 %
P16         1000.00 usec

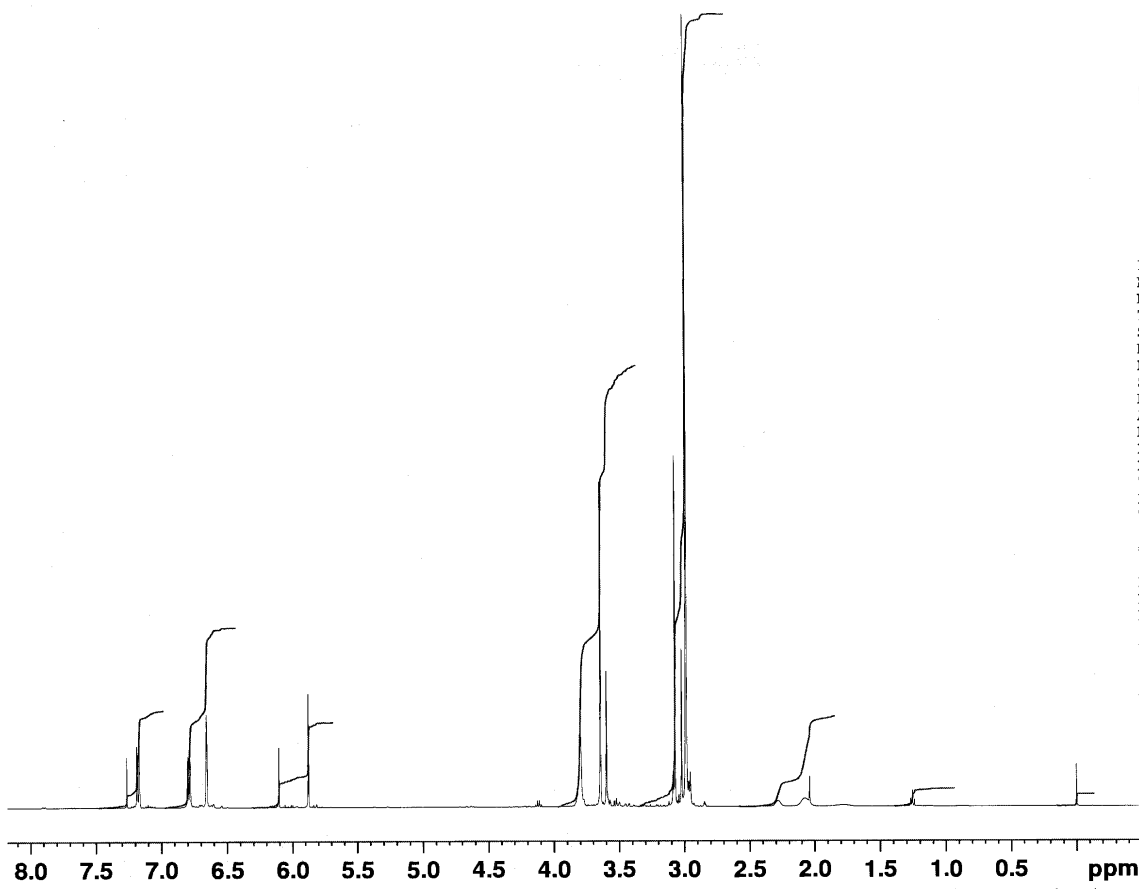
F1 - Acquisition parameters
TD          256
SF01        500.1719 MHz
FIDRES      16.551907 Hz
SW           8.472 PPM
PRMODE      States-TPPI

F2 - Processing parameters
SI          1024
SP          500.1700102 MHz
WDW         COSINE
SSB         2
LB           0 Hz
GB           0
PC           1.00

F1 - Processing parameters
SI          1024
MC2         States-TPPI
SF          500.1700102 MHz
WDW         COSINE
SSB         2
LB           0 Hz
GB           0
  
```



14



```

INSTRUM      spect
PROCDD      5 mm CFFBEO BB
PULPROG      zg30
TD           65536
SOLVENT      CDC13
NS           16
DS           2
SWH          10000.000 Hz
FIDRES       0.152588 Hz
AQ           3.2767999 sec
RG           23.8
DW           50.000 usec
DE           10.00 usec
TE           300.1 K
D1           1.00000000 sec
TDO          1
  
```

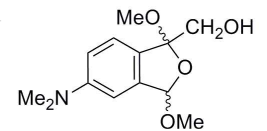
```

----- CHANNEL f1 -----
SFO1         500.1730888 MHz
NUC1          1H
P1            12.00 usec
PLW1         13.50000000 W
  
```

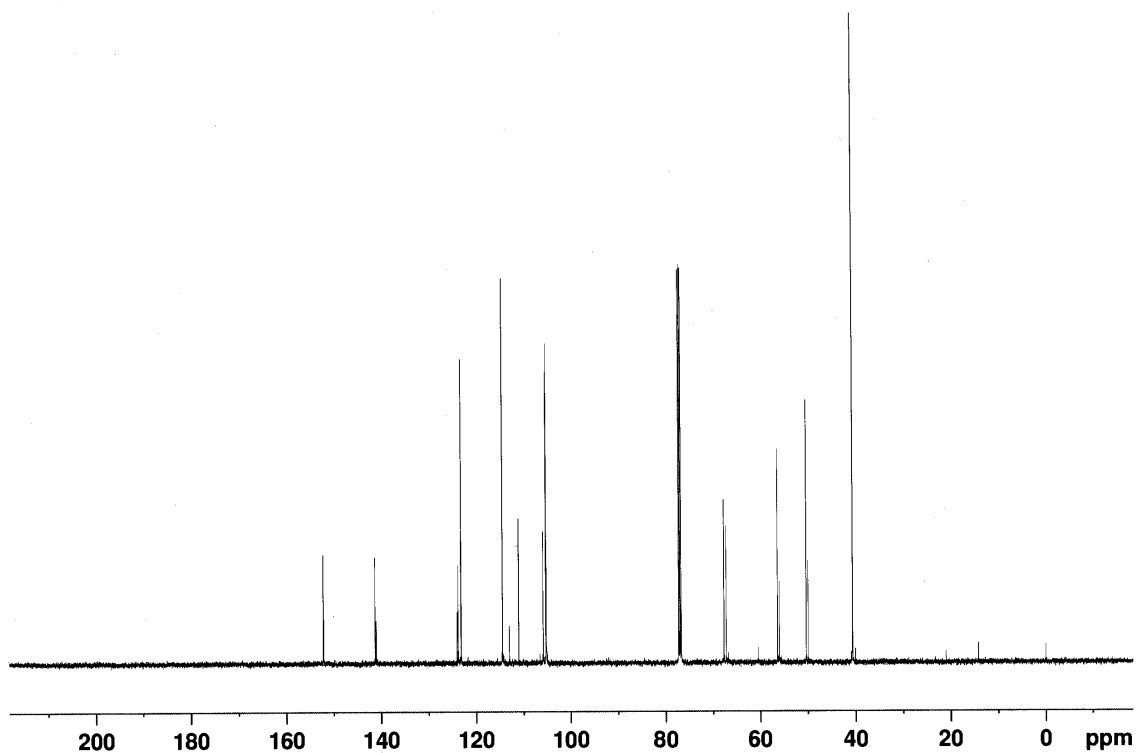
```

F2 - Processing parameters
SI            65536
SF            500.1700095 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

152.275
 152.189
 141.291
 141.085
 124.052
 123.833
 123.256
 123.184
 114.439
 113.019
 111.081
 106.603
 105.931
 105.340
 105.282
 105.258
 105.066
 77.319
 77.065
 76.811
 67.787
 67.331
 66.835
 60.388
 56.408
 56.043
 50.368
 49.968
 40.868
 40.661
 40.076
 21.034
 14.196
 -0.003



14



```

PULPROG      zgpg30
TD           65536
SOLVENT      CDC13
NS           64
DS           4
SWH          29761.904 Hz
FIDRES       0.454131 Hz
AQ           1.1010048 sec
RG           107.18
DW           16.800 usec
DE           11.00 usec
TE           300.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TDO          1
  
```

```

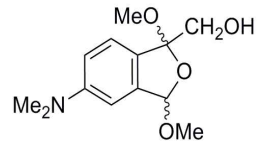
----- CHANNEL f1 -----
SFO1         125.7804227 MHz
NUC1          13C
P1            10.00 usec
PLW1         65.00000000 W
  
```

```

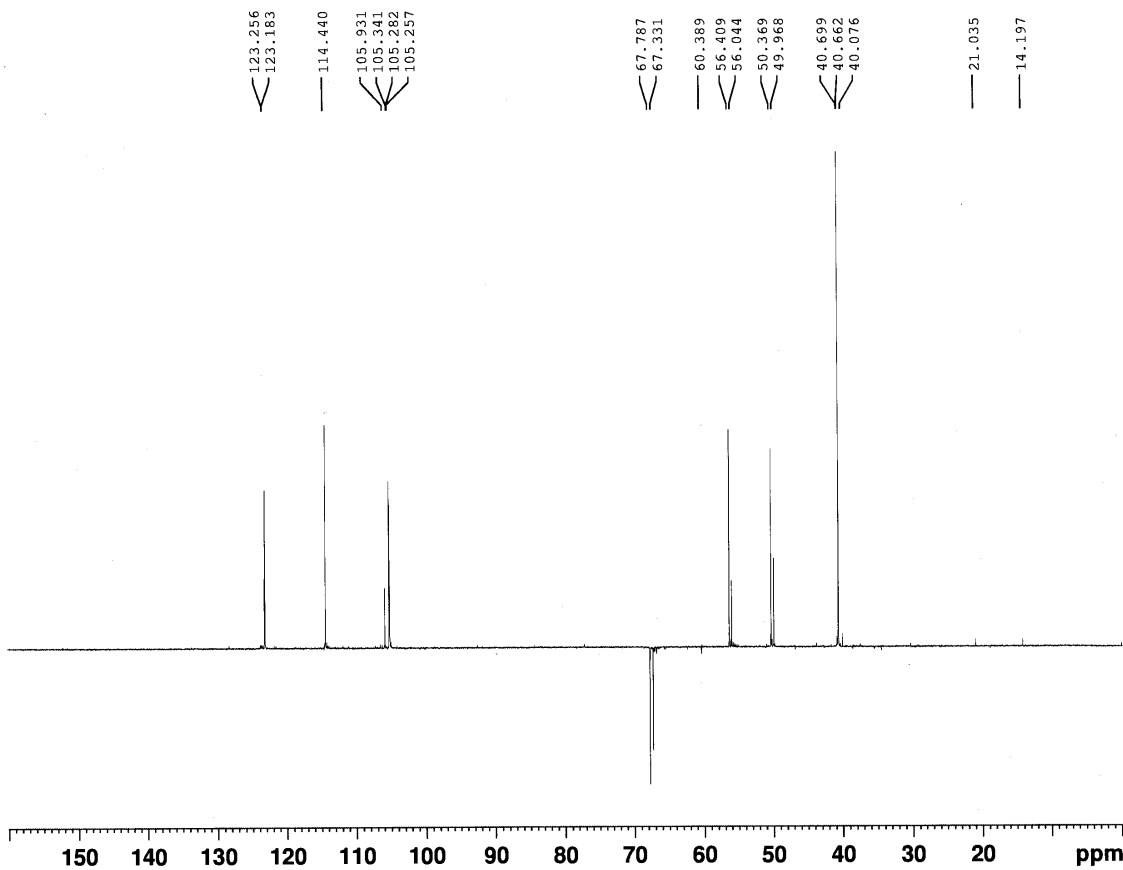
----- CHANNEL f2 -----
SFO2         500.1720007 MHz
NUC2          1H
CPDPRG[2]    waltz16
PCPD2        80.00 usec
PLW2         13.50000000 W
PLW12        0.30375001 W
PLW13        0.19440000 W
  
