# Title: Synthesis of Electron Deficient Acene Derivatives via Bidirectional Iterative Elongation Reaction

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Supporting Information: Syntheses of intermediates **5, 8, 11** and spectroscopic characterization of new compounds

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## General Procedure

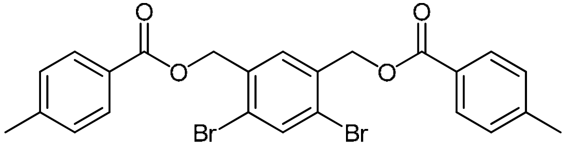
All reactions are performed under 1 atmosphere of dried nitrogen or argon and well mixed with magnetic stirring devices. Reagent grade chemicals and solvents were used in all reactions. Reaction vessels were dried in oven before use. Diethyl ether and tetrahydrofuran were distilled over metallic sodium with benzophenone radical anion as the indicator. Dichloromethane were distilled from $CaH_2$. Flash column chromatography was performed with Merck silica gel 60 (1.11567.9025, 0.040-0.063 mm) as the stationary phase. All reported ratios of mixed eluents are based on volume.

**1,4-diiodo-2,5-dimethylbenzene:** *p*-Xylene (8 g, 0.075 mol) was mixed with potassium iodate (6.5 g, 30 mmol), iodine (21 g, 83 mmol) and 250 mL of acetic acid, 7.5 mL of sulfuric acid and 25 mL of water were added to make a heterogeneous mixture. The reaction was refluxed for 6 hrs. The cooled reaction mixture was slowly poured into ice water. The excess iodine was quenched by adding a saturated solution of sodium thiosulfate. The product was filtered as a crystalline solid in 74%. $^1H$ NMR (400 MHz, $CDCl_3$): δ 2.32 (s, 6H), 7.63 (s, 2H).

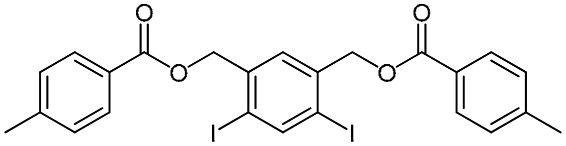
**1,4-bis(bromomethyl)-2,5-diiodobenzene:** 2,5-diiodo-*p*-xylene (10 g, 28 mmol) was dissolved in 100 ml 1,2-dibromoethane. Bromine

(2.88 ml, 56 mmol) was added and it was heated to 135 °C for 6 hours. Another equivalent of Bromine (1.44 ml, 28 mmol) was added. The mixture was stirred over night at 135 °C, cooled to room temperature, poured into a saturated solution of sodium thiosulfate and extracted. In the organic phase a precipitate was formed that was filtered of and recrystallized from chloroform to give the product (3.3 g, 23%). $^1$H NMR (500 MHz, $CDCl_3$): δ 4.46 (s, 4H), 7.87 (s, 2H).

**5, (2,5-diiodo-1,4-phenylene)bis(methylene)bis(4-methylbenzoate):** Potassium carbonate ( 0.14 g, 1.02 mmol) was added to a DMF (15mL) solution of and *p*-toluic acid (0.14 g, 1.02 mmol) and 1,4-bis(bromomethyl)-2,5-diiodobenzene (0.24 g, 0.47 mmol). After the mixture was stirred for overnight, $CH_2Cl_2$ was added and the mixture was washed with water to remove DMF. The organic layer was dried over $MgSO_4$ and concentrated, then purified with flash chromatography ($CH_2Cl_2$/hexane = 2/1) to give pure product (0.23 g, 79%). IR (KBr) ν (cm$^{-1}$): 749, 1110, 1178, 1170, 1609, 1715, 2926, 3034; $^1$H NMR (400 MHz, DMSO-$d_6$): δ 2.38 (s, 6H), 5.27 (s, 4H), 1.39-1.45 (m, 8H), 7.35 (d, *J* = 8.0 Hz, 4H), 7.88 (d, *J* = 8.0 Hz, 4H), 8.04 (s, 2H); $^{13}$C NMR (125 MHz, CDCl3): δ 21.64, 68.92, 97.75, 126.83, 129.18, 129.81, 139.76, 140.37, 144.03, 165.96; HRMS. (MALDI, $[M+Na]^+$), $C_{24}H_{20}I_2O_4Na$, Found: 648.9355.



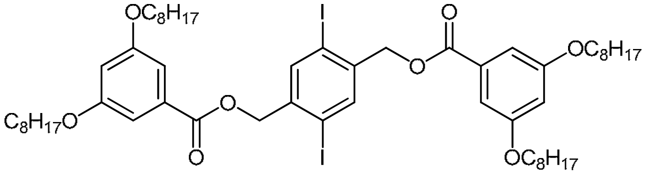
**(4,6-dibromo-1,3-phenylene)bis(methylene) bis(4-methylbenzoate):** DCC (8.13 g, 39.4 mmol) was added to a ice-cooled $CH_2Cl_2$ solution of 1,5-dibromo-2,4-bis-hydroxymethyl-benzene (3 g, 10.1 mmol), *p*-toluic acid (3.59 g, 26.3 mmol) and DMAP (0.32 g, 2.6 mmol). After stirred for 1 hr at 0 °C, the mixture was warmed back to room temperature and then stirred for overnight. The solvent was removed in vacuo and the residual was extracted with $CH_2Cl_2$. Organic layer was dried over $MgSO_4$ and concentrated, then purified with flash chromatography ($CH_2Cl_2$/hexane = 2/1) to give product (3.85 g, 72%, with minor impurities). IR (KBr) $\nu$ ($cm^{-1}$): 749, 1046, 1109, 1176, 1610, 1723, 2851, 2926; $^1H$ NMR (400 MHz, $CDCl_3$): $\delta$ 2.39 (s, 6H), 5.35 (s, 4H), 7.16 (d, *J* = 8.0 Hz, 4H), 7.60 (s, 1H), 7.84(s, 1H), 7.91 (d, *J* = 8.0 Hz, 4H); $^{13}C$ NMR (100 MHz, CDCl3): $\delta$ 21.66, 65.24, 122.82, 126.83, 129.16, 129.72, 130.59, 135.22, 136.16, 143.87, 165.98; HRMS. (MALDI, $[M+Na]^+$), $C_{24}H_{20}Br_2O_4Na$, Calc: 552.9626, Found: 552.9625.



**9, (4,6-diiodo-1,3-phenylene)bis(methylene)bis(4-methylbenzoate):** *N*,*N'*-dimethylethylenediamine (0.02 mL, 0.19 mmol) was added to a dioxane solution (15.0 ml) of (4,6-dibromo-1,3-phenylene)bis(methylene) bis(4-methylbenzoate) (0.50 g, 0.94 mmol), CuI (36 mg, 0.19 mmol) and NaI (0.82 g, 4.69 mmol) under $N_2$ atmosphere. The solution was stirred at 110 °C for 24 hours. Then the second batch of CuI (36 mg, 0.19 mmol), NaI (0.82 g, 4.69 mmol), *N*,*N'*-dmethylethylenediamine (0.02 mL, 0.19 mmol) was added to the solution and the solution was stirred at 110 °C for 66 hours. Dichloromethane (20 mL) was added to the reaction mixture and the solution was washed by 3 % aqueous $NH_3$ (2×30 mL) and $H_2O$ (30mL). The organic solvent was dried over anhydrous $MgSO_4$. The insoluble materials were filtered off and the filtrate was evaporated. The residue was purified by flash chromatography ($CH_2Cl_2$/hexane = 2/1) to give pure product (0.4g, 68%). IR (KBr) ν ($cm^{-1}$): 1068, 1171, 1302, 1422, 1598, 1695, 2872, 2936, 2957; $^1H$ NMR (400 MHz, $CDCl_3$): δ 2.39 (s, 6H), 5.27 (s, 4H), 7.17 (d, *J* = 8.0 Hz, 4H), 7.50 (s, 1H), 7.92 (d, *J* = 8.0 Hz, 4H), 8.36(s, 1H); $^{13}C$ NMR (125 MHz, $CDCl_3$): δ 21.68, 69.42, 97.79, 126.86, 129.06, 129.19, 129.79, 139.22, 143.92, 148.60, 166.00.

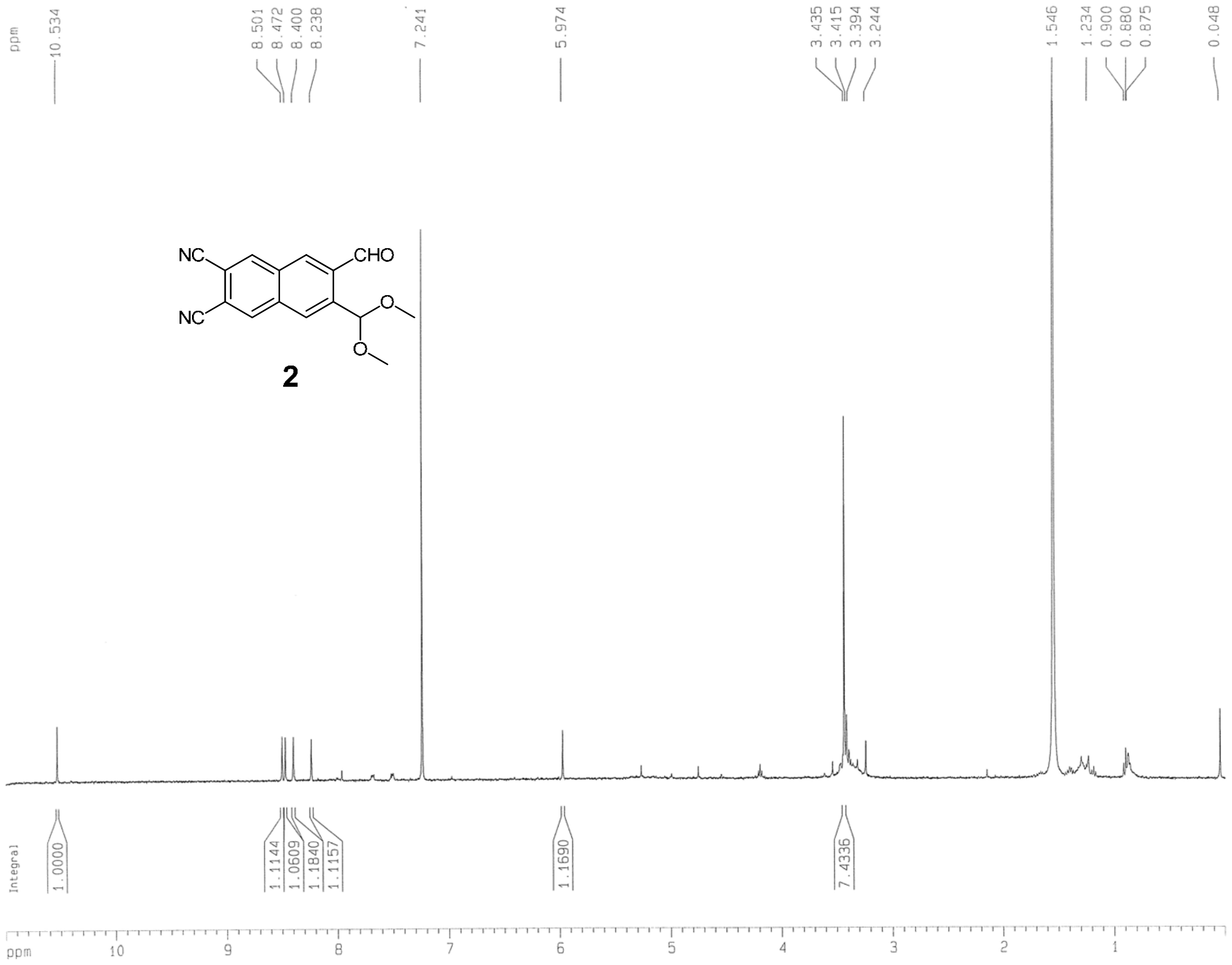
**Methyl 3,5-dioctyloxybenzoate:** A mixture of $K_2CO_3$ (14.80 g, 108 mmol) and methyl 3,5-dihydroxybenzoate (3 g, 18 mmol) in MeCN (60 mL) was refluxed for 30 min under $N_2$ atmosphere. 1-Bomooctane (8.69 g, 0.045 mol) was added dropwise to the mixture, and then refluxed for 24 h. The reaction was cooled to room temperature and filtered. The inorganic residue was washed with $CH_2Cl_2$ (2×50 mL). The filtrate was concentrated under vacuum, the residue dissolved in $CH_2Cl_2$ (75 mL) and washed with a 0.5 M NaOH solution and water, dried over $MgSO_4$ and concentrated in vacuo to give the product (6.25 g, 88%). $^1$H NMR (500 MHz, $CDCl_3$): δ 0.87 (t, *J* = 7.0 Hz, 6H), 1.26-1.30 (m, 16H), 1.40-1.45 (m, 4H), 1.72-1.78 (m, 4H), 3.87(s, 3H), 3.94 (t, *J* = 6.5 Hz, 4H), 6.61 (t, *J* = 2.5 Hz, 1H), 7.13 (d, *J* = 2.5 Hz, 2H).

**3,5-Dioctyloxybenzoic acid:** Methyl 3,5-dioctyloxybenzoate (2.4 g, 6 mmol) was added to a solution of KOH (4.8 g, 84 mmol) in ethyl alcohol (60 mL) and the mixture was refluxed for 5 hrs. The solvent was removed in vacuo. The mixture was then poured into 20 mL of water and acidified with HCl. The mixture was extracted with $CH_2Cl_2$, the combined organic phase was dried over $MgSO_4$ and concentrated to give the product (1.90 g, 82%). $^1$H NMR (400 MHz, $CDCl_3$): δ 0.87 (t, *J* = 6.8 Hz, 6H), 1.27-1.32 (m, 16H), 1.41-1.45 (m, 4H), 1.73-1.80 (m, 4H), 3.96 (t, *J* = 6.8 Hz, 4H), 6.66 (t, *J* = 2.4 Hz, 1H), 7.18 (d, *J* = 2.4 Hz, 2H).



**(2,5-diiodo-1,4-phenylene)bis(methylene) bis(3,5-bis(octyloxy)benzoate):** Potassium carbonate (0.37 g, 2.68 mmol) was added to a DMF (40mL) solution of and methyl 3,5-dioctyloxybenzoate (1.00 g, 2.68 mmol) and 1,4-bis(bromomethyl)-2,5-diiodobenzene (0.60 g, 1.16 mmol). After the mixture was stirred for overnight, $CH_2Cl_2$ was added and the mixture was washed with water to remove DMF. The organic layer was dried over $MgSO_4$ and concentrated, then purified with flash chromatography ($CH_2Cl_2$/hexane = 1/1) to give pure product (0.94 g, 73%). IR (KBr) ν (cm$^{-1}$): 1108, 1170, 1226, 1445, 1608, 1727, 2853, 2921; $^1$H NMR (400 MHz, $CDCl_3$): δ 0.87 (t, *J* = 6.6 Hz, 12H), 1.25-1.32 (m, 32H), 1.39-1.45 (m, 8H), 1.74-1.78 (m, 8H), 3.96 (t, *J* = 6.5 Hz, 8H), 5.28 (s, 4H), 6.64 (t, *J* = 2.2 Hz, 2H), 7.19 (d, *J* = 2.2 Hz, 4H); $^{13}$C

NMR (100 MHz, $CDCl_3$): δ 14.07, 22.62, 25.99, 29.14, 29.20, 29.30, 31.78, 68.29, 69.07, 97.72, 106.83, 107.78, 131.15, 139.74, 140.27, 160.18, 165.73; HRMS. (FAB, $M^+$), $C_{54}H_{80}I_2O_8$, Calc: 1110.3943, Found: 1110.3949.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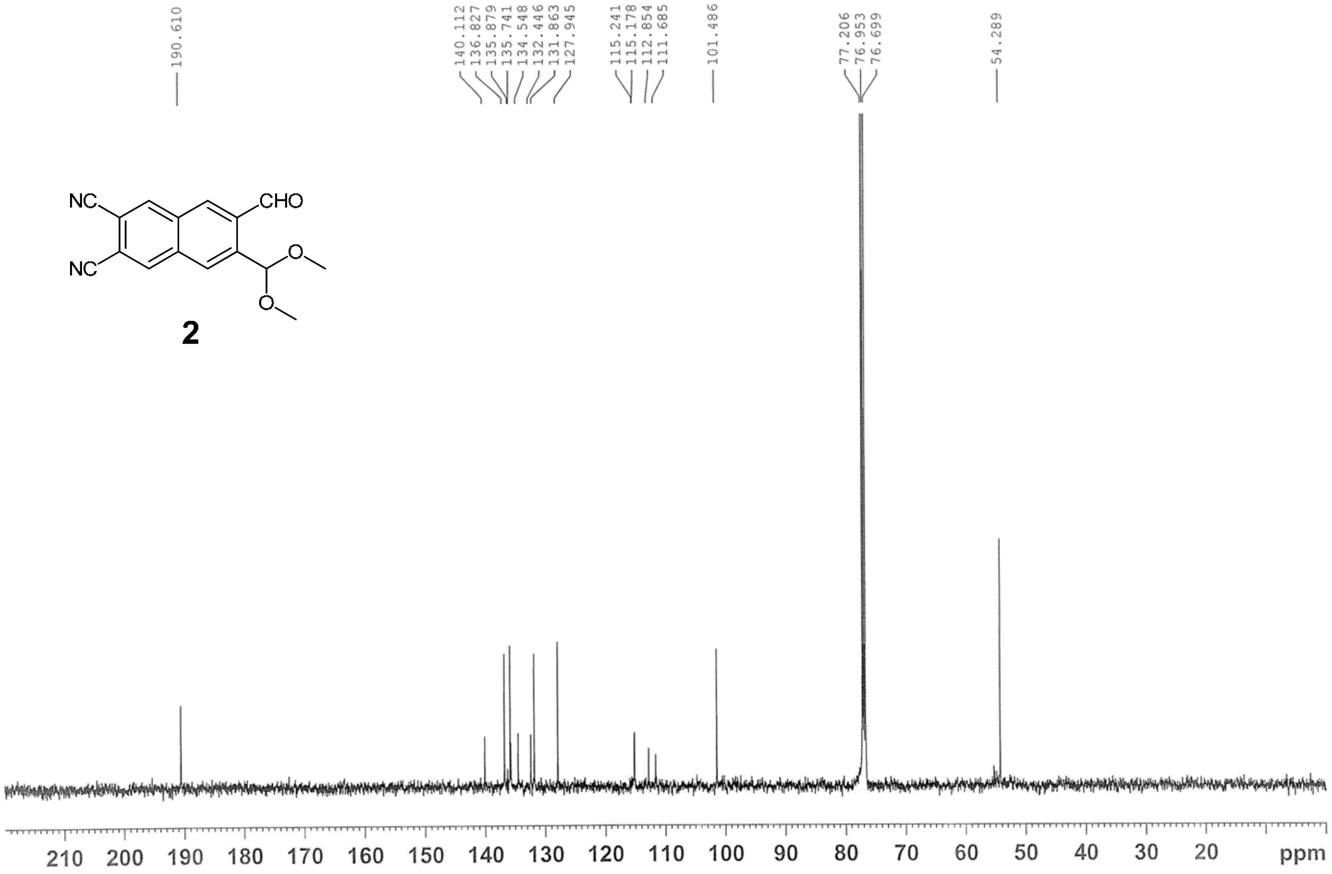