```

```

F2 - Processing parameters
SI            32768
SF            125.7678470 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```



14

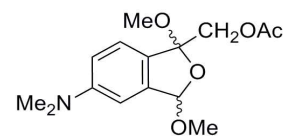


SOLVENT CDC13
 NS 168
 DS 4
 SWH 20161.291 Hz
 FIDRES 0.307637 Hz
 AQ 1.6252928 sec
 RG 189.66
 DW 24.800 usec
 DE 11.00 usec
 TE 300.2 K
 CNST2 145.0000000
 D1 2.000000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1

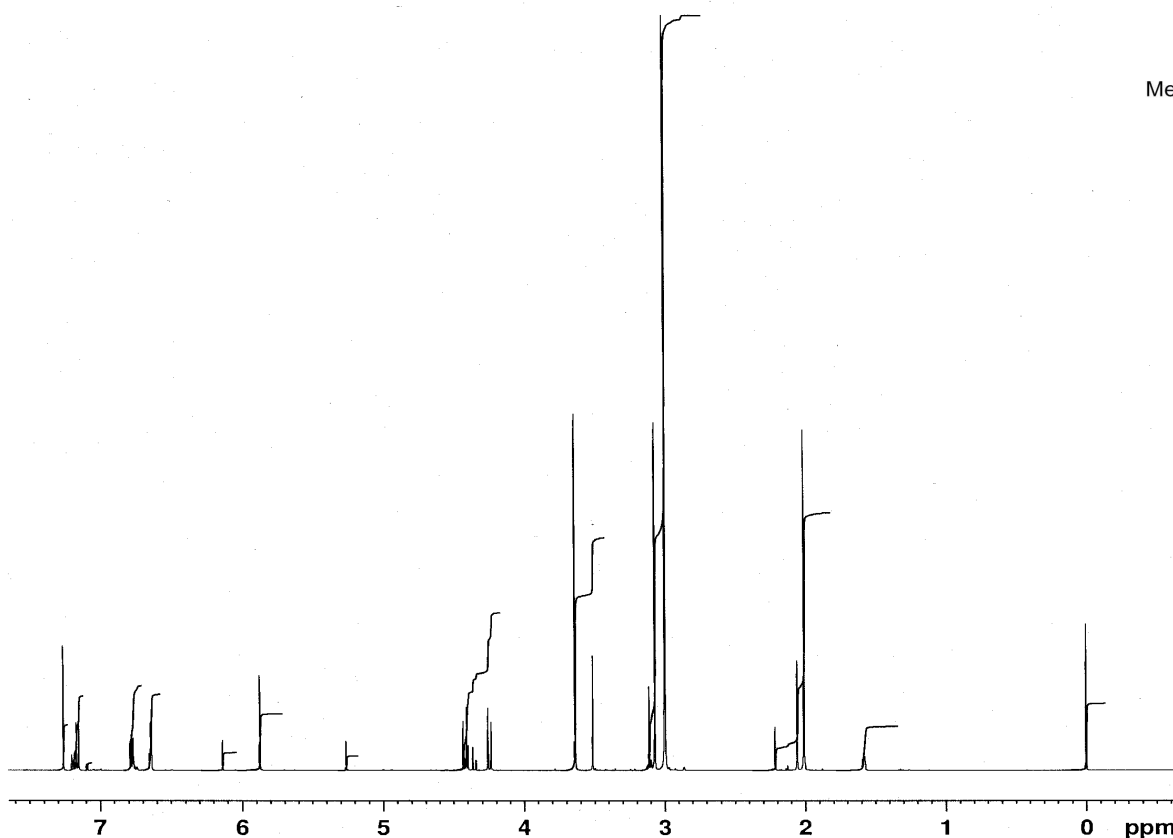
===== CHANNEL f1 =====
 SFO1 125.7779074 MHz
 NUC1 13C
 P1 10.00 usec
 P13 2000.00 usec
 PLW0 0 W
 PLW1 65.00000000 W
 SPNAM[5] Crp60comp.4
 SPOAL5 0.500
 SPOFFS5 0 Hz
 SPW5 9.93130016 W

===== CHANNEL f2 =====
 SFO2 500.1715996 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 F3 12.00 usec
 F4 24.00 usec
 PCPD2 80.00 usec
 PLW2 13.50000000 W
 PLW12 0.30375001 W

F2 - Processing parameters
 SI 32768
 SF 125.7678470 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0



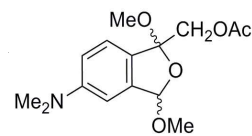
10



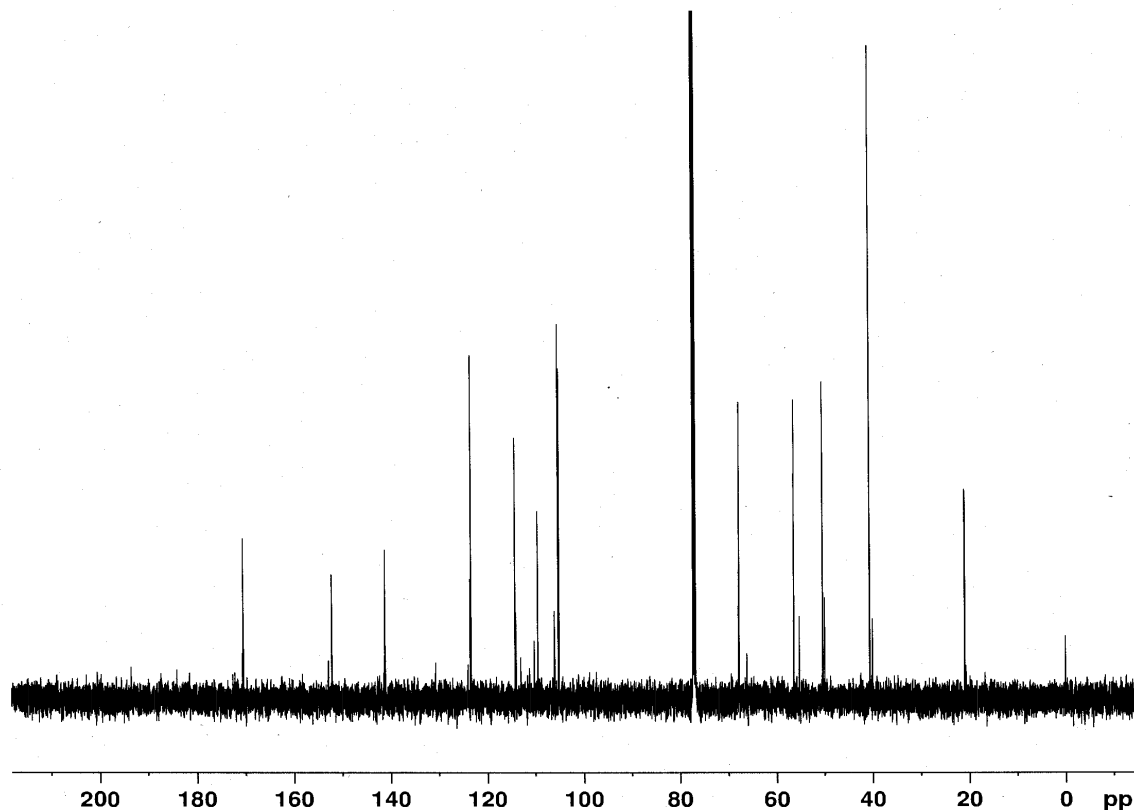
PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.29
 DW 50.000 usec
 DE 10.00 usec
 TE 300.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1730888 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 13.50000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1700109 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



10



```

time 15.23
INSTRUM spect
PROBHD 5 mm QNPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 32
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

```

```

===== CHANNEL f1 =====
SFO1 125.7804227 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W

```

```

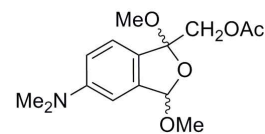
===== CHANNEL f2 =====
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W

```

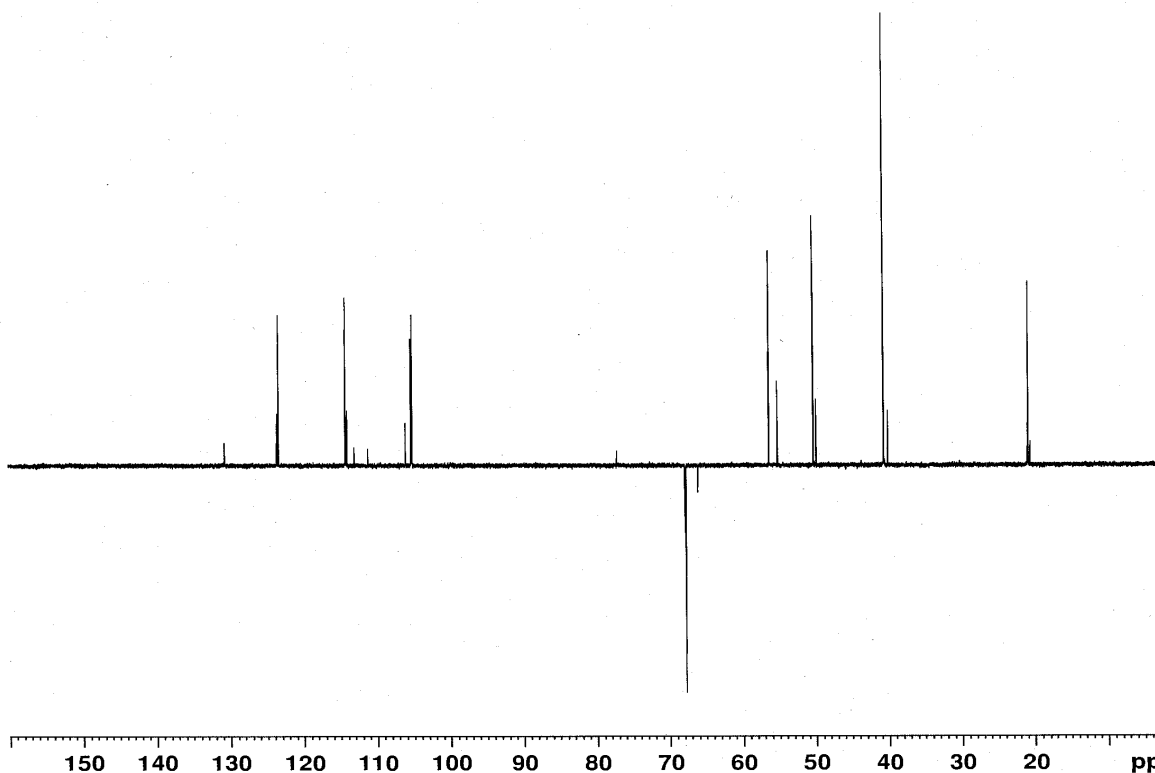
```