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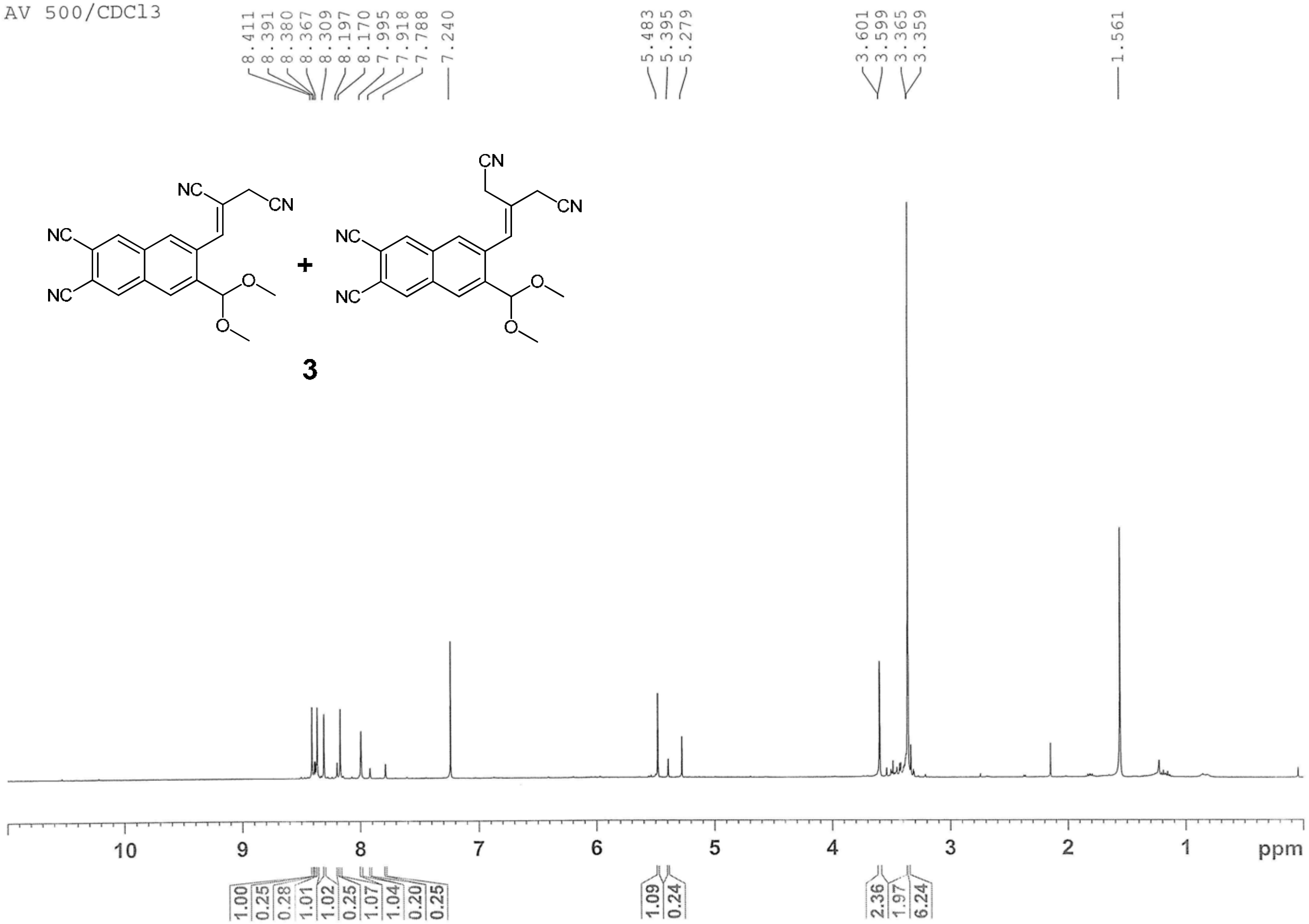
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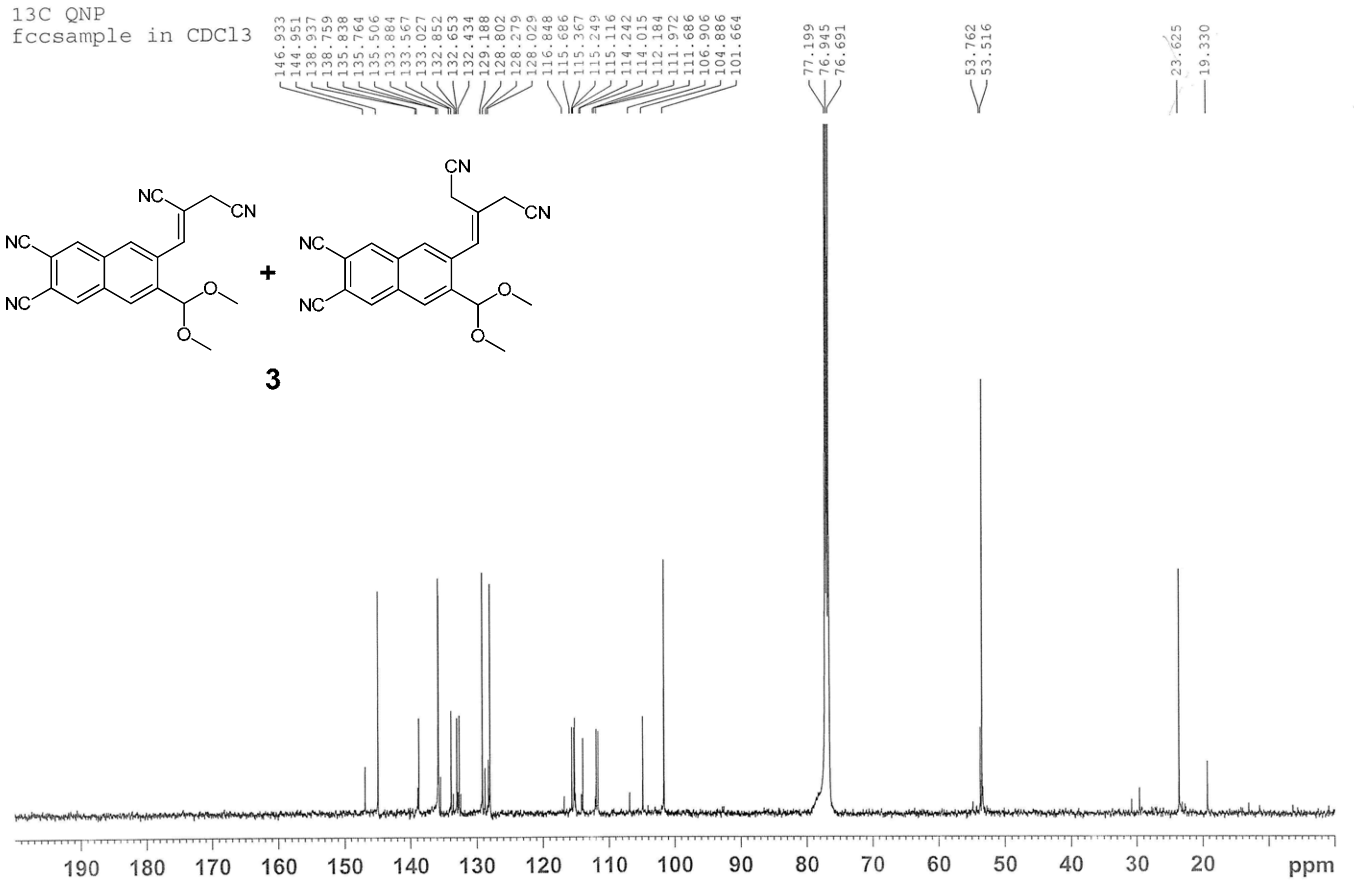
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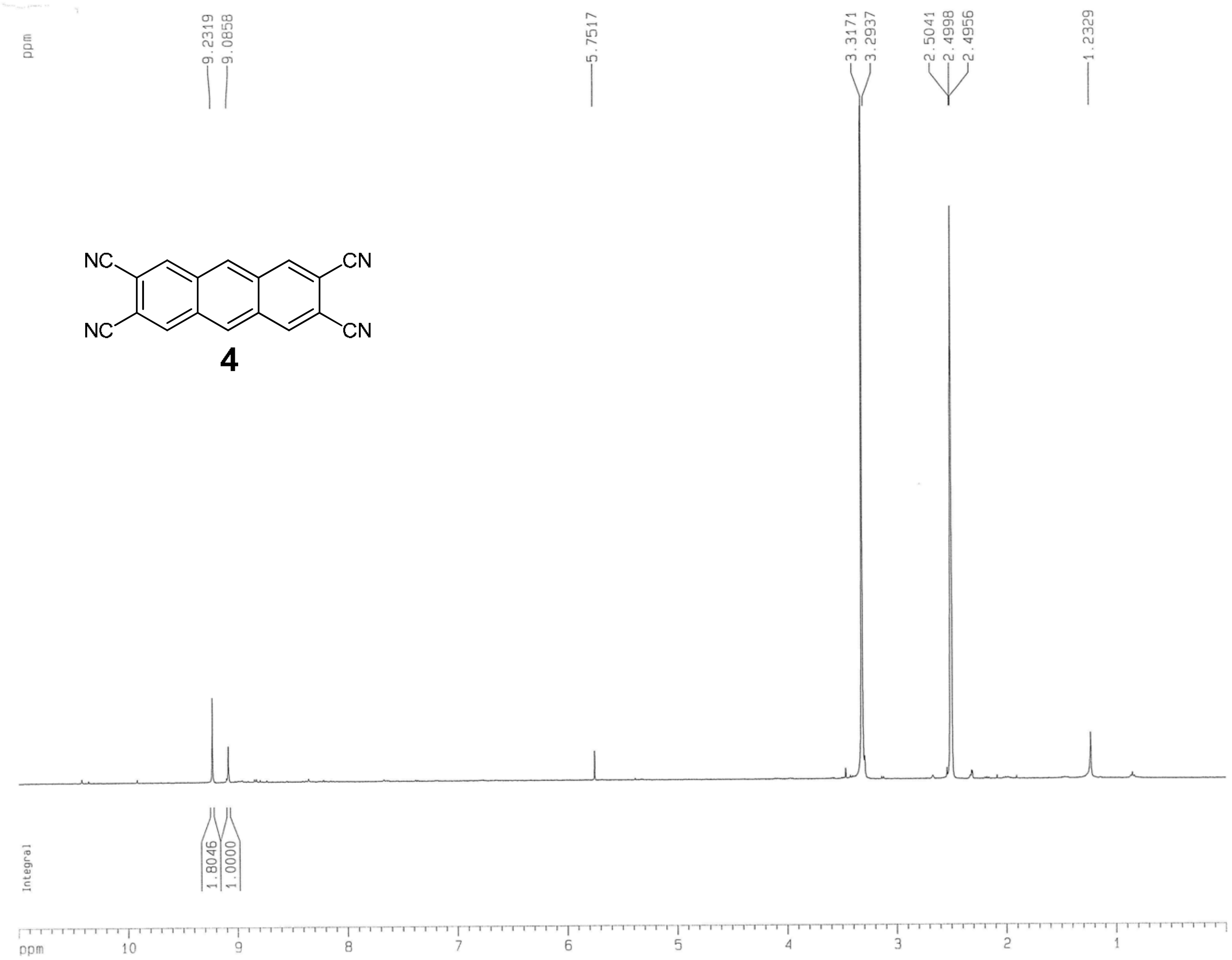
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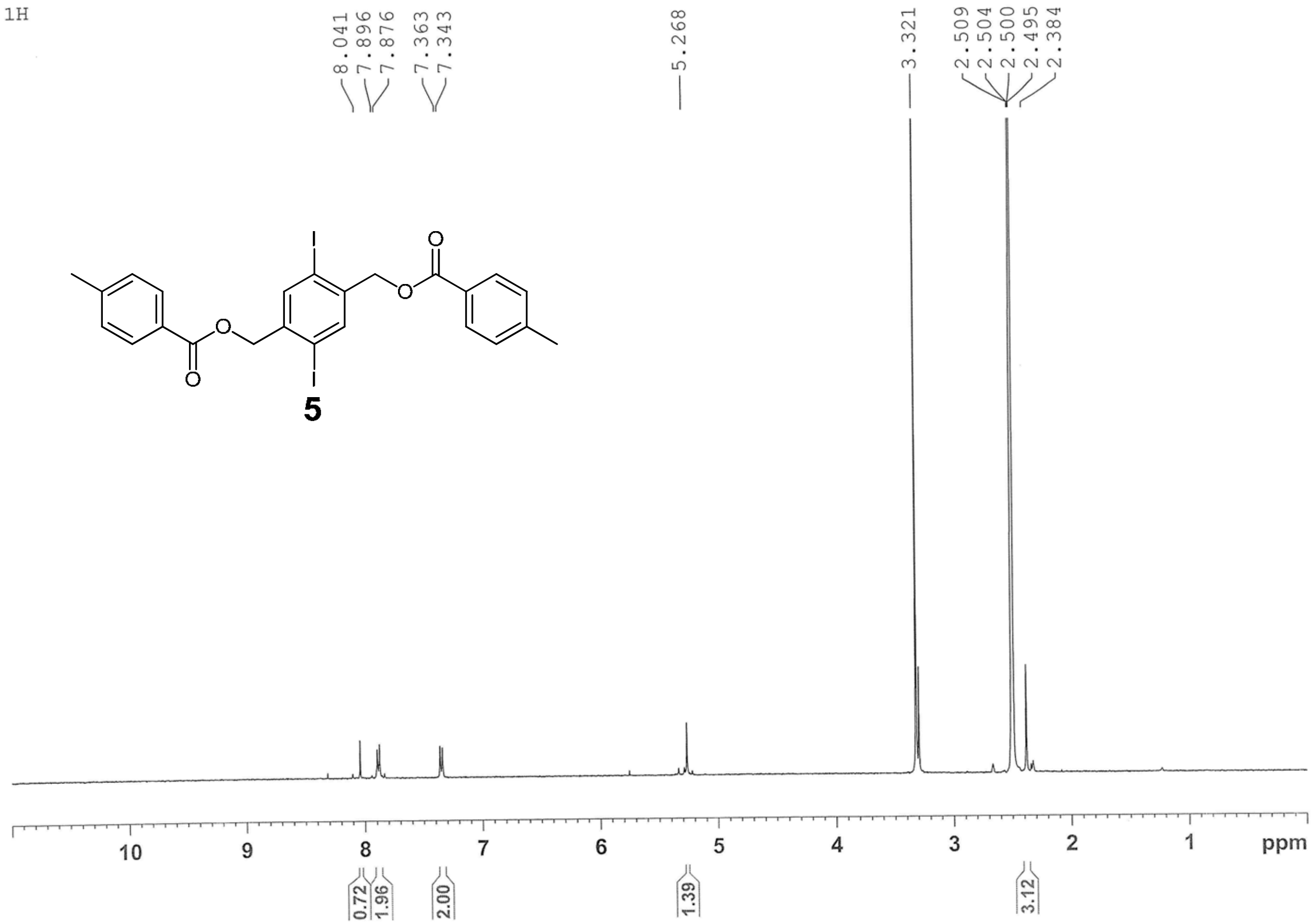
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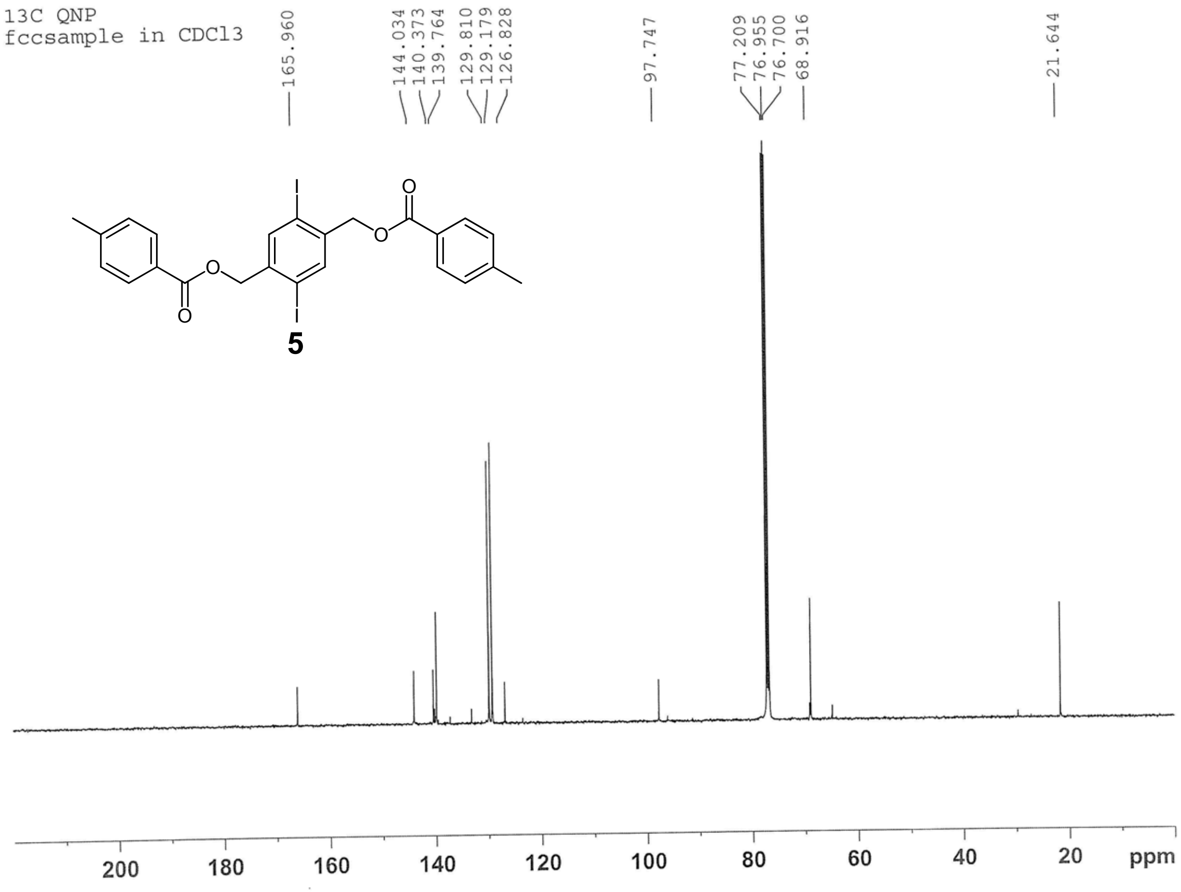

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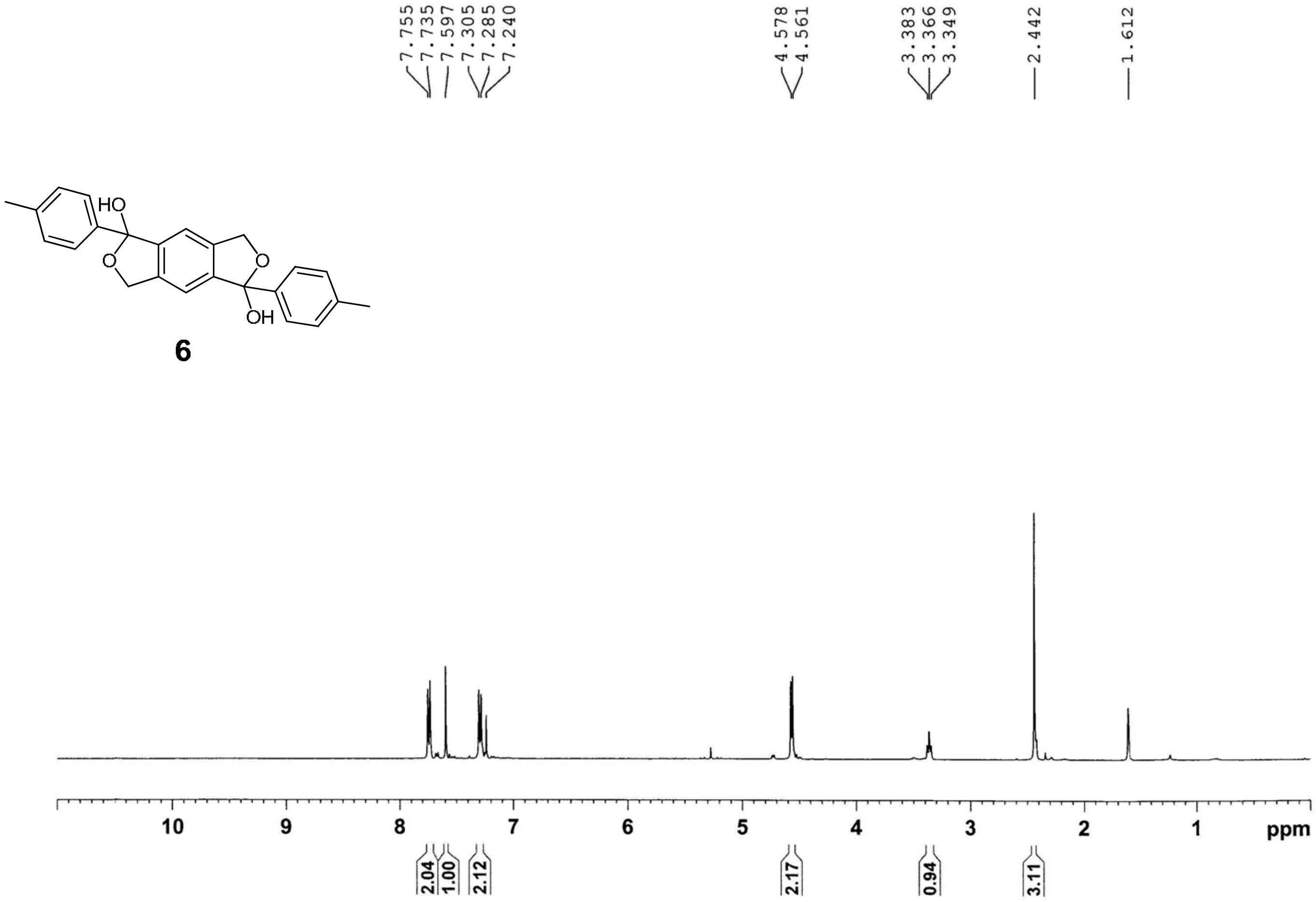
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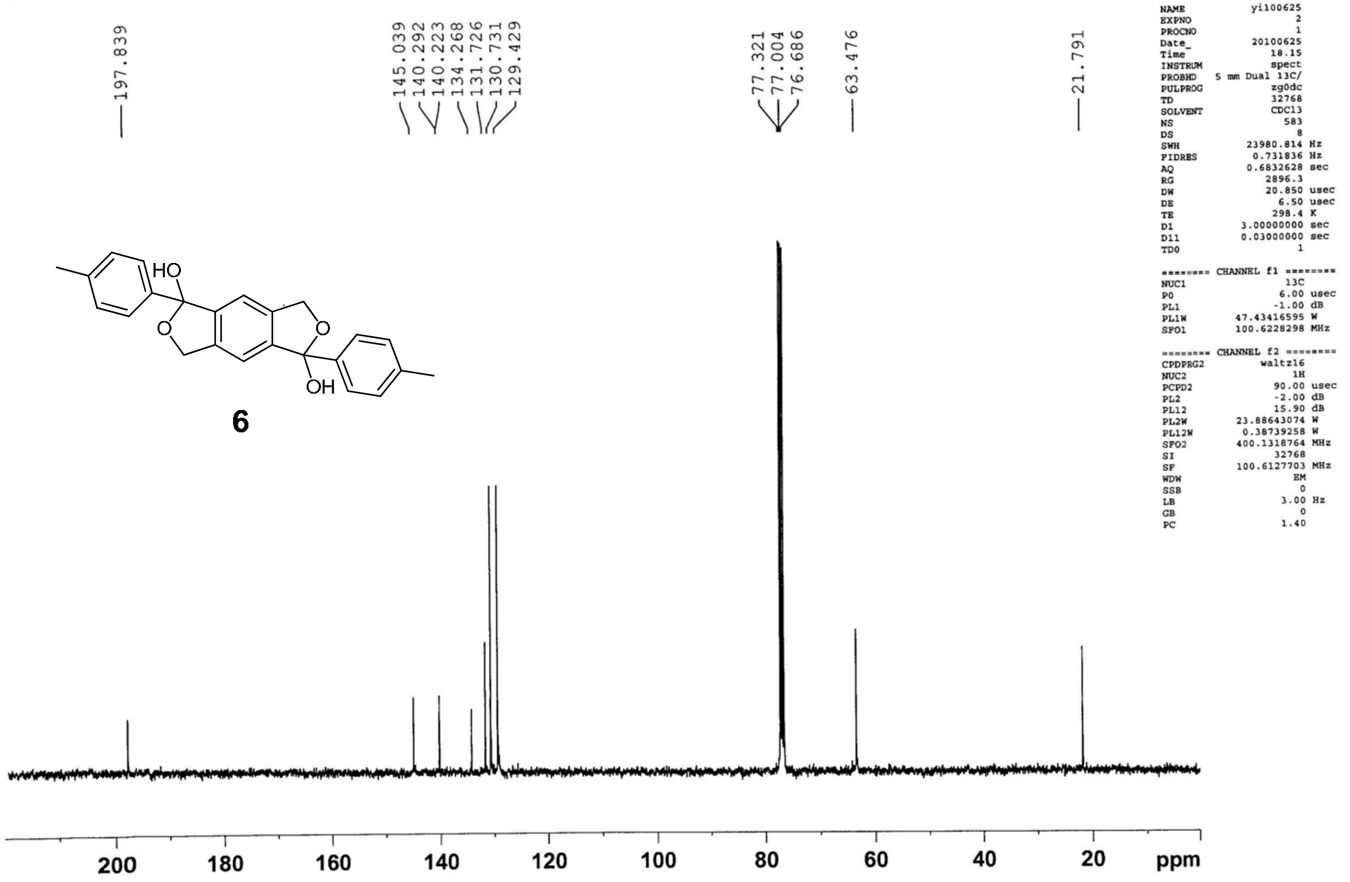

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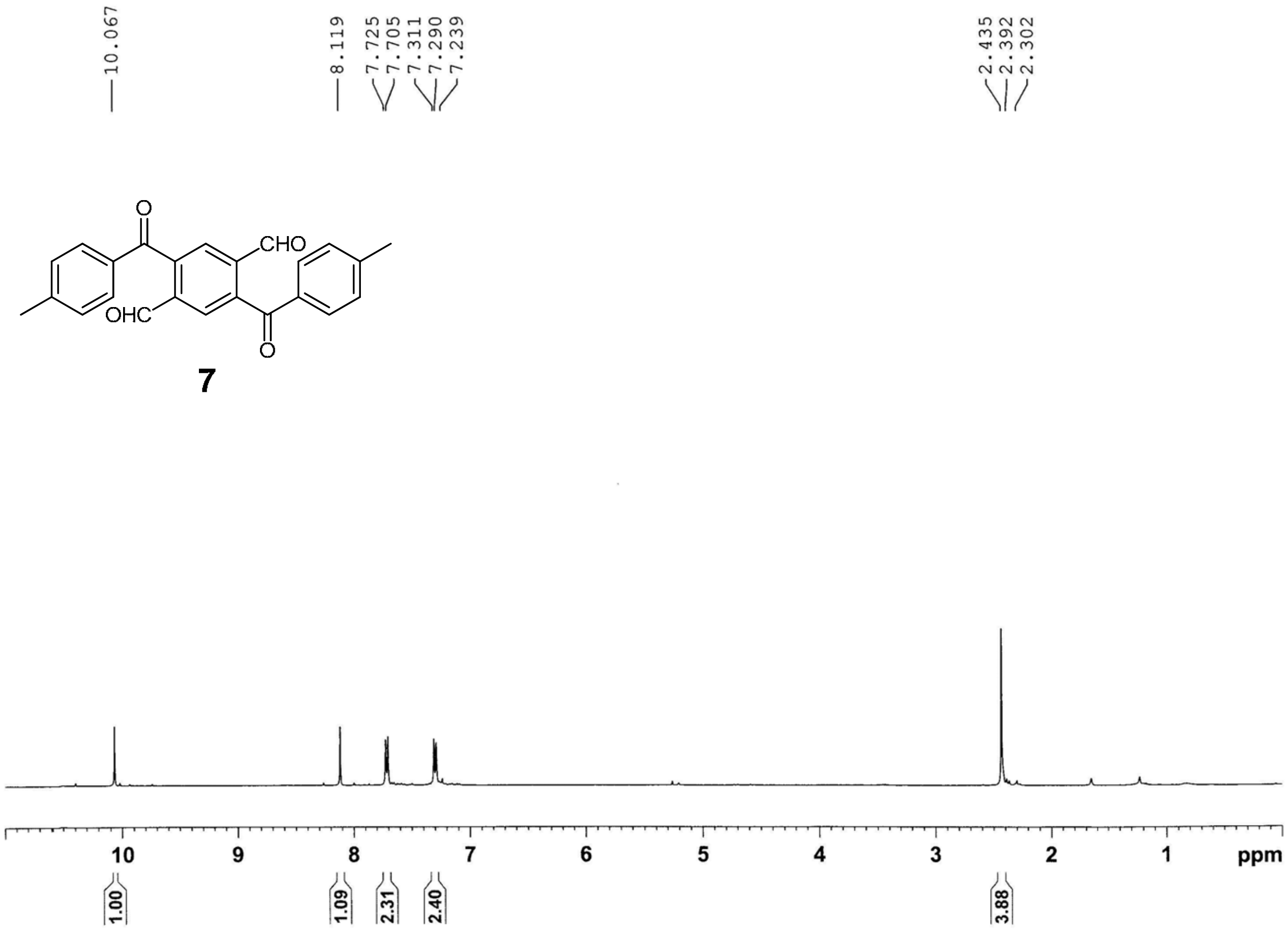
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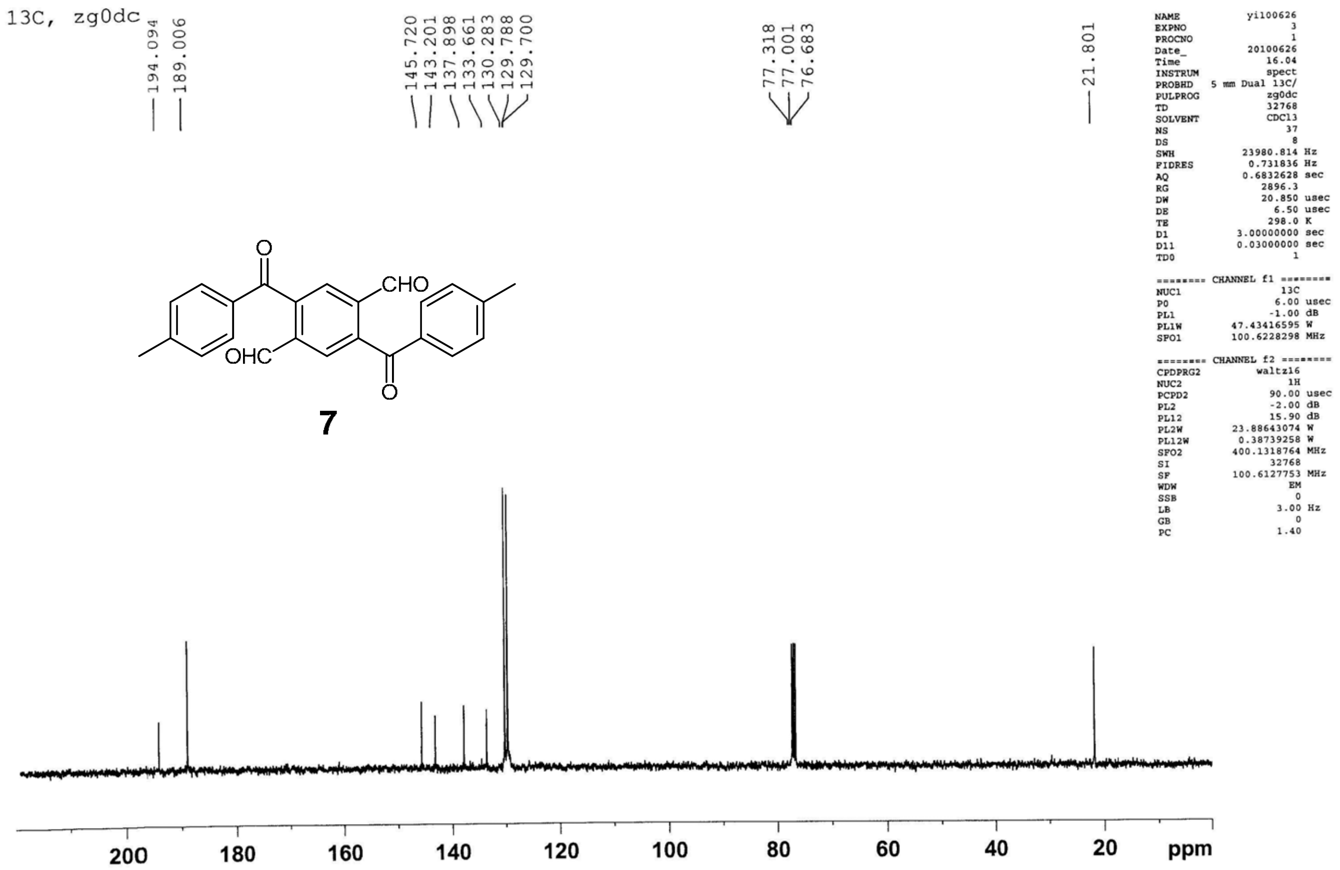