F2 - Processing parameters
SI 32768
SF 125.7678470 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```



10



```

PROBHD 5 mm CPPBBO BB
PULPROG deptsp135
TD 65536
SOLVENT CDC13
NS 249
DS 4
SWH 20161.291 Hz
FIDRES 0.307637 Hz
AQ 1.6252928 sec
RG 189.66
DW 24.800 usec
DE 11.00 usec
TE 300.2 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

```

```

===== CHANNEL f1 =====
SFO1 125.7779074 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 65.00000000 W
SPNAM[5] Crp60comp_4
SPOALS 0.500
SPOFFS5 0 Hz
SPW5 9.93130016 W

```

```

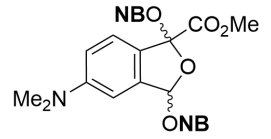
===== CHANNEL f2 =====
SFO2 500.1715996 MHz
NUC2 1H
CPDPRG[2] waltz16
P3 12.00 usec
P4 24.00 usec
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W

```

```

F2 - Processing parameters
SI 32768
SF 125.7678464 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

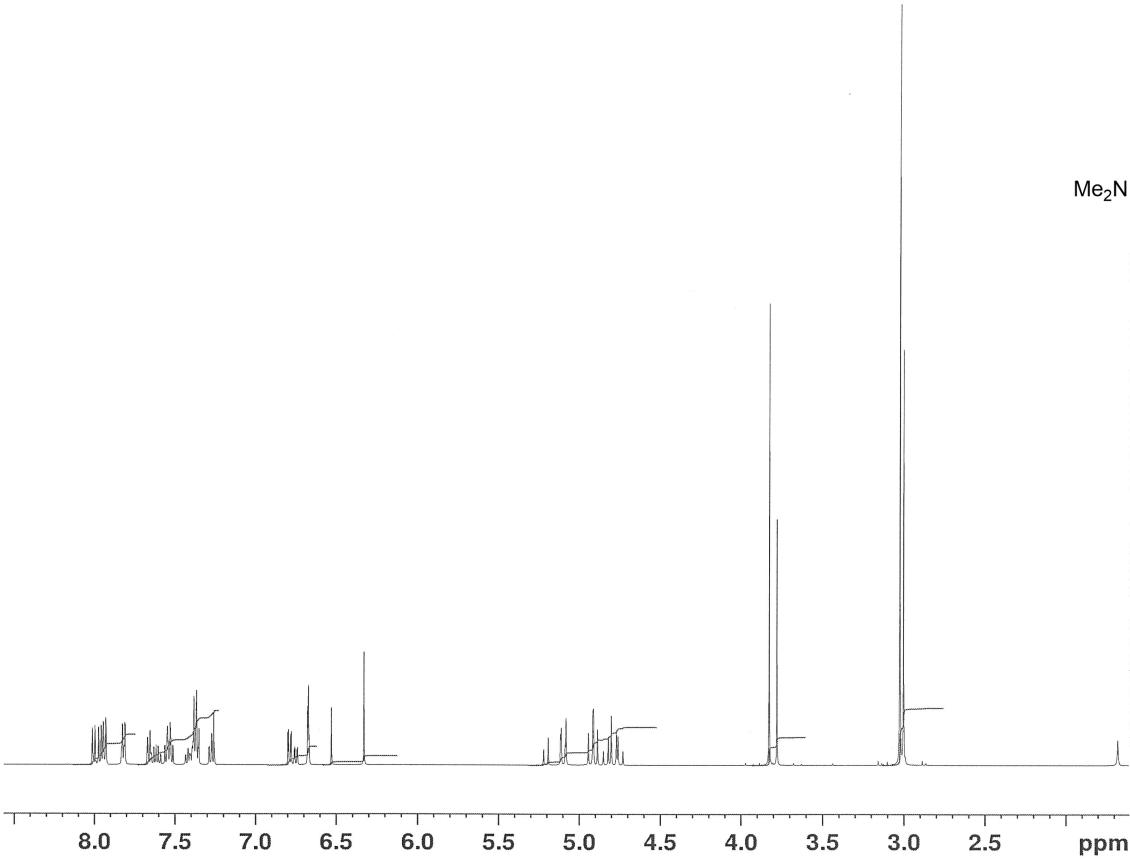
```



PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 22.23
 DW 50.000 usec
 DE 10.00 usec
 TE 300.2 K
 D1 1.00000000 sec
 TD0 1

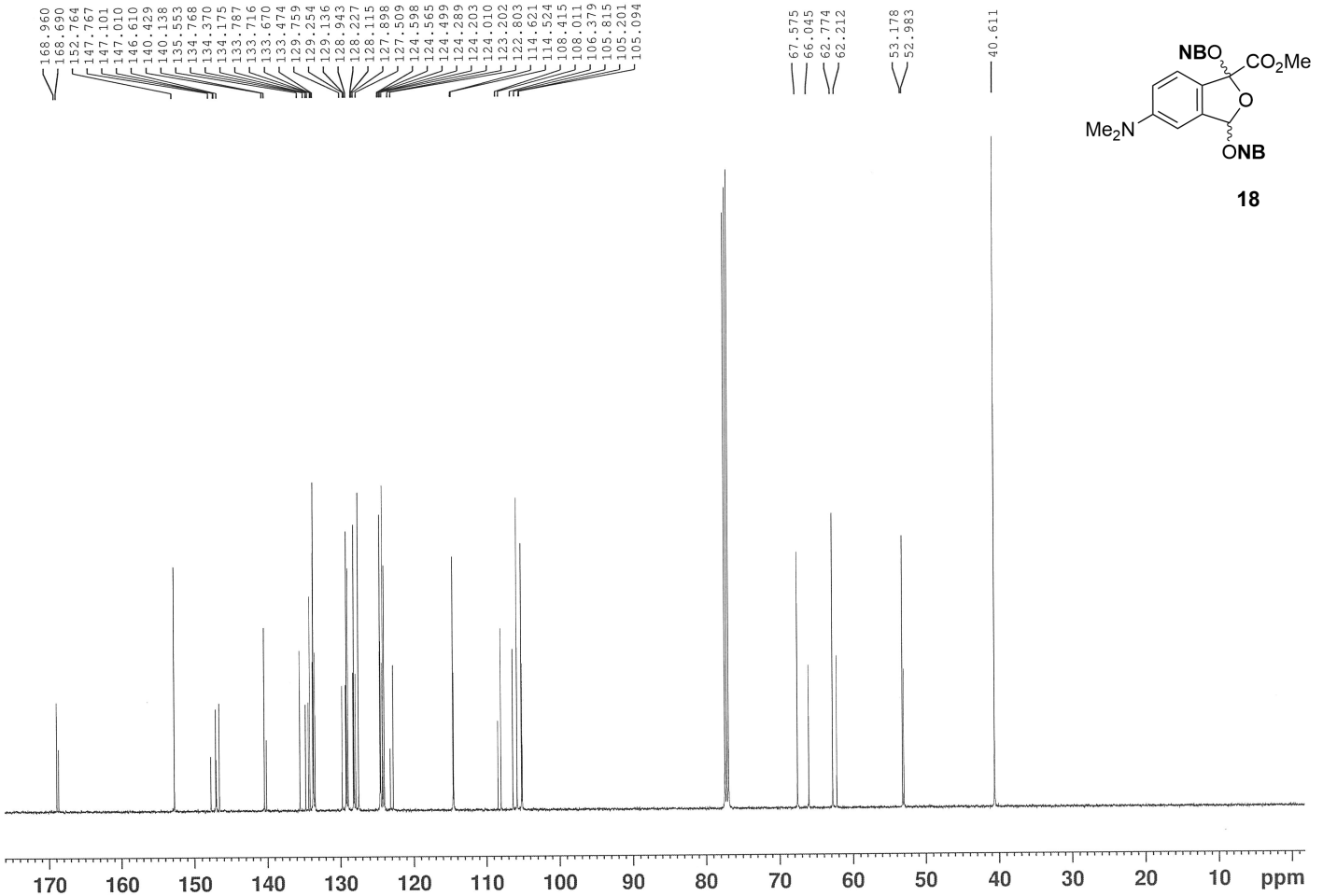
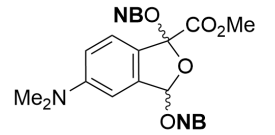
===== CHANNEL f1 =====
 SFO1 500.1730888 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 13.50000000 W