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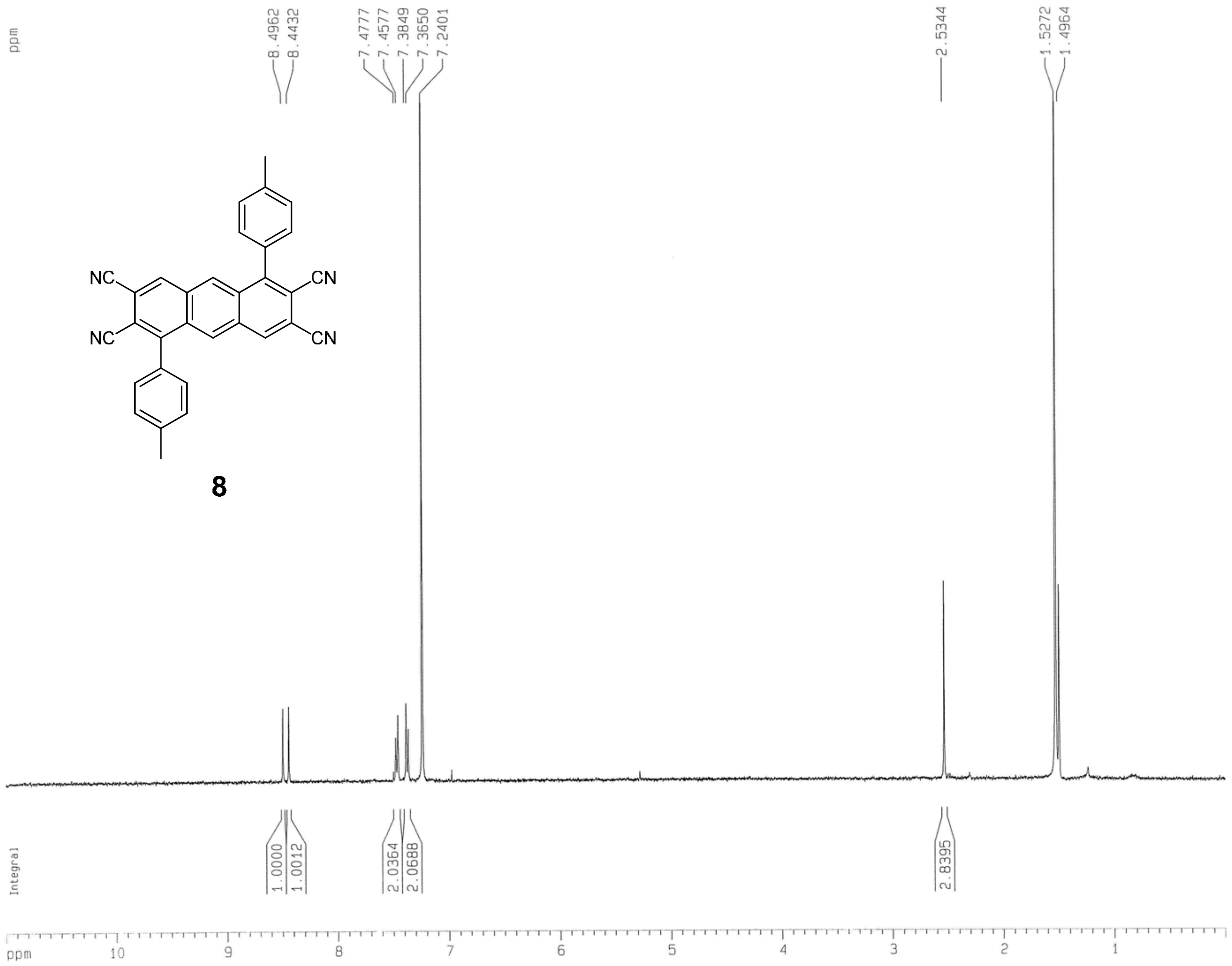
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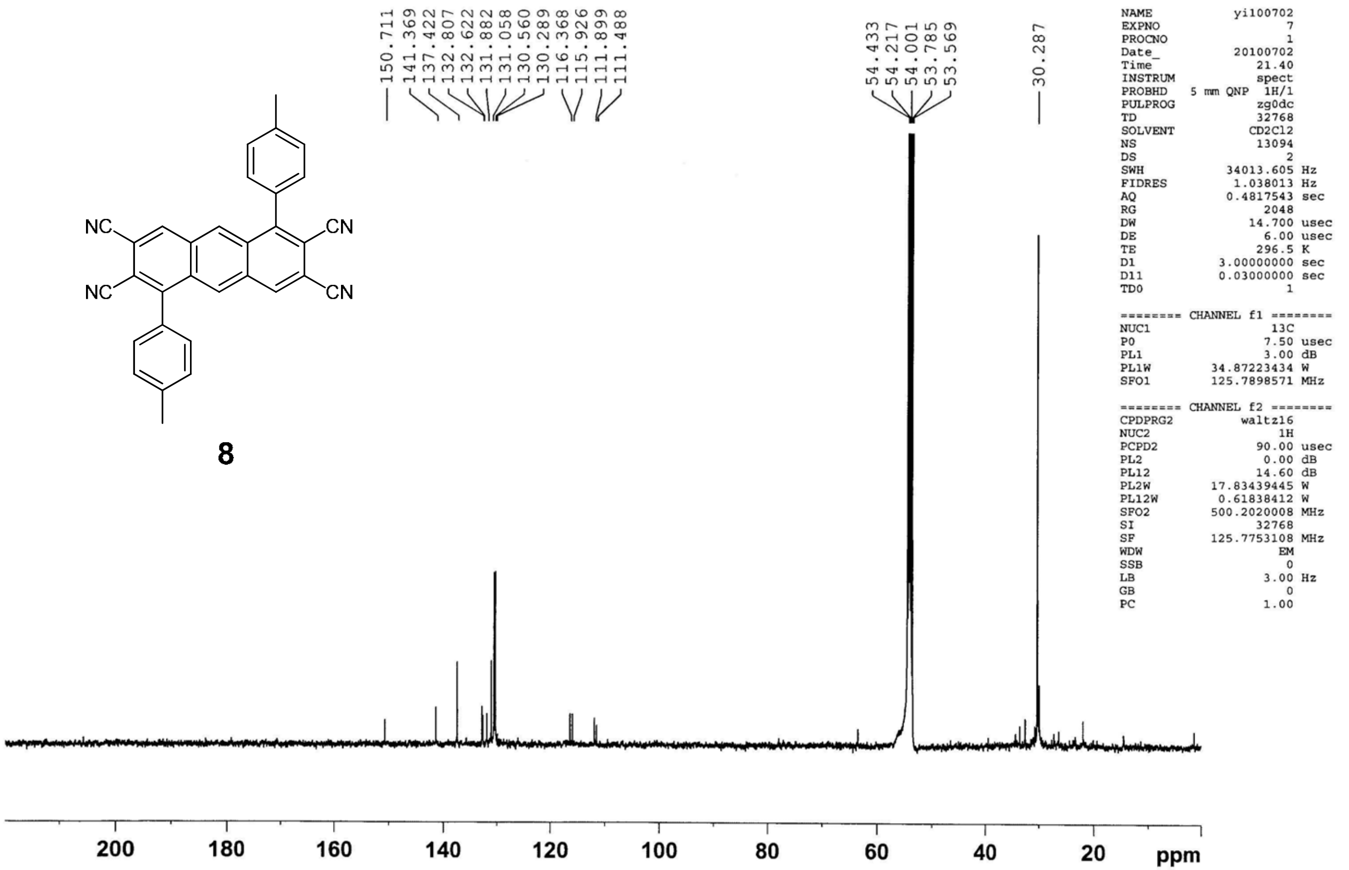
**8**



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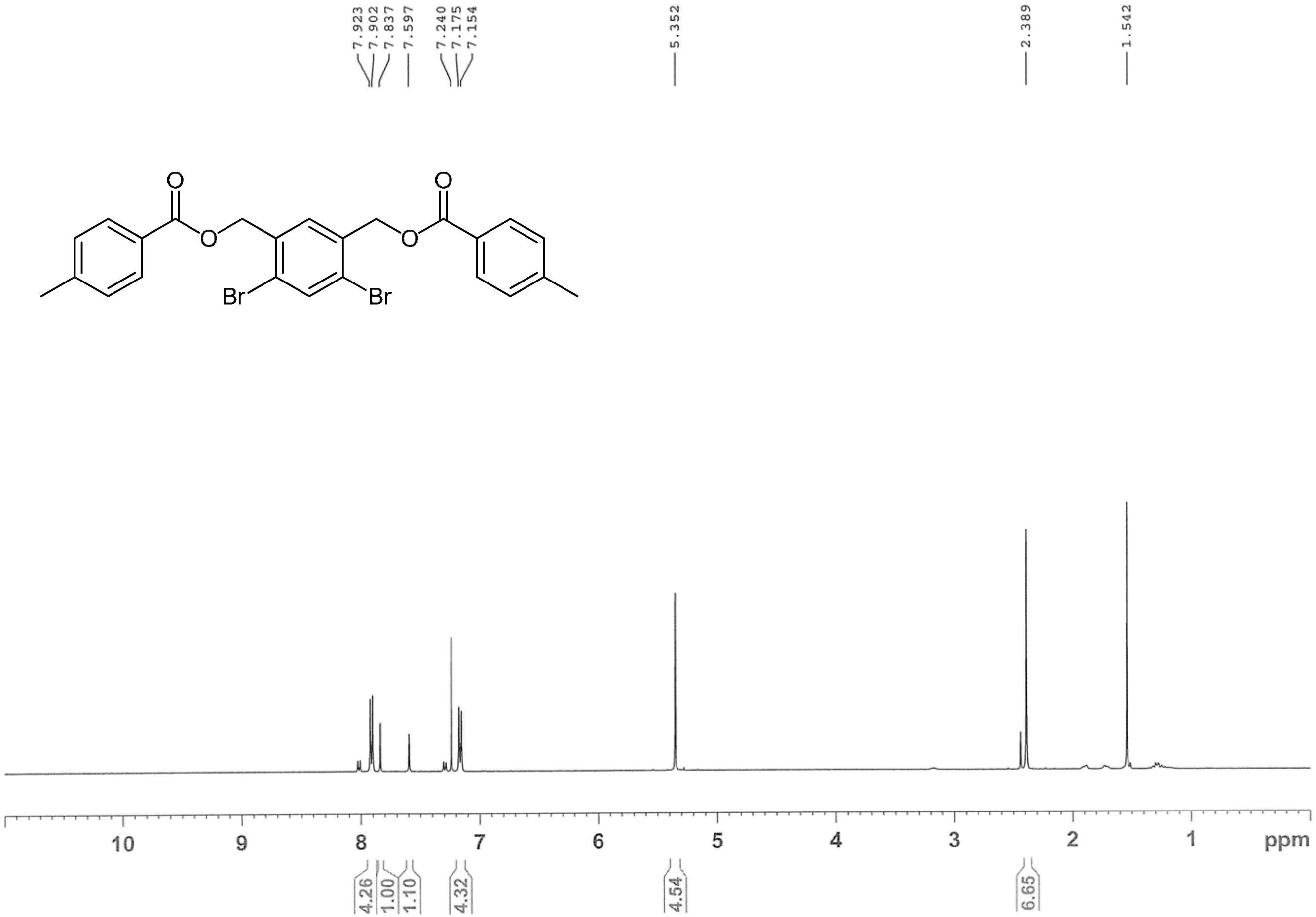
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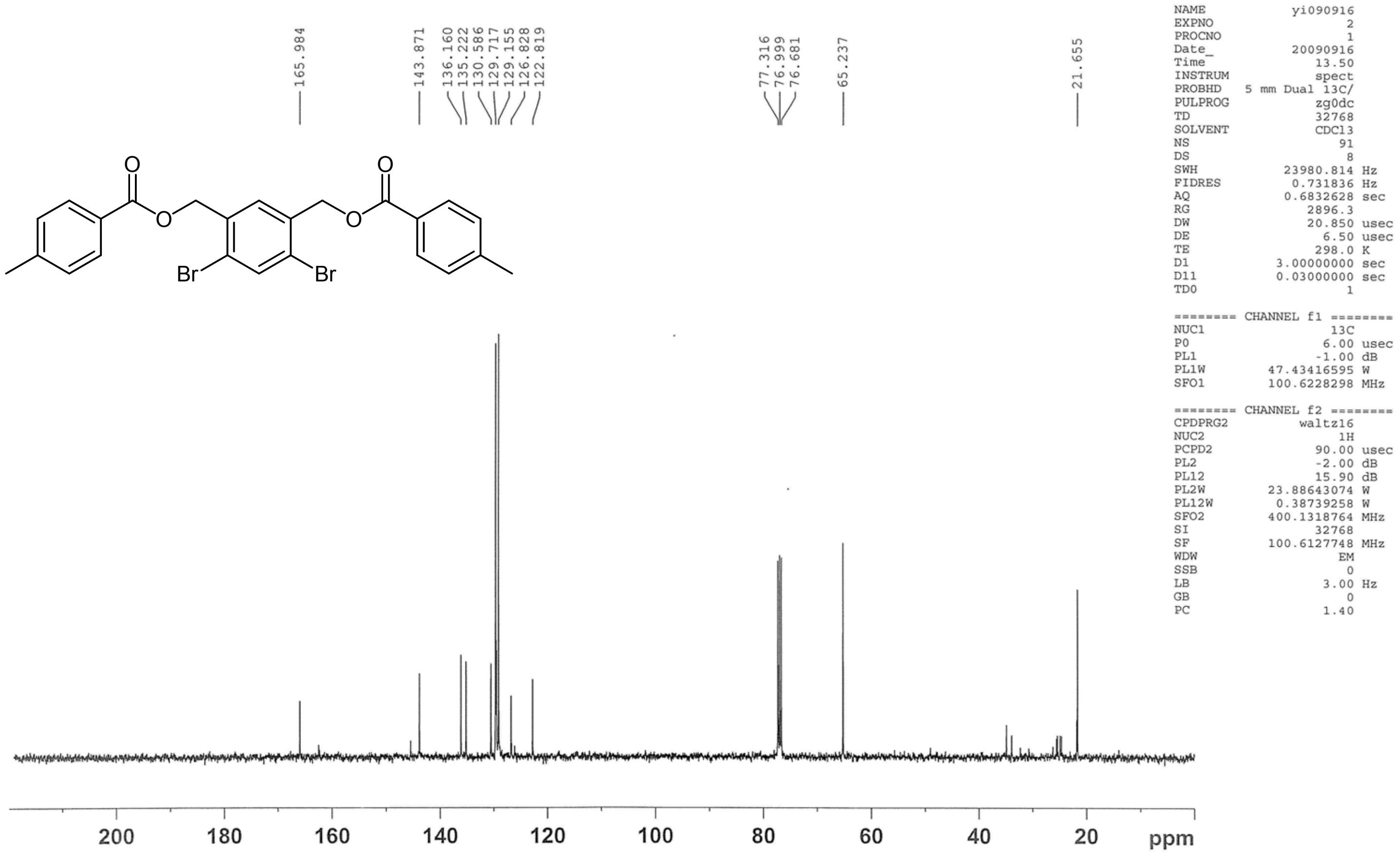
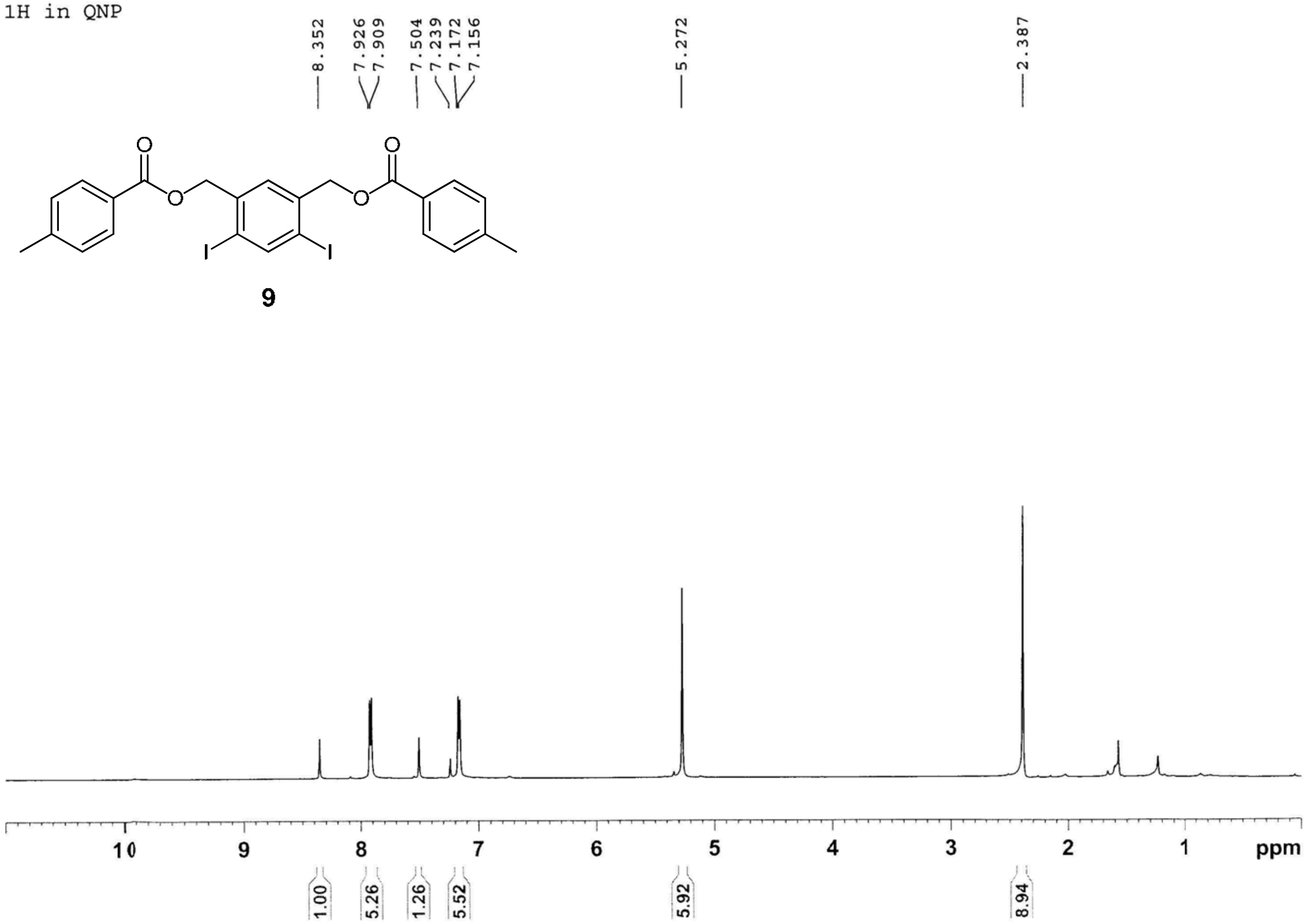
4.32
4.54
6.65

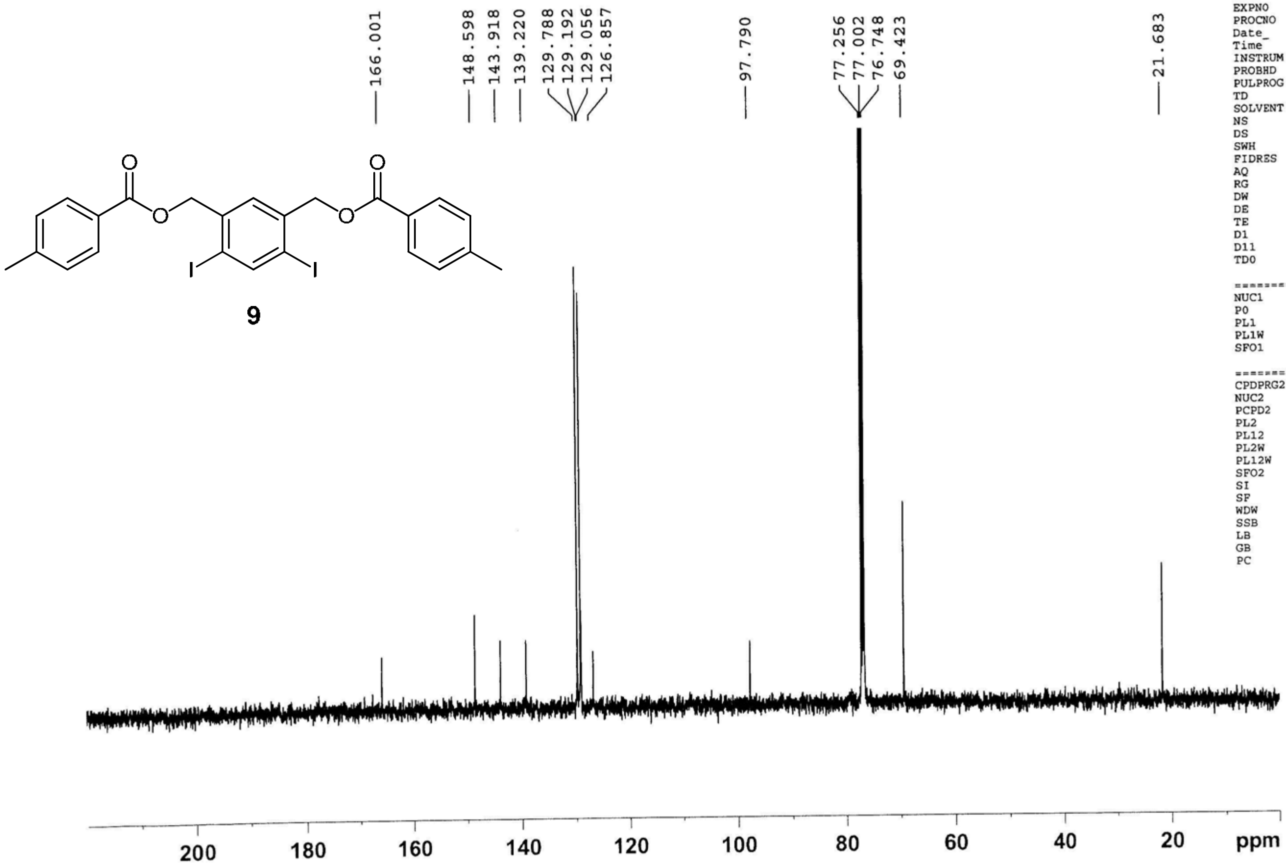


```
NAME              yi090916
EXPNO                    2
PROCNO                   1
Date_             20090916
Time                 13.50
INSTRUM              spect
PROBHD   5 mm Dual 13C/
PULPROG             zg0dc
TD                   32768
SOLVENT              CDCl3
NS                      91
DS                       8
SWH              23980.814 Hz
FIDRES            0.731836 Hz
AQ               0.6832628 sec
RG                  2896.3
DW                  20.850 usec
DE                    6.50 usec
TE                   298.0 K
D1              3.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P0                    6.00 usec
PL1                  -1.00 dB
PL1W           47.43416595 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  -2.00 dB
PL12                 15.90 dB
PL2W           23.88643074 W
PL12W           0.38739258 W
SFO2          400.1318764 MHz
SI                   32768
SF            100.6127748 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.40
```

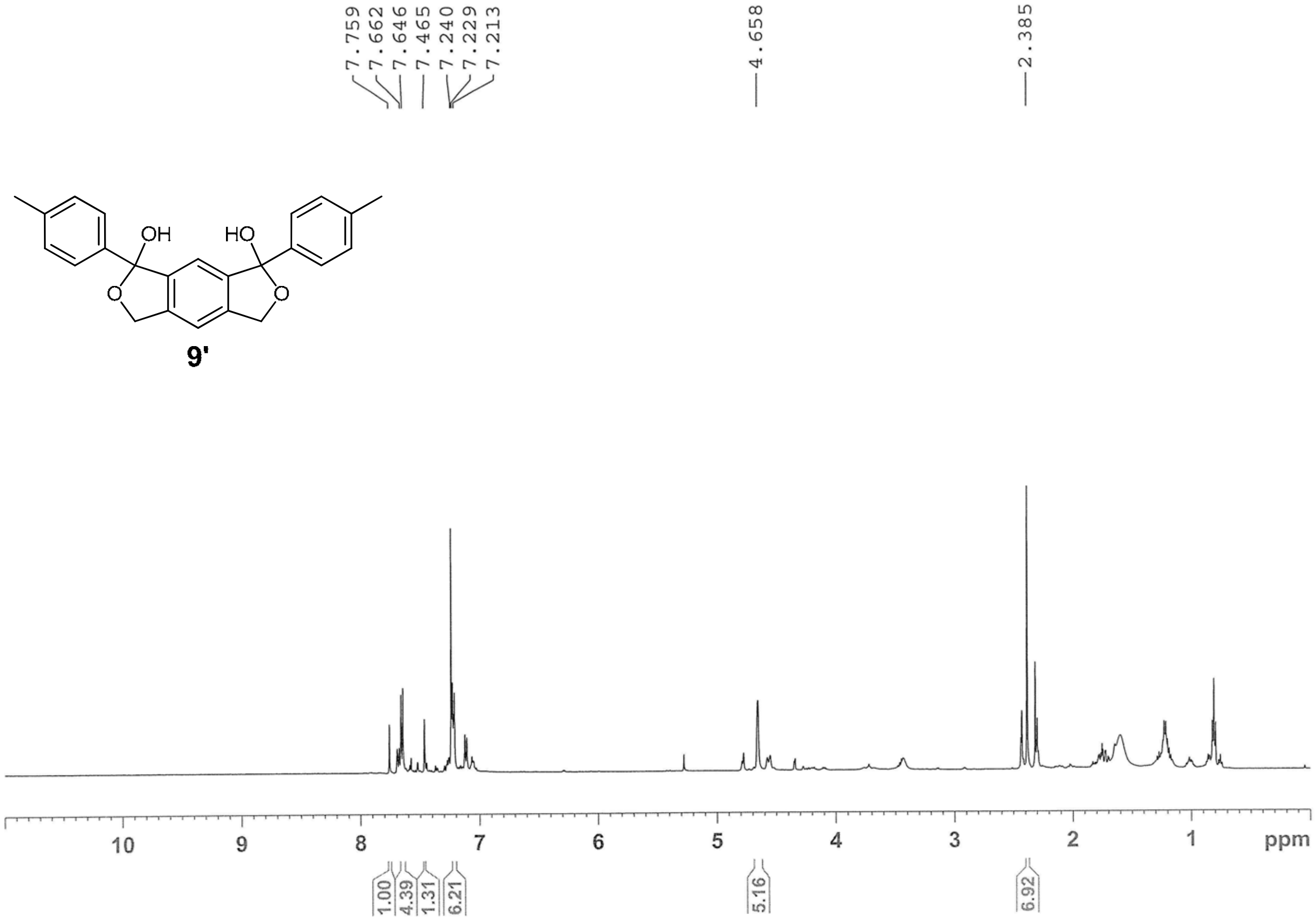

1H in QNP
8.352
7.926
7.909
7.504
7.239
7.172
7.156
5.272
2.387
O
O
O
O
I
I
10
9
8
7
6
5
4
3
2
1
ppm
1.00
5.26
1.26
5.52
5.92
8.94

**9**

**9**

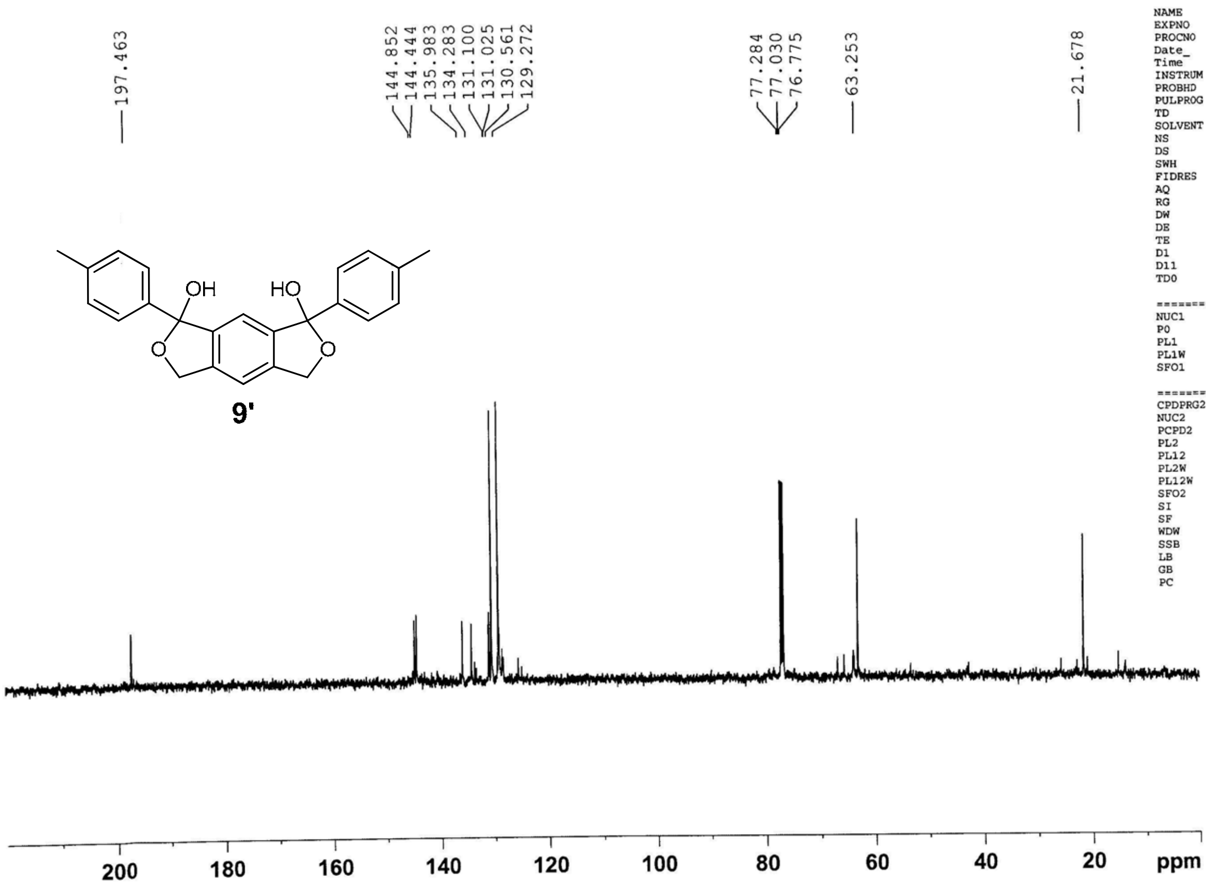


```
NAME           yi100626
EXPNO                 2
PROCNO                1
Date_          20100626
Time              20.43
INSTRUM           spect
PROBHD   5 mm QNP  1H/1
PULPROG          zg0dc
TD                32768
SOLVENT           CDCl3
NS                   90
DS                    2
SWH           34013.605 Hz
FIDRES         1.038013 Hz
AQ            0.4817543 sec
RG                 2048
DW               14.700 usec
DE                 6.00 usec
TE                296.2 K
D1           3.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P0                 7.50 usec
PL1                3.00 dB
PL1W        34.87223434 W
SFO1        125.7898571 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 0.00 dB
PL12               14.60 dB
PL2W         17.83439445 W
PL12W         0.61838412 W
SFO2         500.2020008 MHz
SI                 32768
SF           125.7753925 MHz
WDW                   EM
SSB                    0
LB                  3.00 Hz
GB                     0
PC                  1.00
```