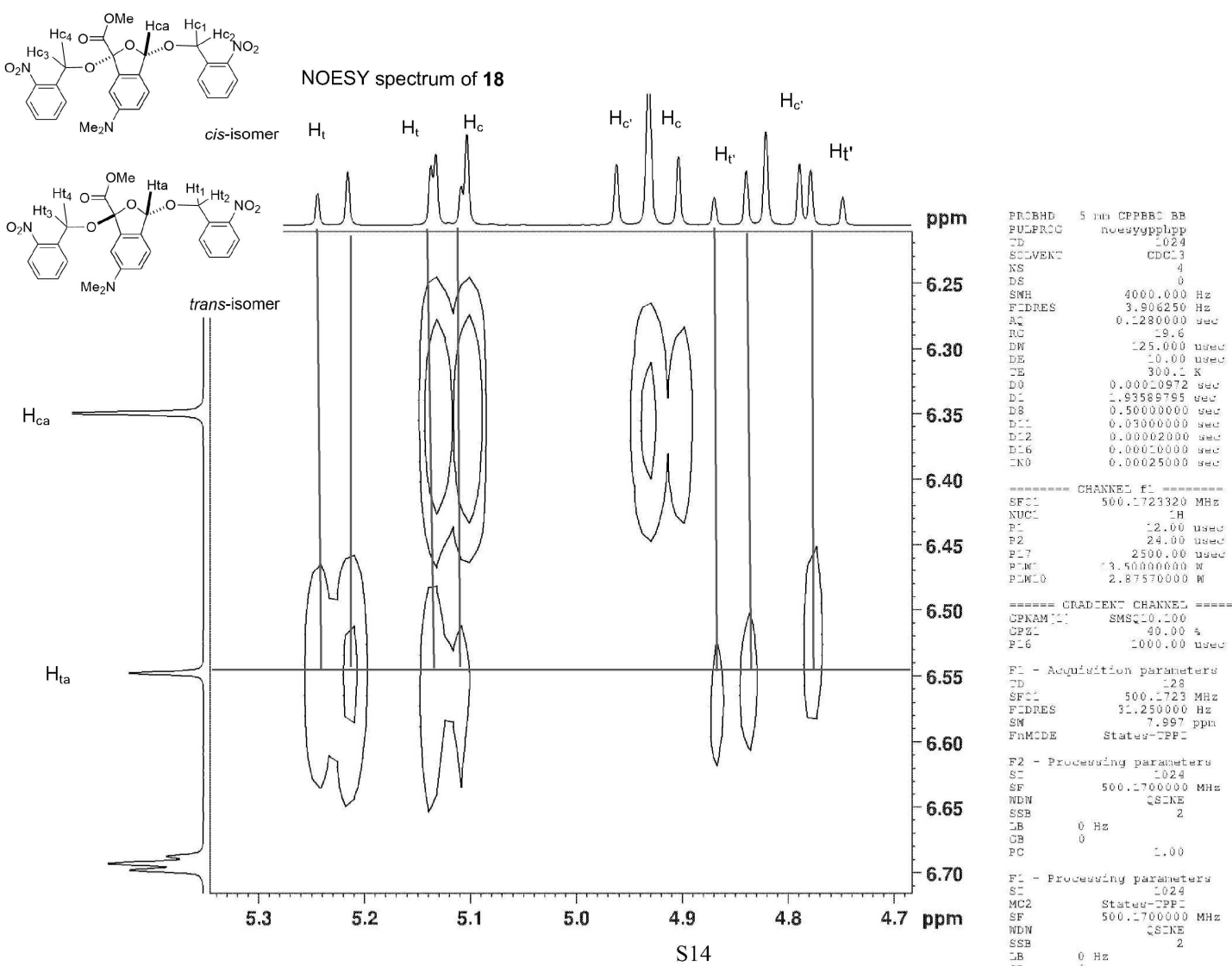
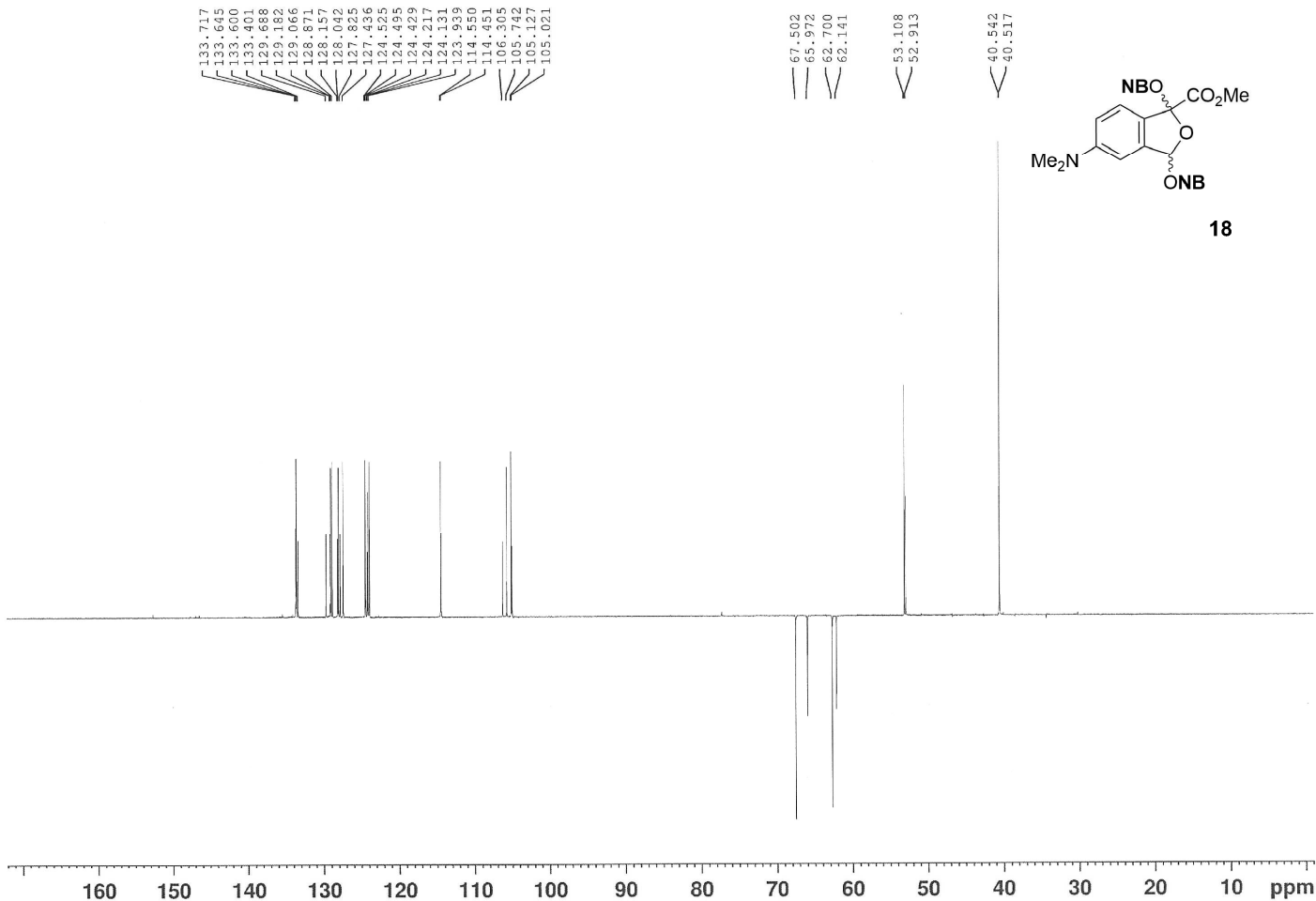
F2 - Processing parameters
 SI 65536
 SF 500.1700124 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

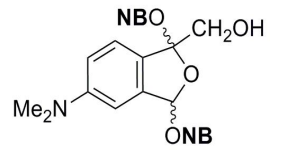


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 134.398
 134.390
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 133.767
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 133.474
 129.759
 129.284
 129.156
 128.933
 128.297
 128.115
 127.898
 127.598
 124.598
 124.525
 124.499
 124.289
 124.203
 124.010
 123.202
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 114.621
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 108.011
 106.379
 105.815
 105.201
 105.094

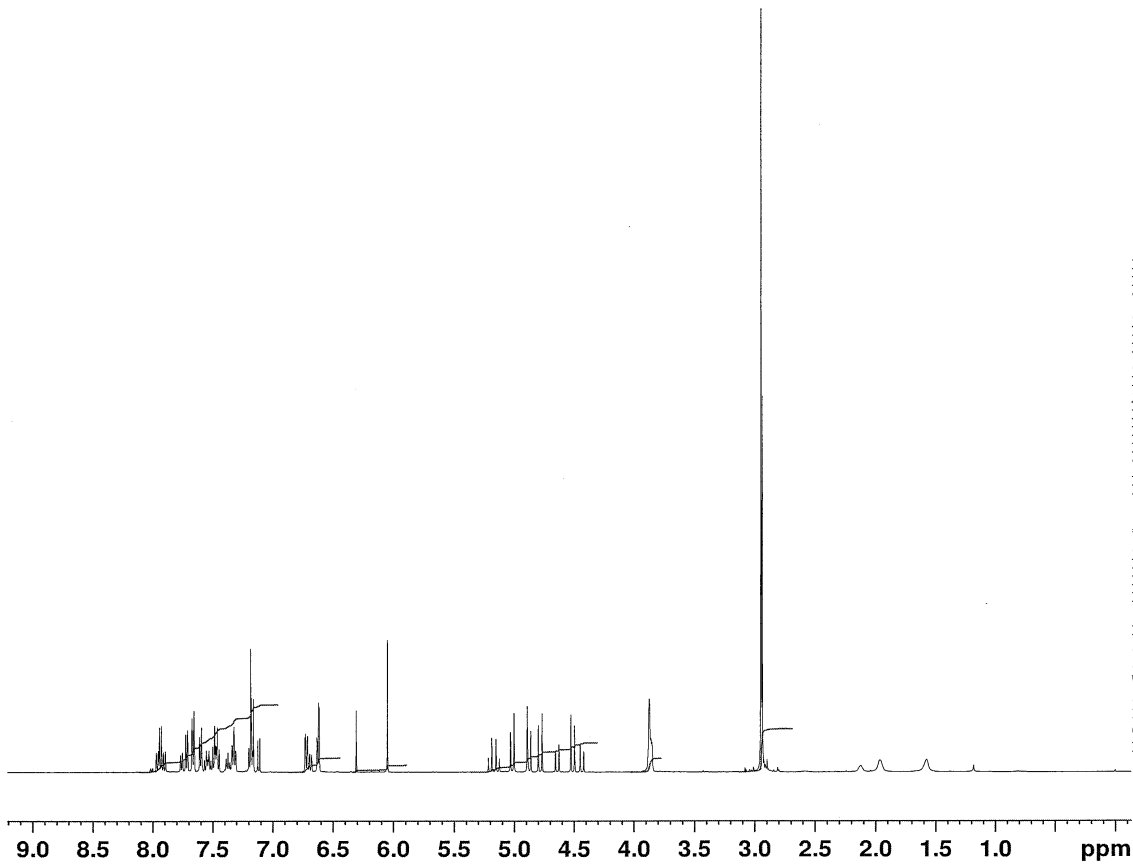
67.575
 66.045
 62.774
 62.212
 53.178
 52.983