OH
HO
O
O

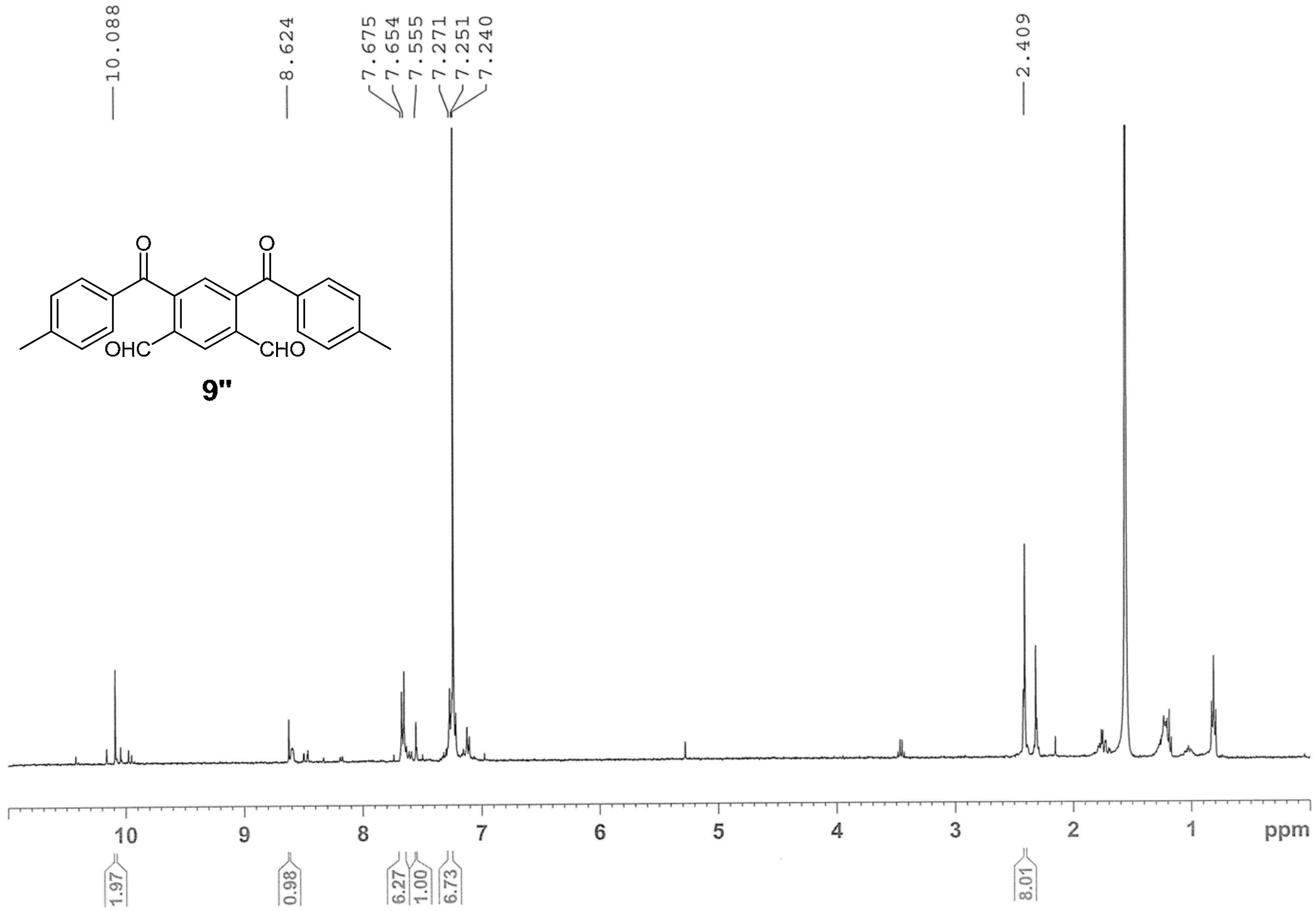
**9'**

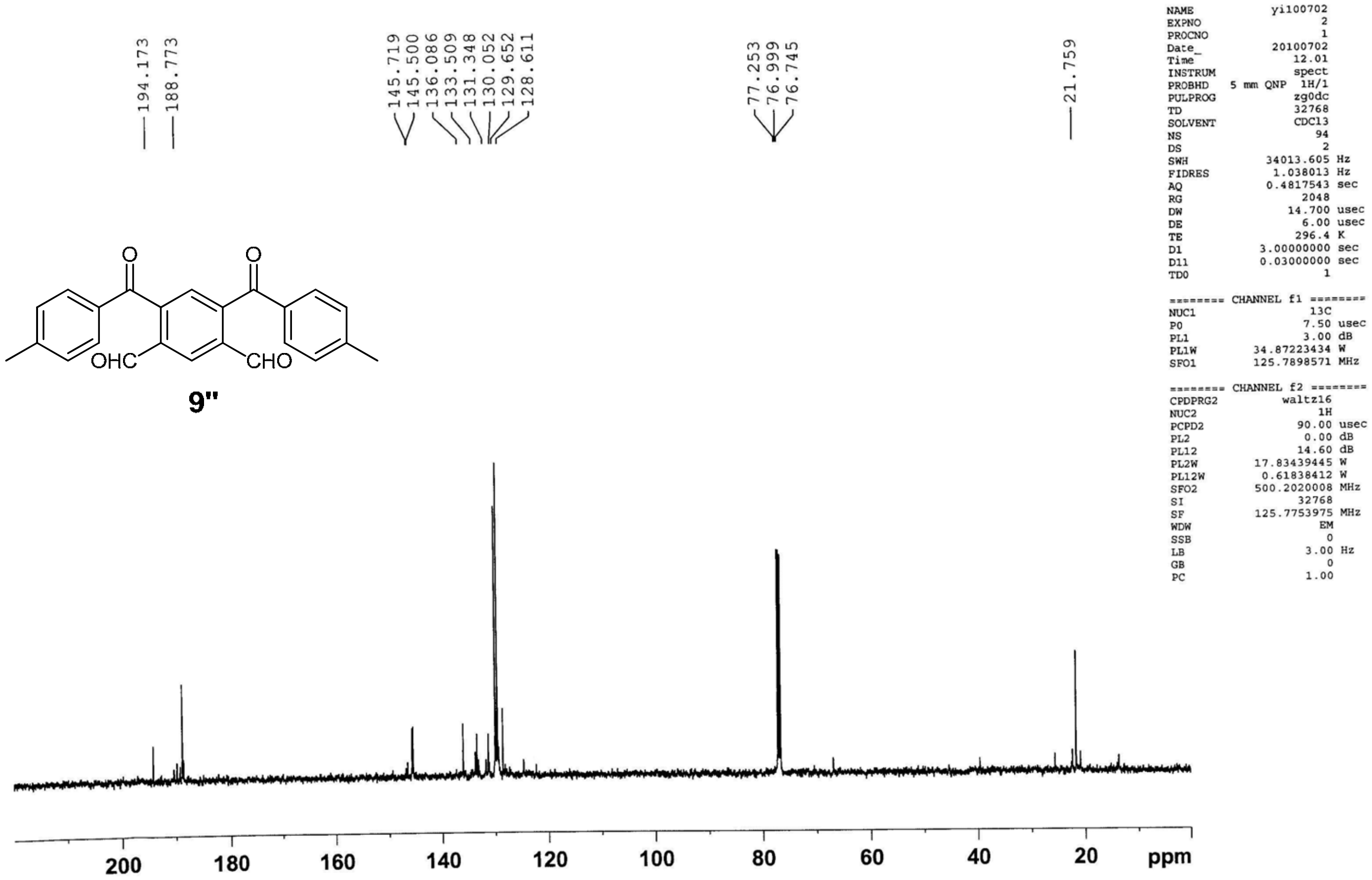
7.759
7.662
7.646
7.465
7.240
7.229
7.213
4.658
2.385
10
9
8
7
6
5
4
3
2
1
ppm
1.00
4.39
1.31
6.21
5.16
6.92



9'

```
NAME          yi100701
EXPNO                4
PROCNO               1
Date_         20100701
Time             22.03
INSTRUM          spect
PROBHD   5 mm QNP  1H/1
PULPROG         zg0dc
TD               32768
SOLVENT          CDCl3
NS                  44
DS                   2
SWH          34013.605 Hz
FIDRES        1.038013 Hz
AQ           0.4817543 sec
RG                2048
DW              14.700 usec
DE                6.00 usec
TE               296.6 K
D1          3.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1               13C
P0                7.50 usec
PL1               3.00 dB
PL1W       34.87223434 W
SFO1       125.7898571 MHz

======== CHANNEL f2 ========
CPDPRG2        waltz16
NUC2                1H
PCPD2            90.00 usec
PL2               0.00 dB
PL12             14.60 dB
PL2W       17.83439445 W
PL12W       0.61838412 W
SFO2       500.2020008 MHz
SI               32768
SF         125.7753975 MHz
WDW                 EM
SSB                  0
LB                3.00 Hz
GB                   0
PC                1.00
```


10.088
8.624
7.675
7.654
7.555
7.271
7.251
7.240
2.409
O
O
OHC
CHO
9''
10
9
8
7
6
5
4
3
2
1
ppm
1.97
0.98
6.27
1.00
6.73
8.01



**9''**

```
NAME             yi100702
EXPNO                   2
PROCNO                  1
Date_            20100702
Time                12.01
INSTRUM             spect
PROBHD   5 mm QNP  1H/1
PULPROG            zg0dc
TD                  32768
SOLVENT             CDCl3
NS                     94
DS                      2
SWH             34013.605 Hz
FIDRES           1.038013 Hz
AQ              0.4817543 sec
RG                   2048
DW                 14.700 usec
DE                   6.00 usec
TE                  296.4 K
D1             3.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P0                   7.50 usec
PL1                  3.00 dB
PL1W          34.87223434 W
SFO1          125.7898571 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               90.00 usec
PL2                  0.00 dB
PL12                14.60 dB
PL2W          17.83439445 W
PL12W          0.61838412 W
SFO2          500.2020008 MHz
SI                  32768
SF            125.7753975 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.00
```

Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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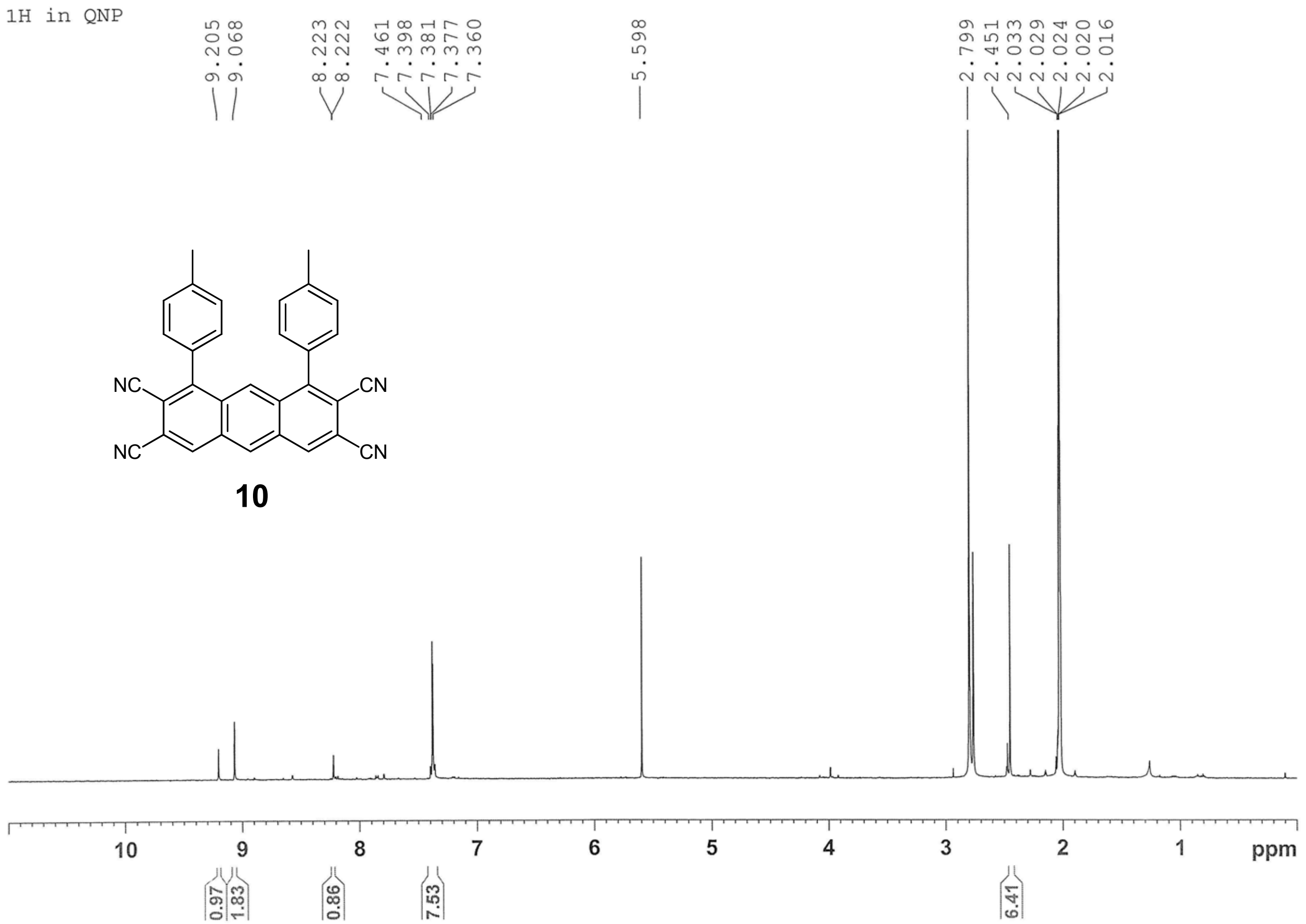
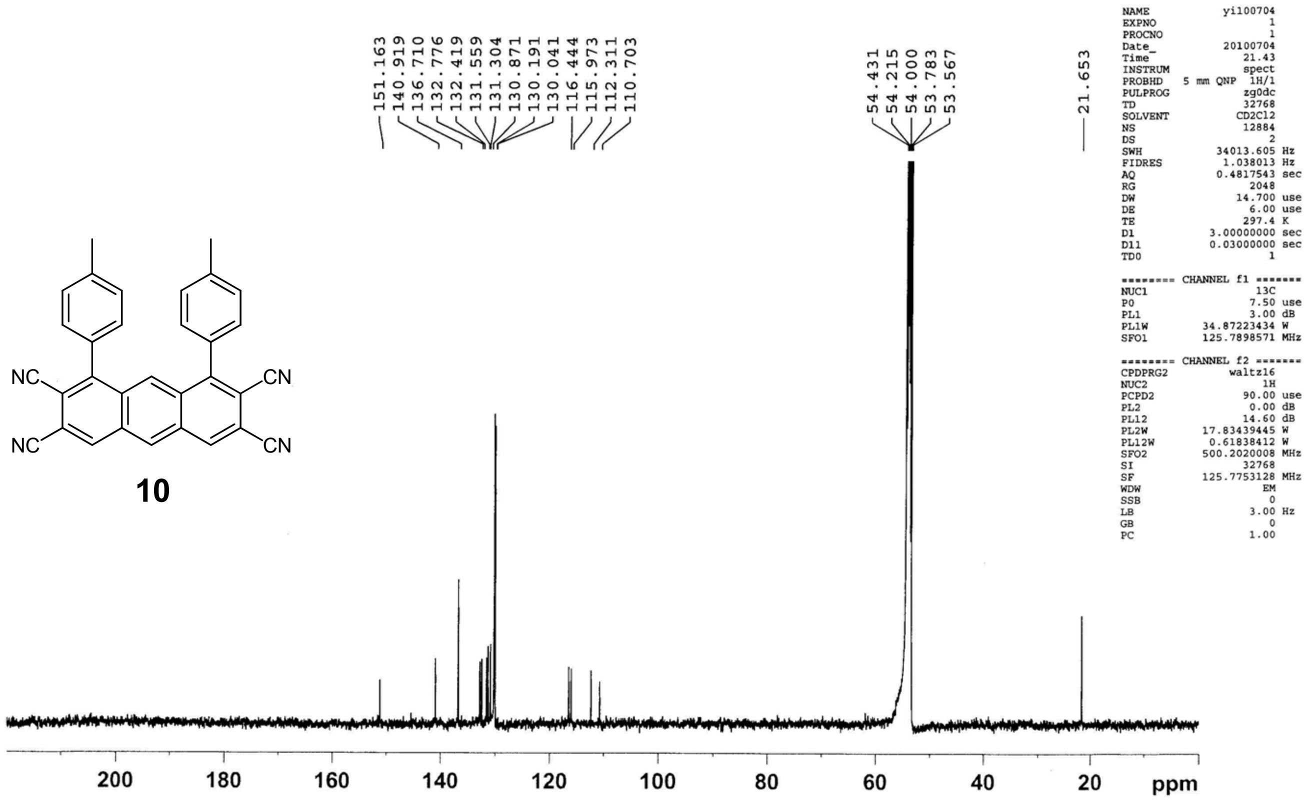
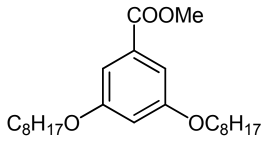