17



```

INSIRUM          spect
PROBHD           5 mm CPPBBO BB
PULPROG          zg30
TD               65536
SOLVENT          CDC13
NS               16
DS               2
SWH              10000.000 Hz
FIDRES           0.152588 Hz
AQ               3.2767999 sec
RG               31.29
DW               50.000 usec
DE               10.00 usec
TE               300.2 K
D1               1.00000000 sec
TD0              1

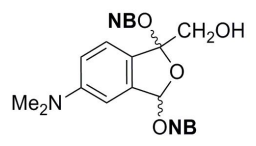
===== CHANNEL f1 =====
SFO1             500.1730888 MHz
NUC1              1H
P1                12.00 usec
PLW1             13.50000000 W

F2 - Processing parameters
SI                65536
SF               500.1700505 MHz
WDW              EM
SSB              0
LB                0.30 Hz
GB               0
PC                1.00
  
```

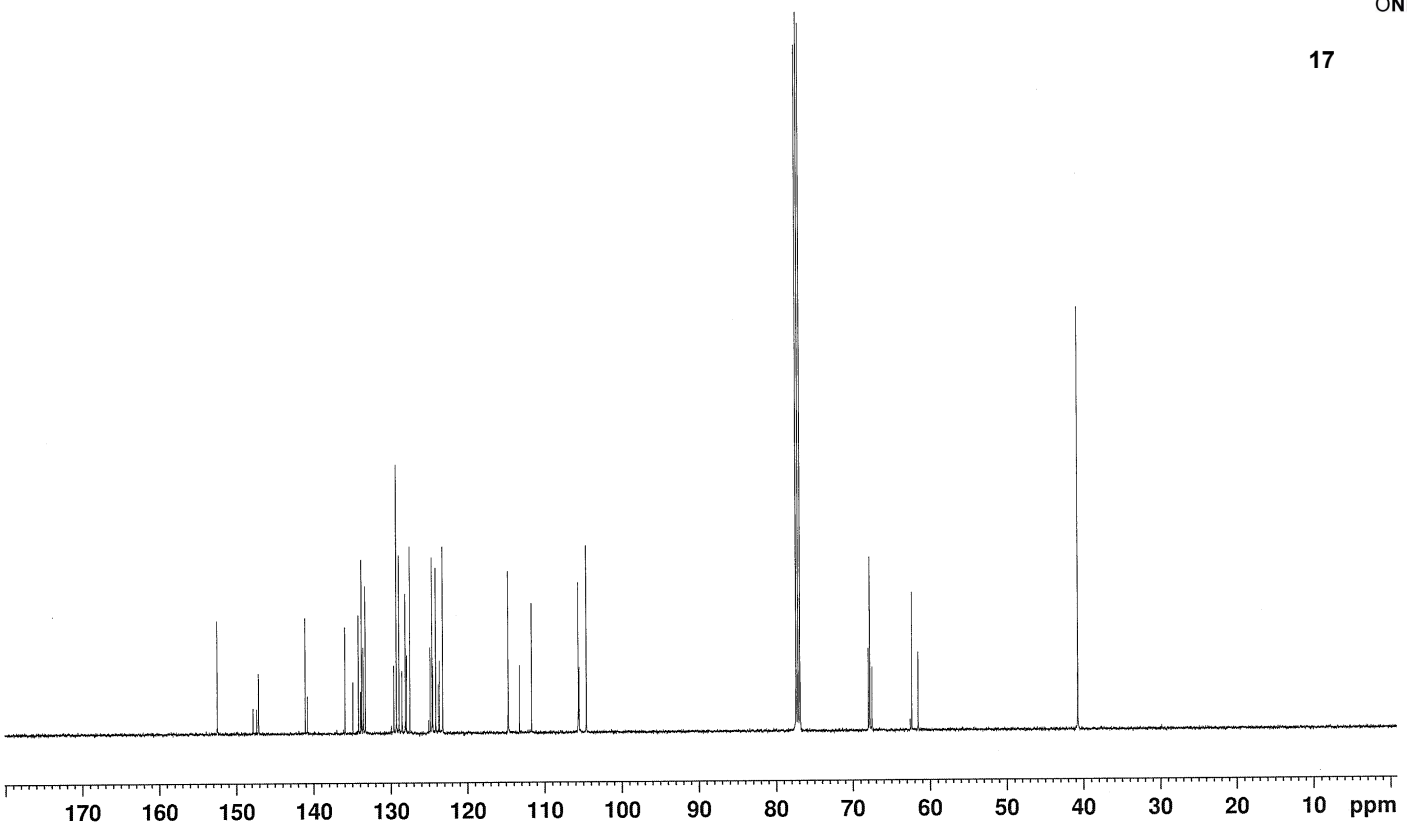
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147.393
147.175
147.126
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135.973
134.948
134.240
134.221
133.943
133.830
133.641
133.613
133.343
129.978
129.629
129.301
128.948
128.576
128.127
127.958
127.532
125.086
124.882
124.635
124.160
123.820
123.678
123.242
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114.733
113.297
111.717
105.673
105.611
105.559
104.632

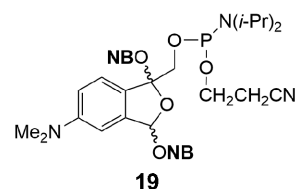
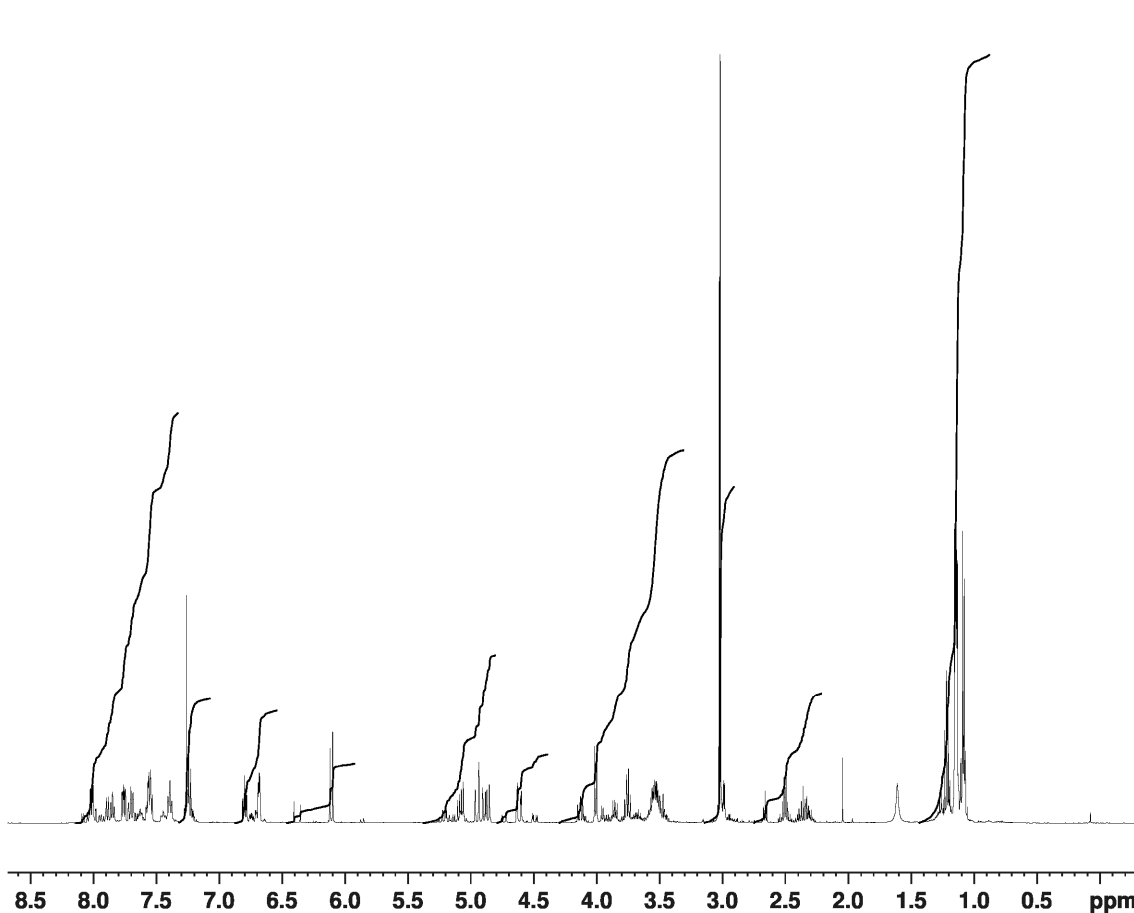
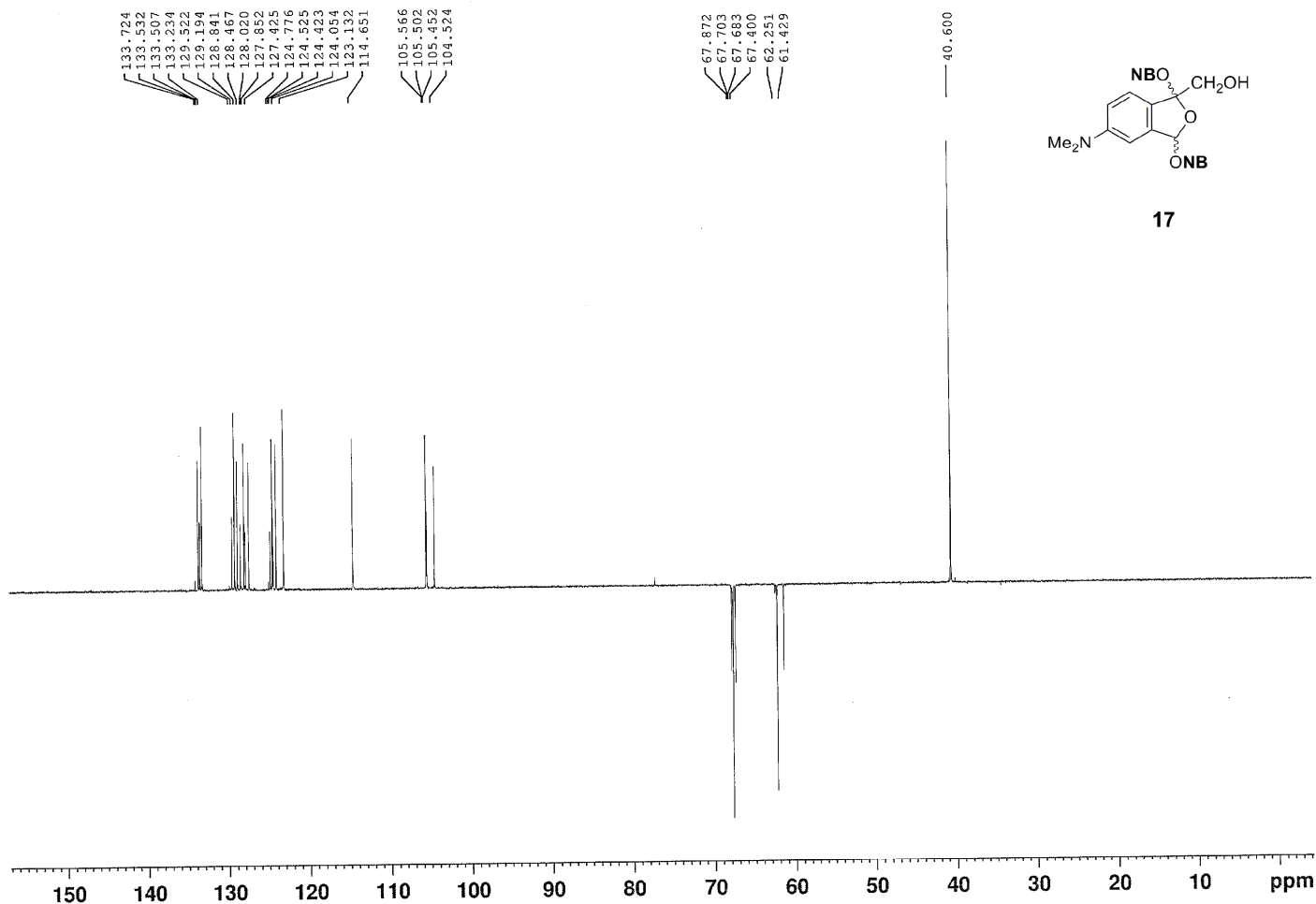
67.981
67.809
67.793
67.507
62.359
61.539

40.741



17



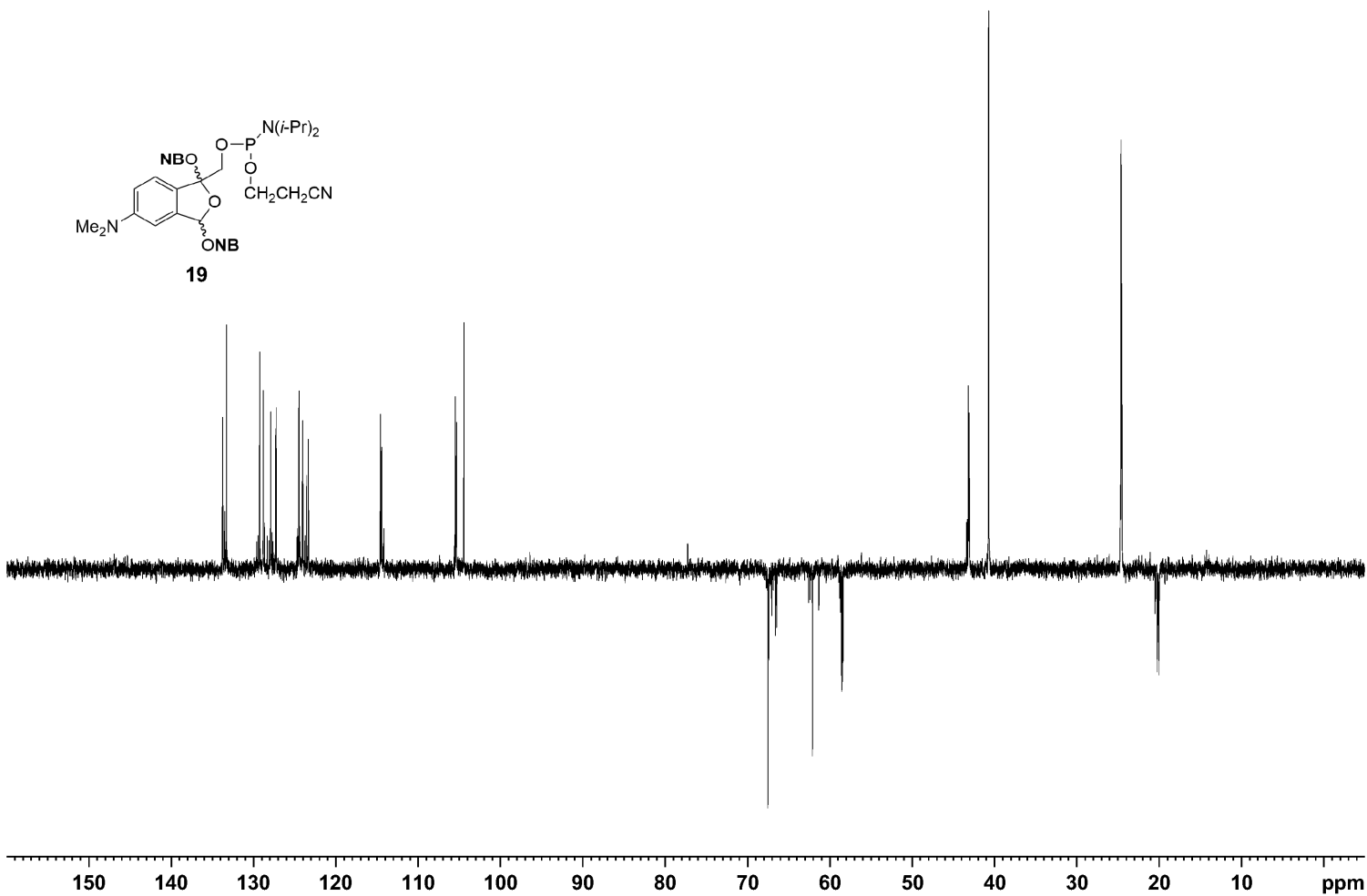
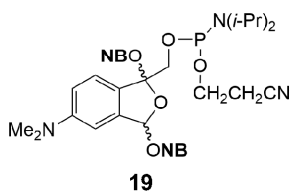
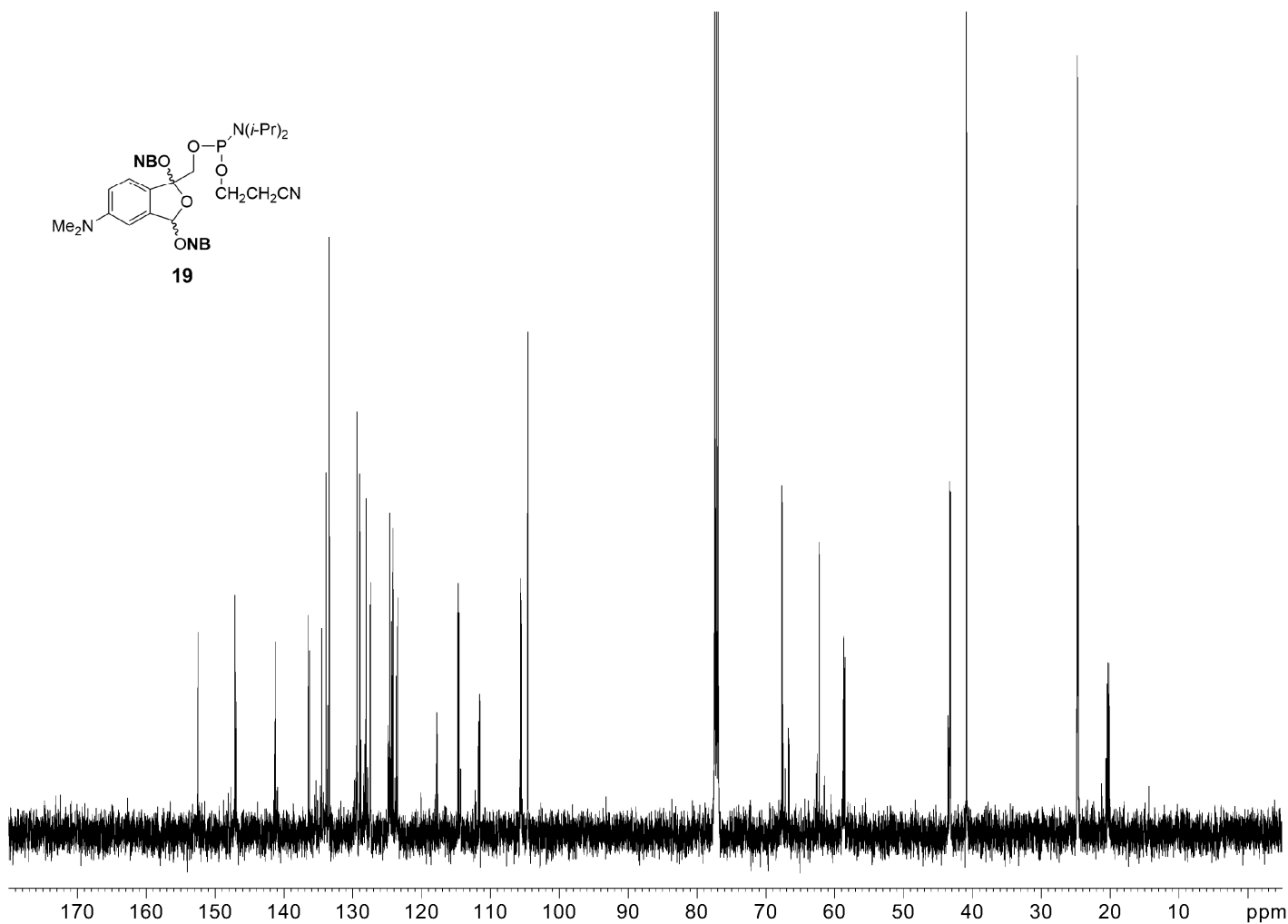
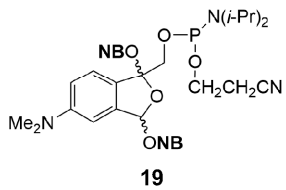