**10**

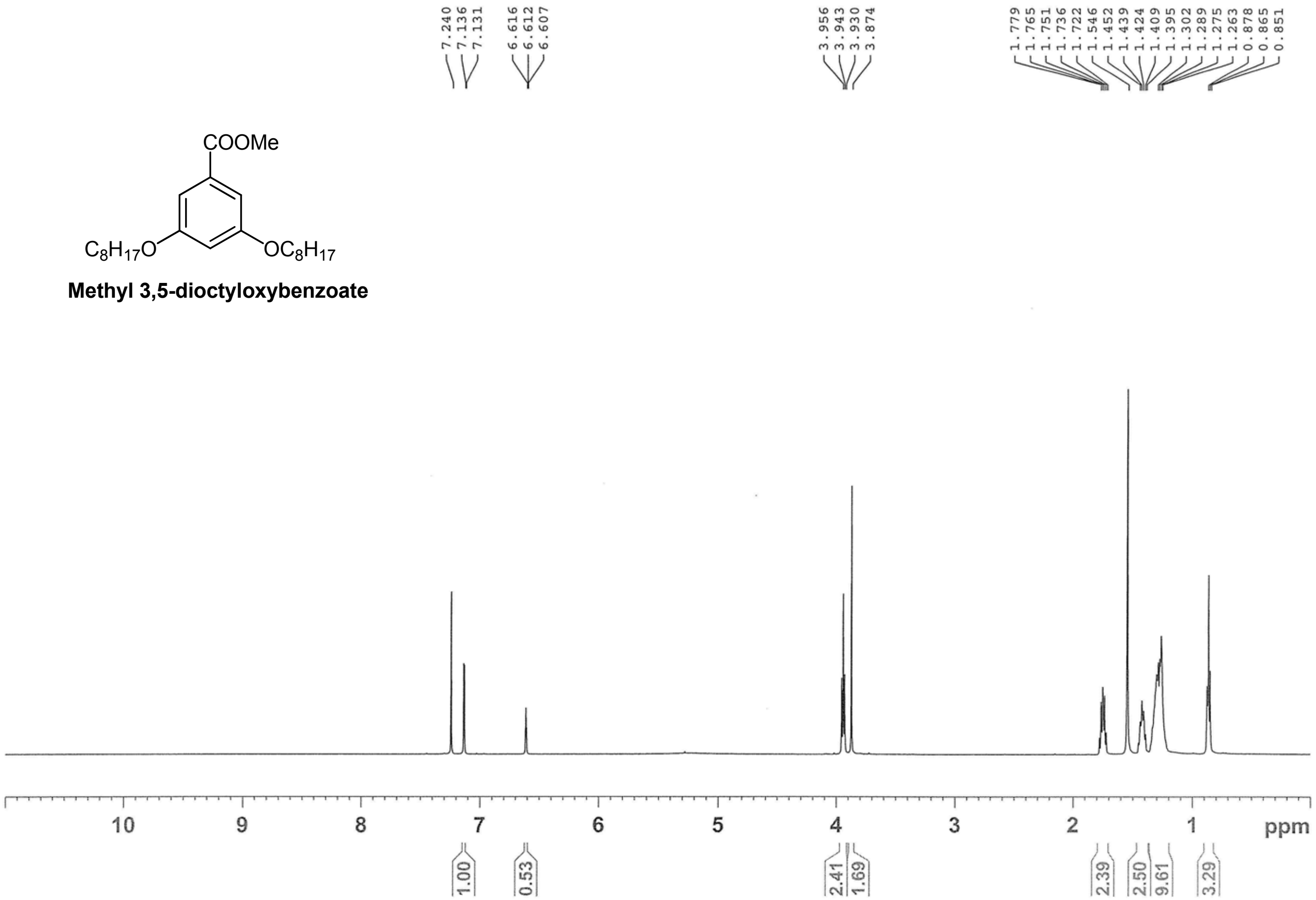


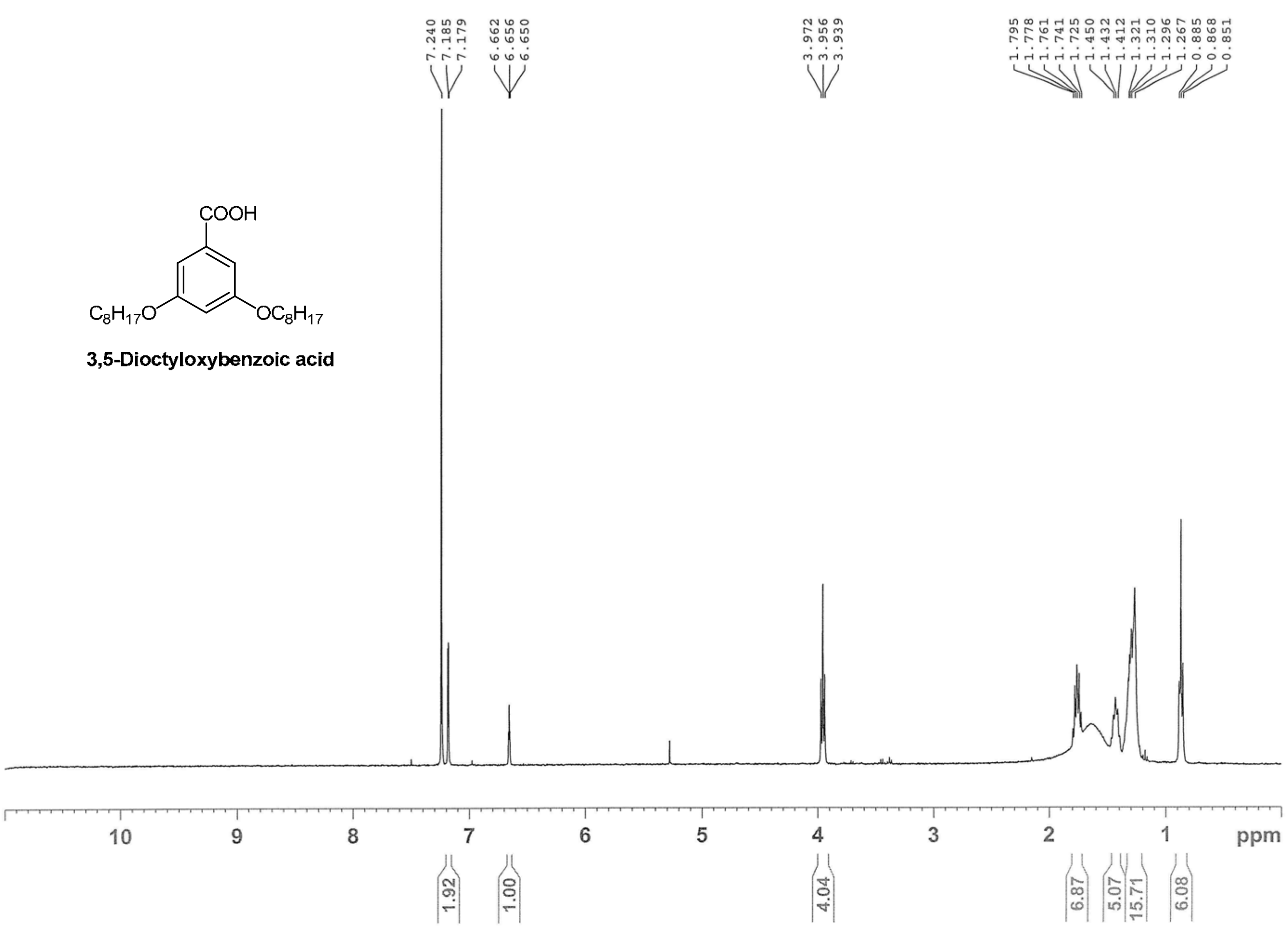
**10**

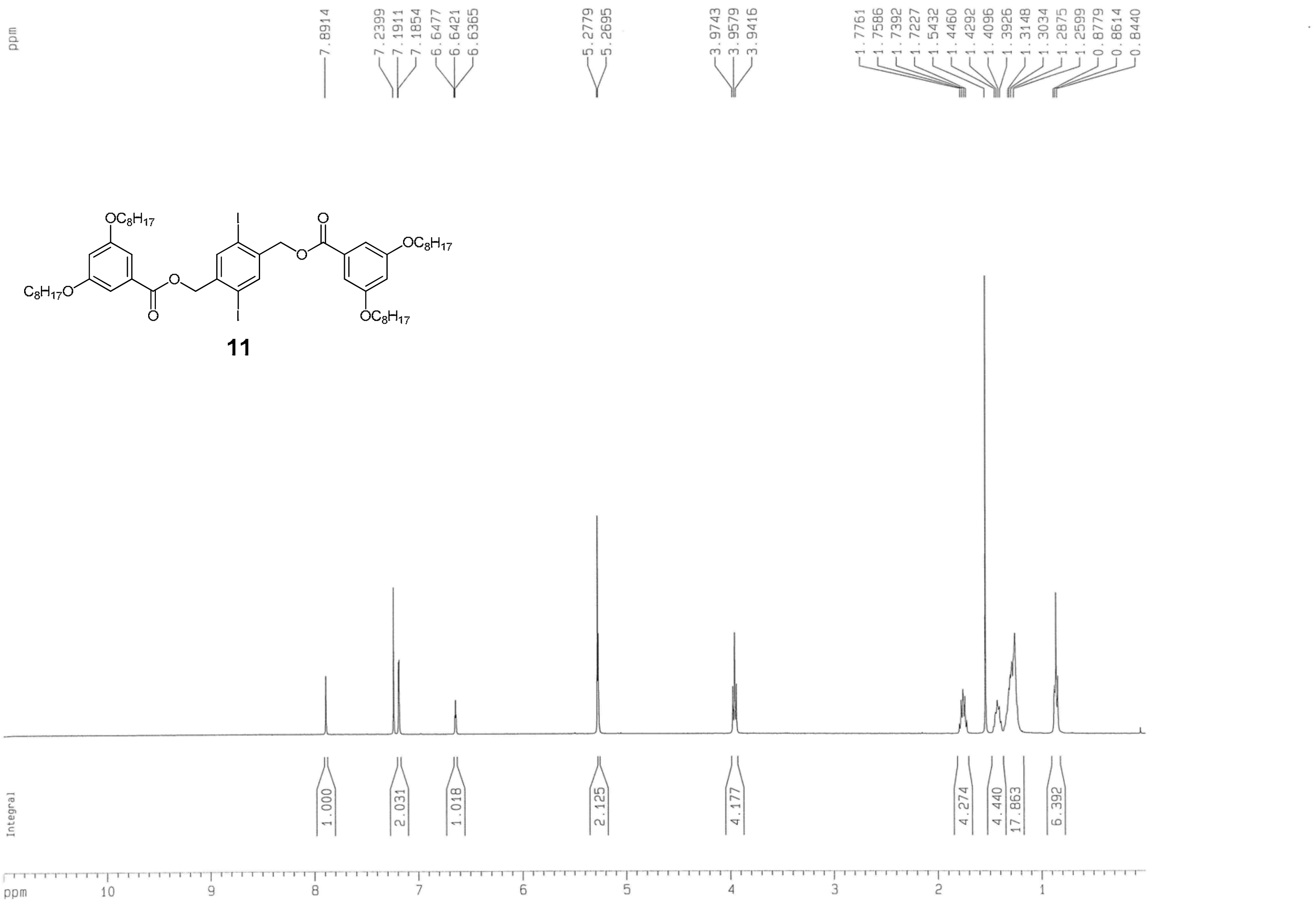
```
NAME           yi100704
EXPNO                 1
PROCNO                1
Date_          20100704
Time              21.43
INSTRUM           spect
PROBHD   5 mm QNP  1H/1
PULPROG           zg0dc
TD                32768
SOLVENT          CD2Cl2
NS                12884
DS                    2
SWH           34013.605 Hz
FIDRES         1.038013 Hz
AQ            0.4817543 sec
RG                 2048
DW               14.700 use
DE                 6.00 use
TE                297.4 K
D1           3.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 =======
NUC1                13C
PO                 7.50 use
PL1                3.00 dB
PL1W        34.87223434 W
SFO1        125.7898571 MHz

======== CHANNEL f2 =======
CPDPRG2         waltz16
NUC2                 1H
PCPD2             90.00 use
PL2                0.00 dB
PL12              14.60 dB
PL2W        17.83439445 W
PL12W        0.61838412 W
SFO2        500.2020008 MHz
SI                32768
SF          125.7753128 MHz
WDW                  EM
SSB                   0
LB                 3.00 Hz
GB                    0
PC                 1.00
```



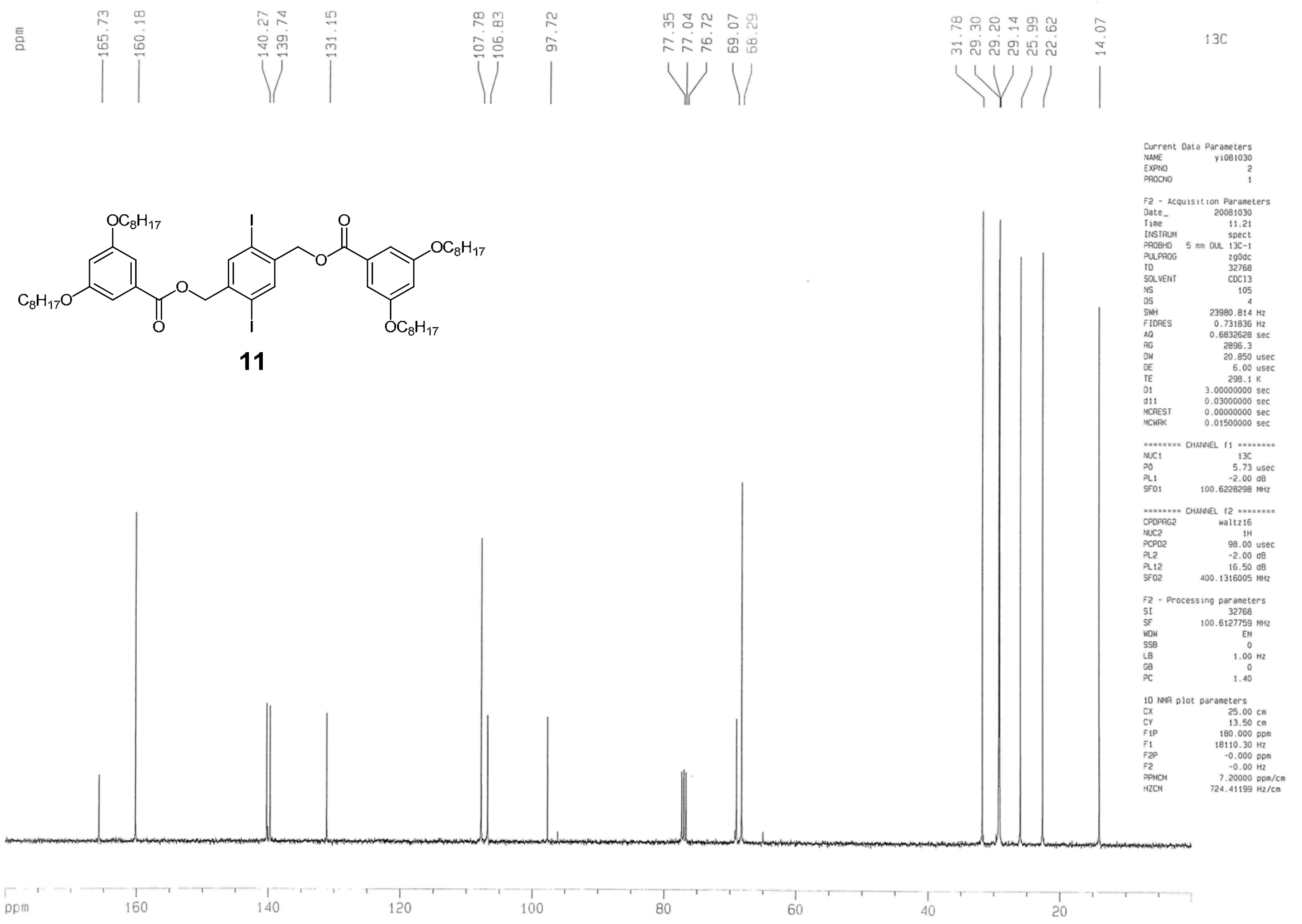
**Methyl 3,5-dioctyloxybenzoate**




**3,5-Dioctyloxybenzoic acid**

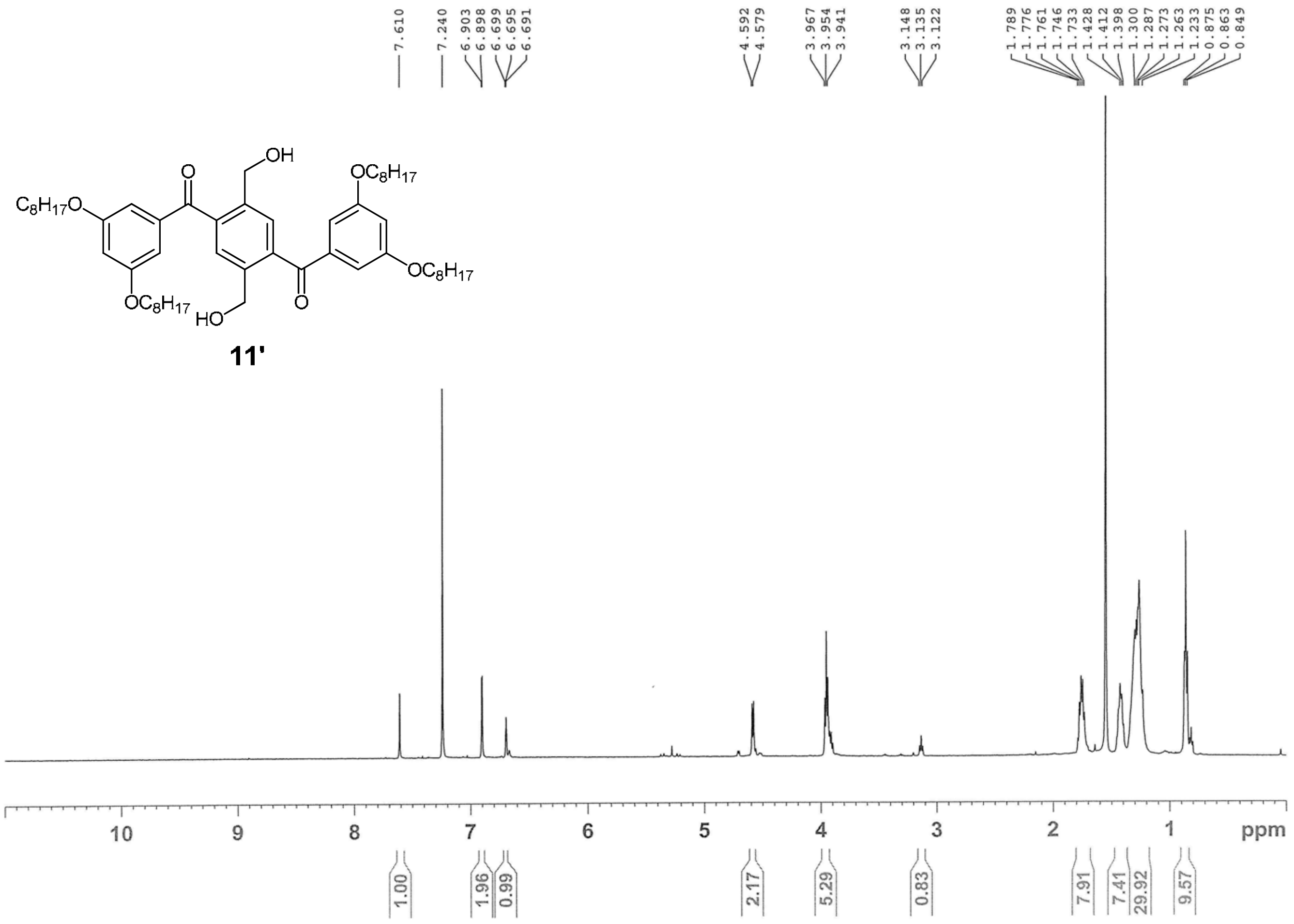

ppm
7.8914
7.2399
7.1911
7.1854
6.6477
6.6421
6.6365
5.2779
5.2695
3.9743
3.9579
3.9416
1.7761
1.7586
1.7392
1.7227
1.5432
1.4460
1.4292
1.4096
1.3926
1.3148
1.3034
1.2875
1.2599
0.8779
0.8614
0.8440
OC8H17
C8H17O
I
O
Integral
1.000
2.031
1.018
2.125
4.177
4.274
4.440
17.863
6.392
ppm
10
9
8
7
6
5
4
3
2
1