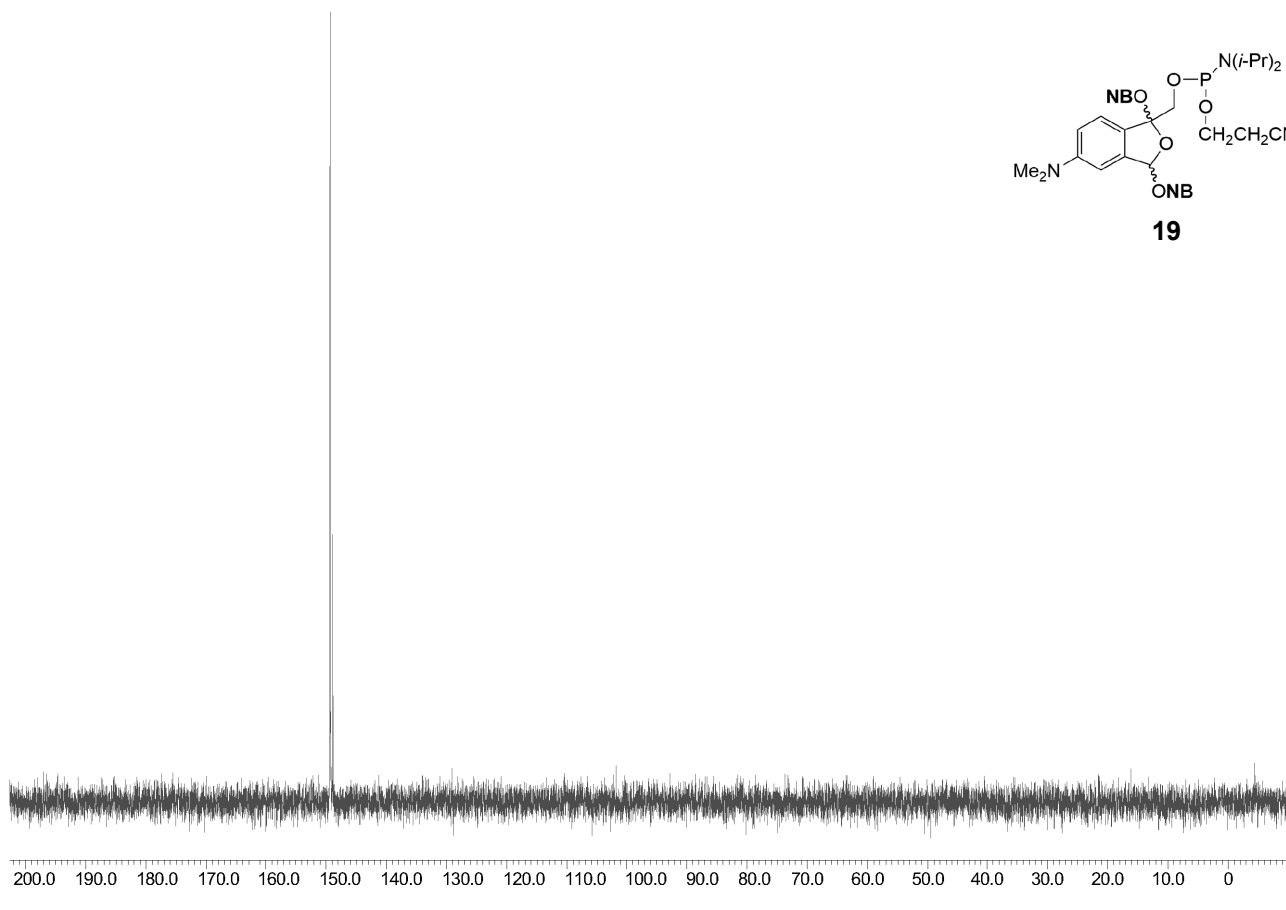
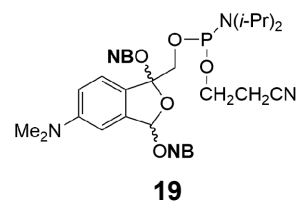
19

Current Data Parameters
 NAME amidite2
 EXPNO 10
 PROCNO 1

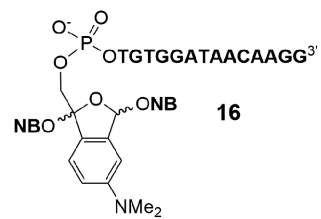
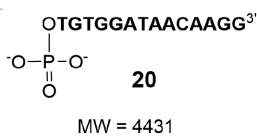
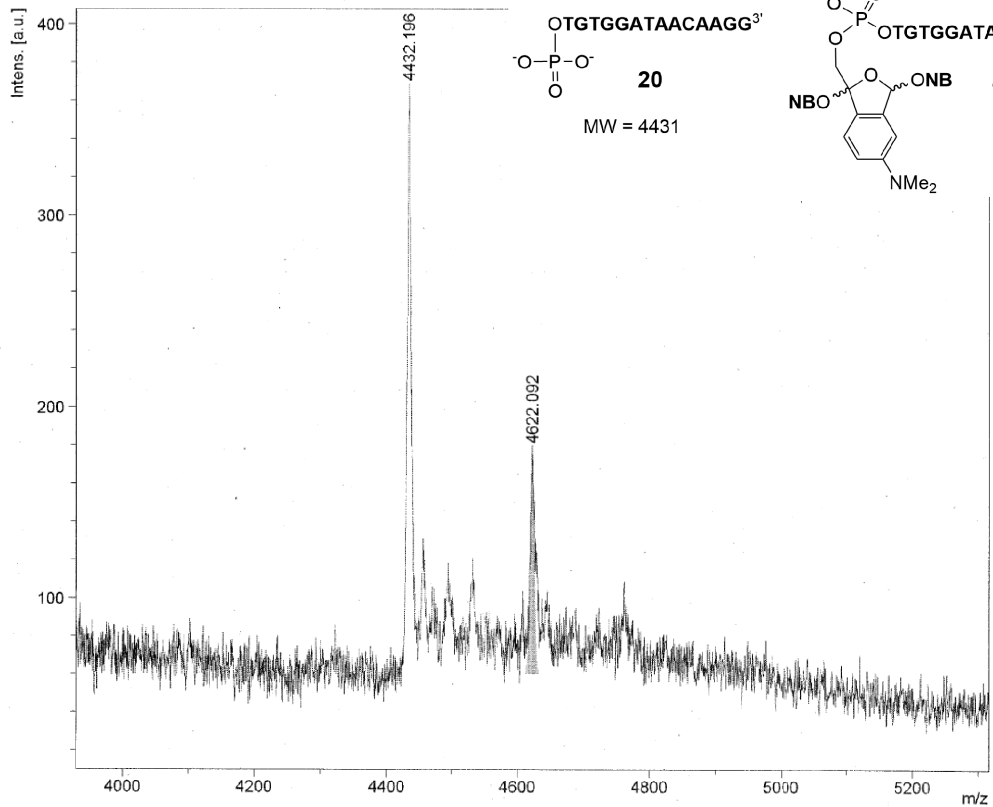
F2 - Acquisition Parameters
 Date_ 20230912
 Time 21.05 h
 INSTRUM spect
 PROBHD z119470_0344 (
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 65.87
 DW 50.000 usec
 DE 13.13 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1730885 MHz
 NUC1 1H
 P0 4.83 usec
 P1 14.50 usec
 PLW1 10.80000019 W

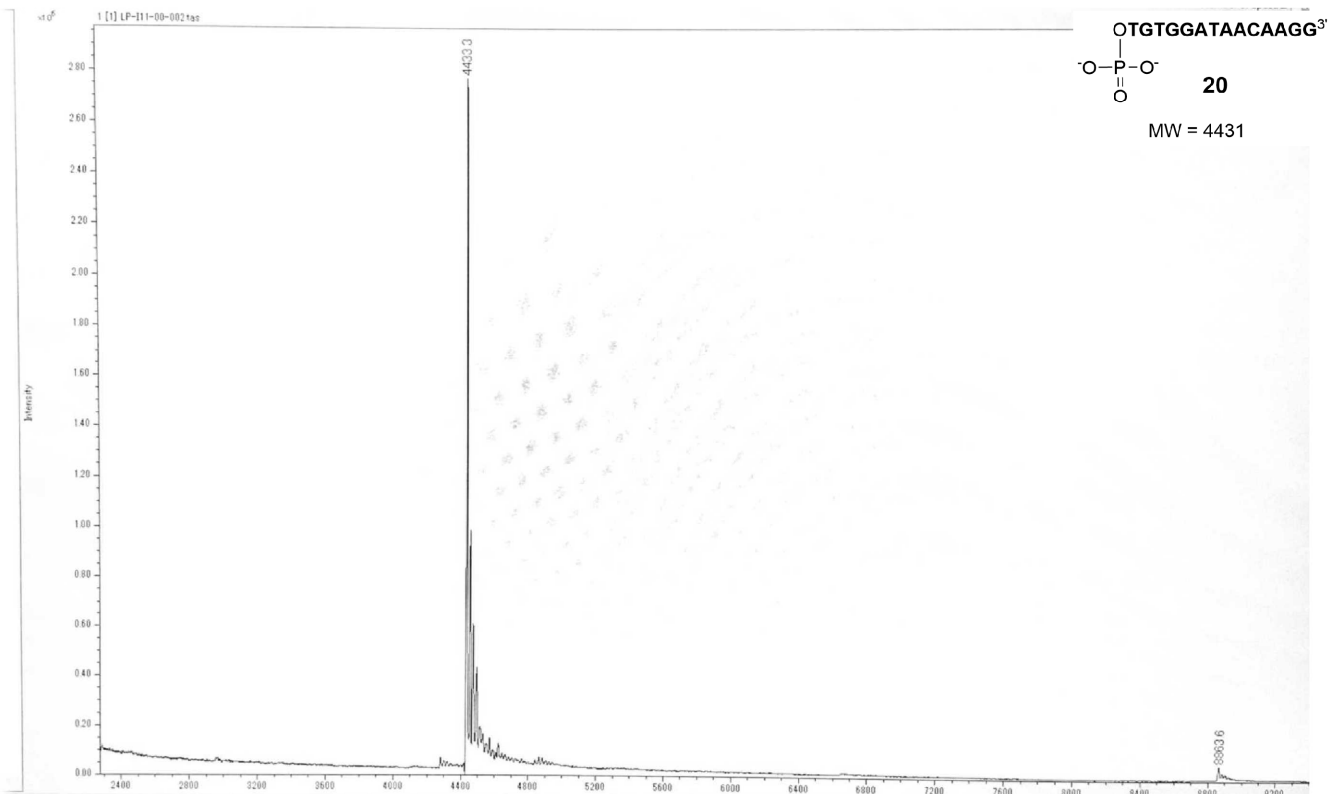
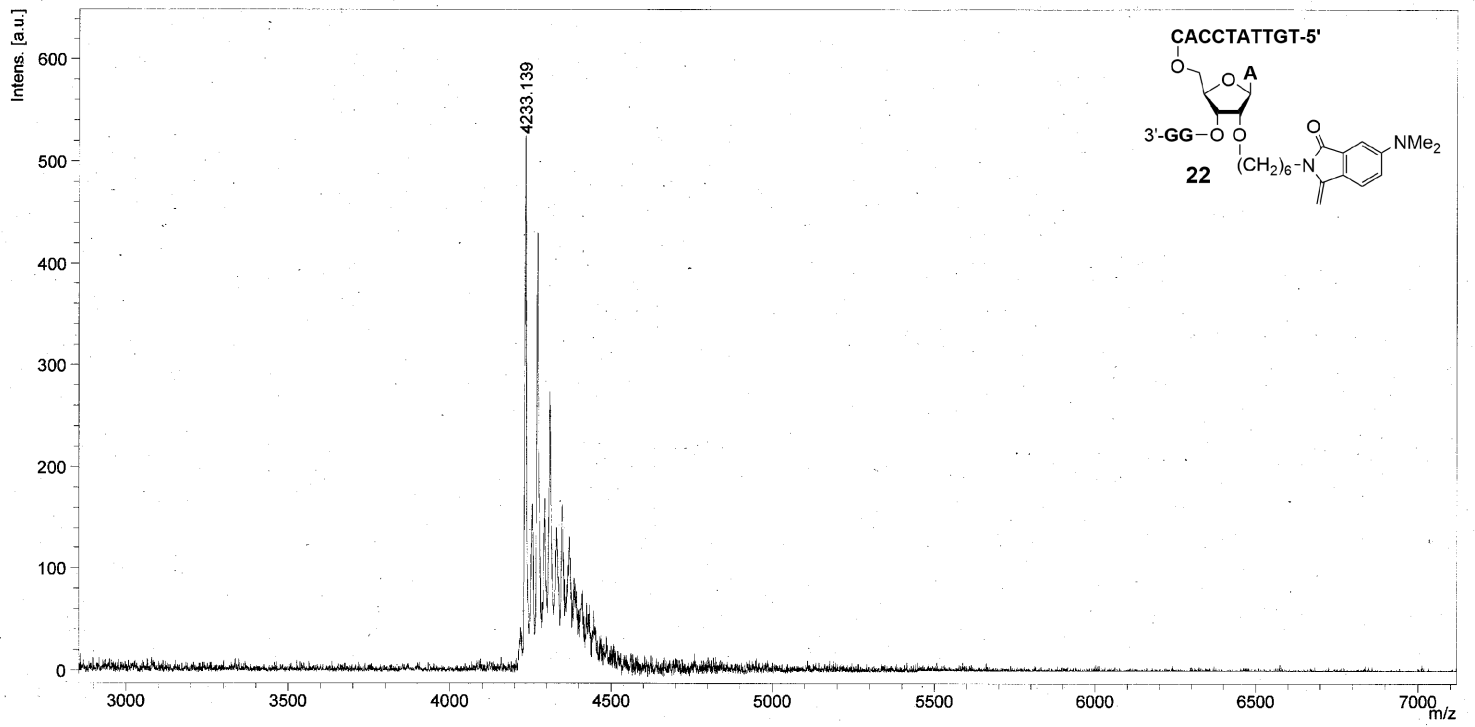
F2 - Processing parameters
 SI 65536
 SF 500.1700129 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





Comment 2





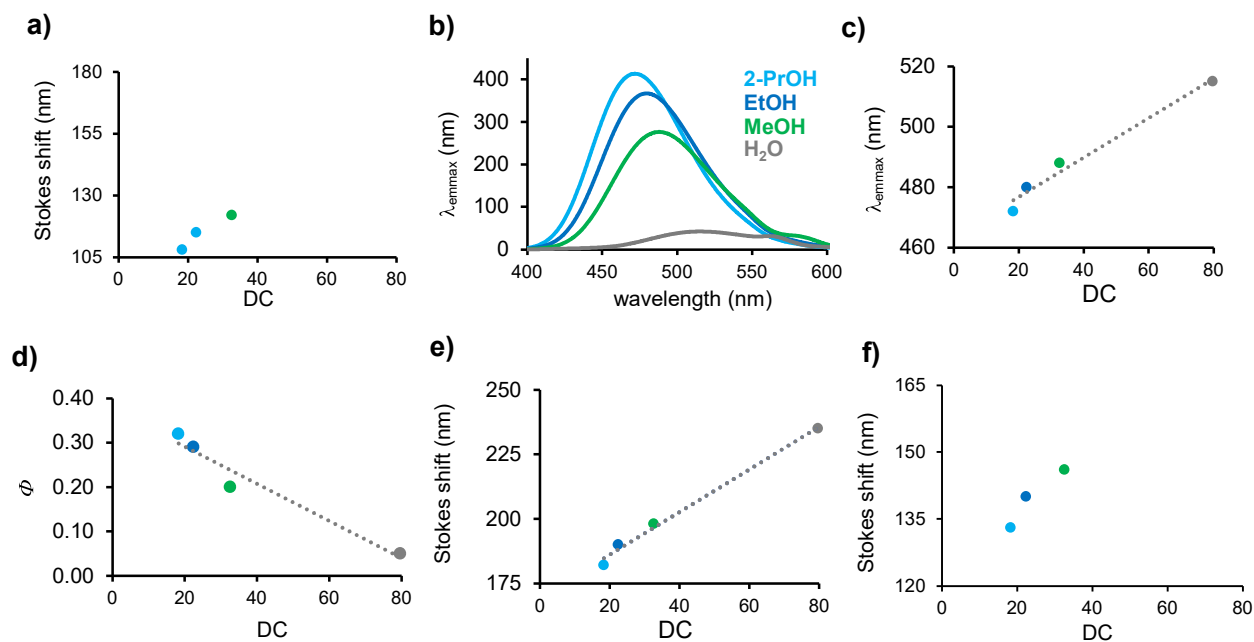


Fig. S1. Plots of data for **7** and **4b**. solvent; **2-PrOH**, **EtOH**, **MeOH**, and **H₂O**.

a) Stokes shift versus solvent dielectric constant (DC), data of **7** (0.1 μM solution,

$\lambda_{\text{ex}} \cong 365$ nm, Table 1)

b) fluorescence spectra of **7** (0.1 μM solution, $\lambda_{\text{ex}} = 280$ or 290 nm, Table 1)

c) λ_{emmax} versus DC, data of **7** (0.1 μM solution, $\lambda_{\text{ex}} = 280$ or 290 nm, Table 1)

d) fluorescence quantum yield versus DC, data of **7** (0.1 μM solution, $\lambda_{\text{ex}} = 280$ or 290 nm, Table 1)

e) Stokes shift versus DC, data of **7** (0.1 μM solution, $\lambda_{\text{ex}} = 280$ or 290 nm, Table 1)

f) Stokes shift versus DC, data of **4b** (Table S2, $\lambda_{\text{ex}} = 396$ nm)

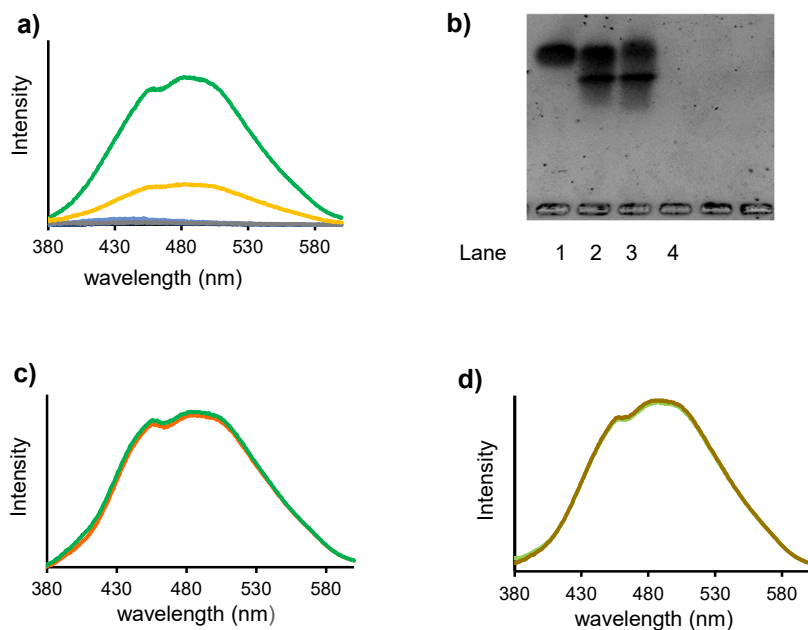


Fig. S2. a) Fluorescence spectra of the reaction of DIV-IV and reactive ODN (—), reactive ODN (—), unmodified ODN (—), and unmodified DIV-IV (—).
 b) 1% Agarose electrophoresis;
 lane 1. reactive ODN,
 lane 2. reaction mixture for DIV modification,
 lane 3. reaction mixture for DIV modification after addition of DNase,
 lane 4. reaction mixture for DIV modification after addition of DNase and CaCl_2
 c) Fluorescence spectra of the reaction of DIV-IV and reactive ODN (—) and after addition of DNase and EDTA (—),
 d) Fluorescence spectra of the reaction mixture (—) and after addition of CaCl_2 (—).

Table S1. Photophysical data of **4** (R = -(CH₂)₁₀-CO₂H) in protic solvents^{a)}

solvent (dielectric constant, 20 °C ^a)	Fluorescence $\lambda_{\text{max}}/\text{nm}$ (λ_{ex})	Φ^b (λ_{ex})
1-BuOH (18.2)	527(410)	0.037
1-PrOH (20.1)	530(410)	0.025
EtOH (22.4)	532 (410)	0.013
MeOH (32.6)	535 (410)	0.006
H ₂ O (79.7)	575 (410)	0.001

^{a)} Saroja, G.; Ramachandram, B.; Saha, S.; Samanta, A., *J. Phys. Chem. B* **1999**, *103*, 2906.

Table S2. Photophysical data of **4** (R = -(CH₂)₆-OH) in protic solvents

solvent (dielectric constant ^a)	UV-Vis absorption $\lambda_{\text{max}}/\text{nm}$ ($\lambda_{\text{og}} \epsilon$)	Fluorescence $\lambda_{\text{max}}/\text{nm}$ (λ_{ex})	Φ^b (λ_{ex})	Stokes shift (λ_{ex})	Brightness $\Phi \times \epsilon$
2-PrOH (18.3)	268 (4.3)	527 (268)	0.031 (268)	259 (268)	600
	324 (3.9)	530 (324)	0.047 (324)	206 (324)	360
	396 (3.8)	529 (396)	0.044 (396)	133 (396)	240
EtOH (22.4)	268 (4.3)	530 (268)	0.014 (268)	262 (268)	260
	324 (3.9)	536 (324)	0.020 (324)	212 (324)	150
	396 (3.7)	536 (396)	0.019 (396)	140 (396)	100
MeOH (32.6)	268 (4.3)	527 (268)	0.006 (268)	259 (268)	110
	324 (3.9)	542 (324)	0.008 (324)	218 (324)	60
	396 (3.7)	542 (396)	0.007 (396)	146 (396)	40
H ₂ O (79.7)	274 (4.3)	553 (274)	0.001 (274)	279 (274)	10
	327 (3.7)	512 (327)	0.002 (327)	185 (327)	

^a20 °C, Handbook of organic solvents properties I. M. Smallwood, 1996 Arnold.

^bRelative quantum yields were obtained from comparison with quinine