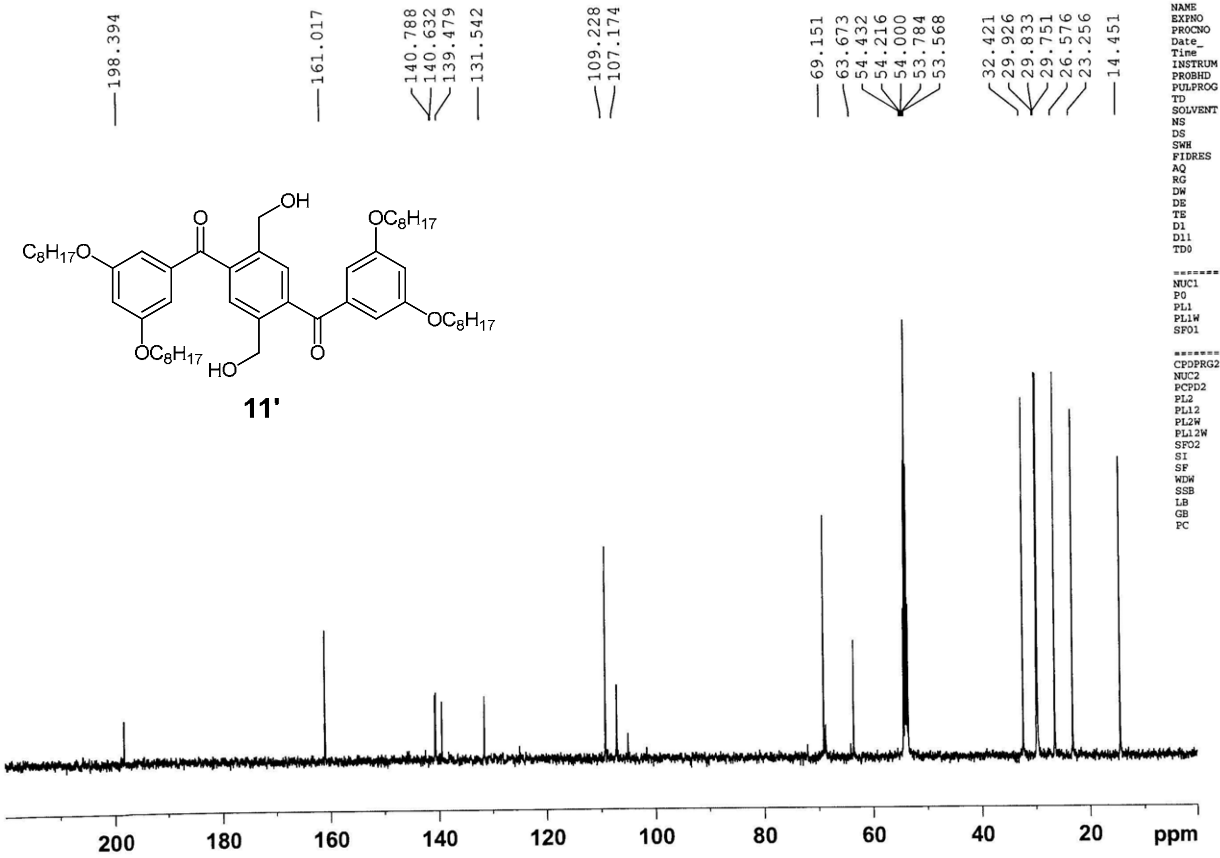
**11**



**11**

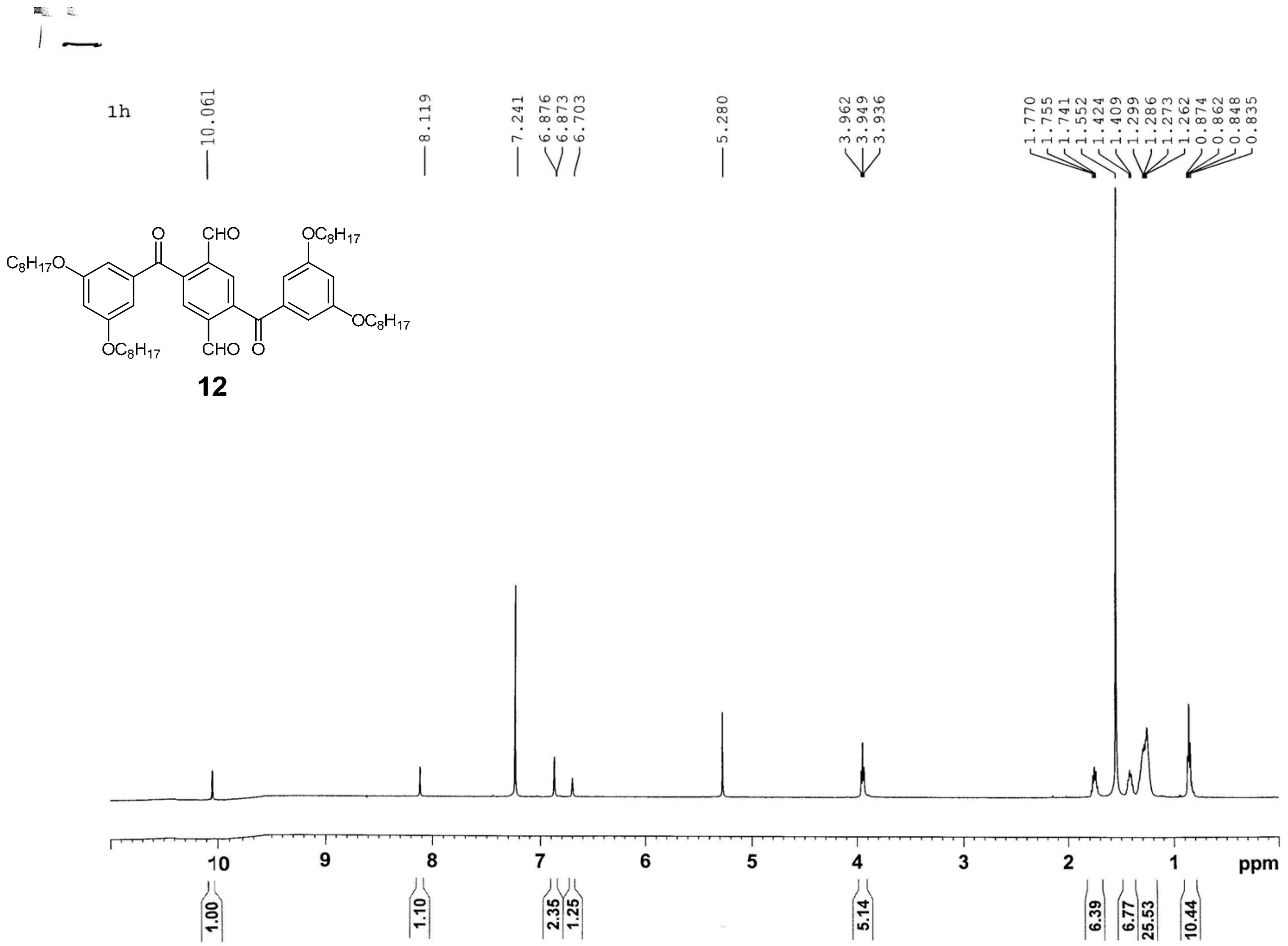
```
Current Data Parameters
NAME             yi081030
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20081030
Time                11.21
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG            zg0dc
TD                  32768
SOLVENT             CDCl3
NS                    105
DS                      4
SWH             23980.814 Hz
FIDRES           0.731836 Hz
AQ              0.6832628 sec
RG                 2896.3
DW                 20.850 usec
DE                   6.00 usec
TE                  298.1 K
D1             3.00000000 sec
d11            0.03000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P0                   5.73 usec
PL1                 -2.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               98.00 usec
PL2                 -2.00 dB
PL12                16.50 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF            100.6127759 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40

1D NMR plot parameters
CX                  25.00 cm
CY                  13.50 cm
F1P               180.000 ppm
F1               18110.30 Hz
F2P                -0.000 ppm
F2                  -0.00 Hz
PPMCM             7.20000 ppm/cm
HZCM            724.41199 Hz/cm
```

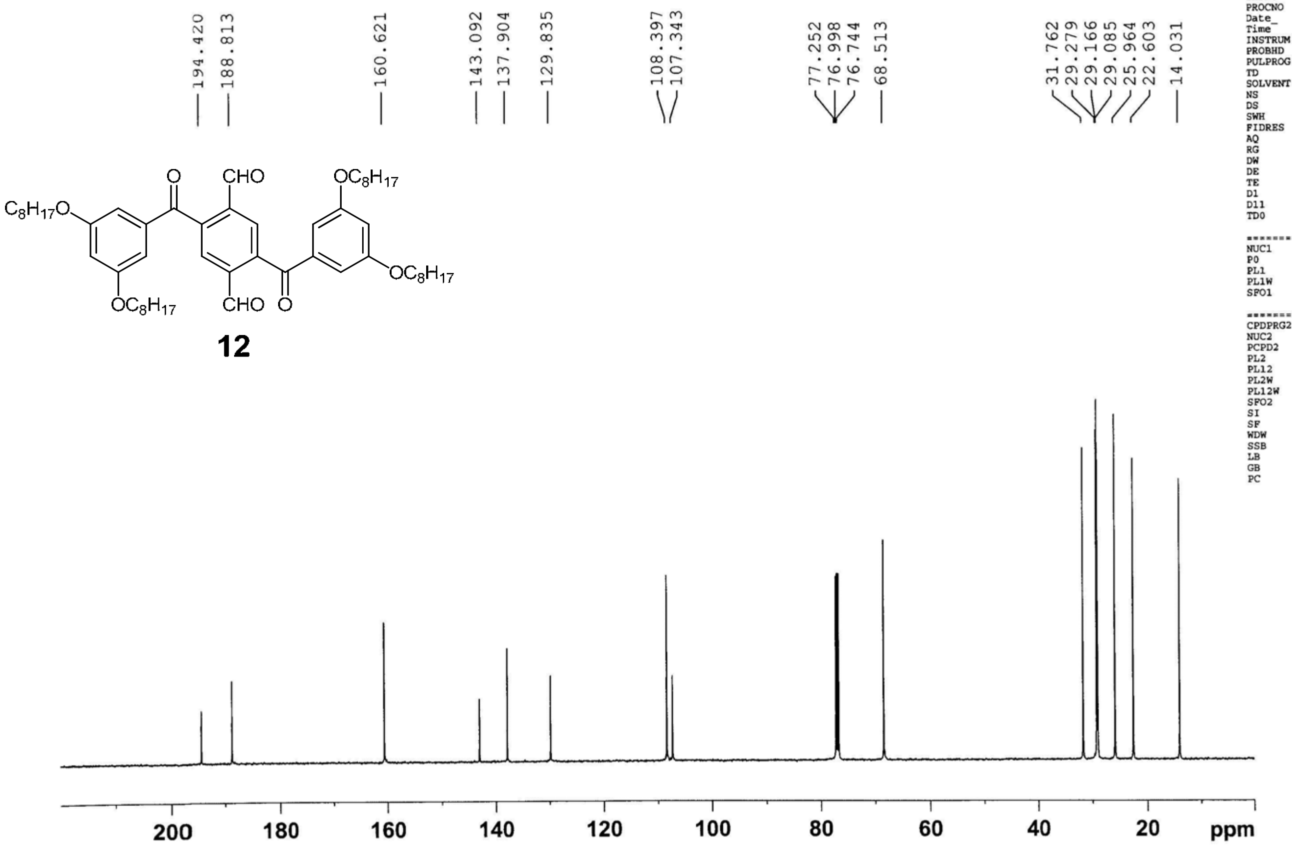

7.610
7.240
6.903
6.898
6.699
6.695
6.691
4.592
4.579
3.967
3.954
3.941
3.148
3.135
3.122
1.789
1.776
1.761
1.746
1.733
1.428
1.412
1.398
1.300
1.287
1.273
1.263
1.233
0.875
0.863
0.849
OH
O
OC8H17
C8H17O
OC8H17
OC8H17
HO
O
11'
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.96
0.99
2.17
5.29
0.83
7.91
7.41
29.92
9.57



**11'**

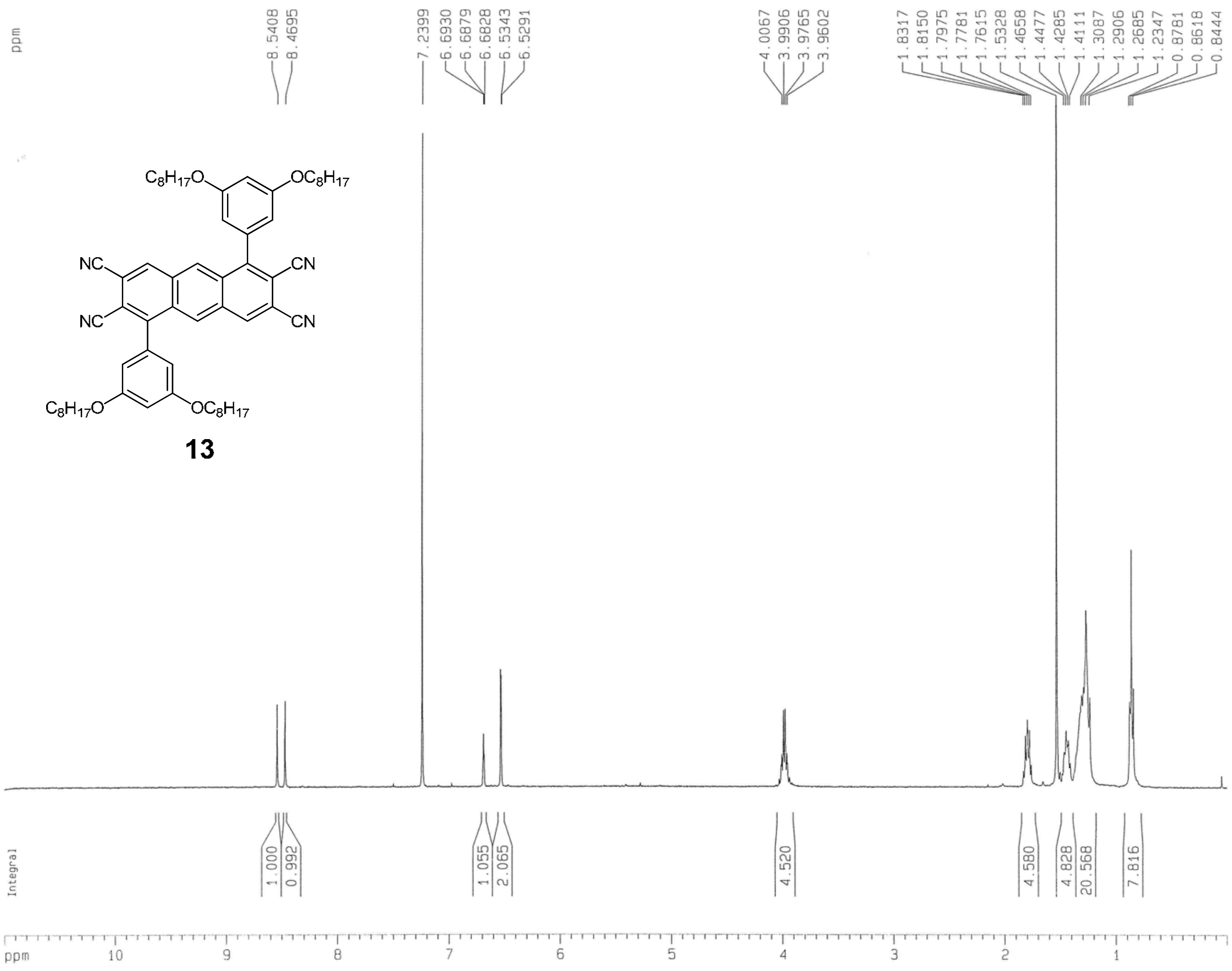
```
NAME              yi100624
EXPNO                    8
PROCNO                   1
Date_             20100624
Time                 19.44
INSTRUM              spect
PROBHD   5 mm QNP  1H/1
PULPROG             zg0dc
TD                   32768
SOLVENT             CD2Cl2
NS                      98
DS                       2
SWH              34013.605 Hz
FIDRES            1.038013 Hz
AQ               0.4817543 sec
RG                    2048
DW                  14.700 usec
DE                    6.00 usec
TE                   296.4 K
D1              3.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P0                    7.50 usec
PL1                   3.00 dB
PL1W           34.87223434 W
SFO1           125.7898571 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                   0.00 dB
PL12                 14.60 dB
PL2W           17.83439445 W
PL12W           0.61838412 W
SFO2           500.2020008 MHz
SI                   32768
SF             125.7753129 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.00
```

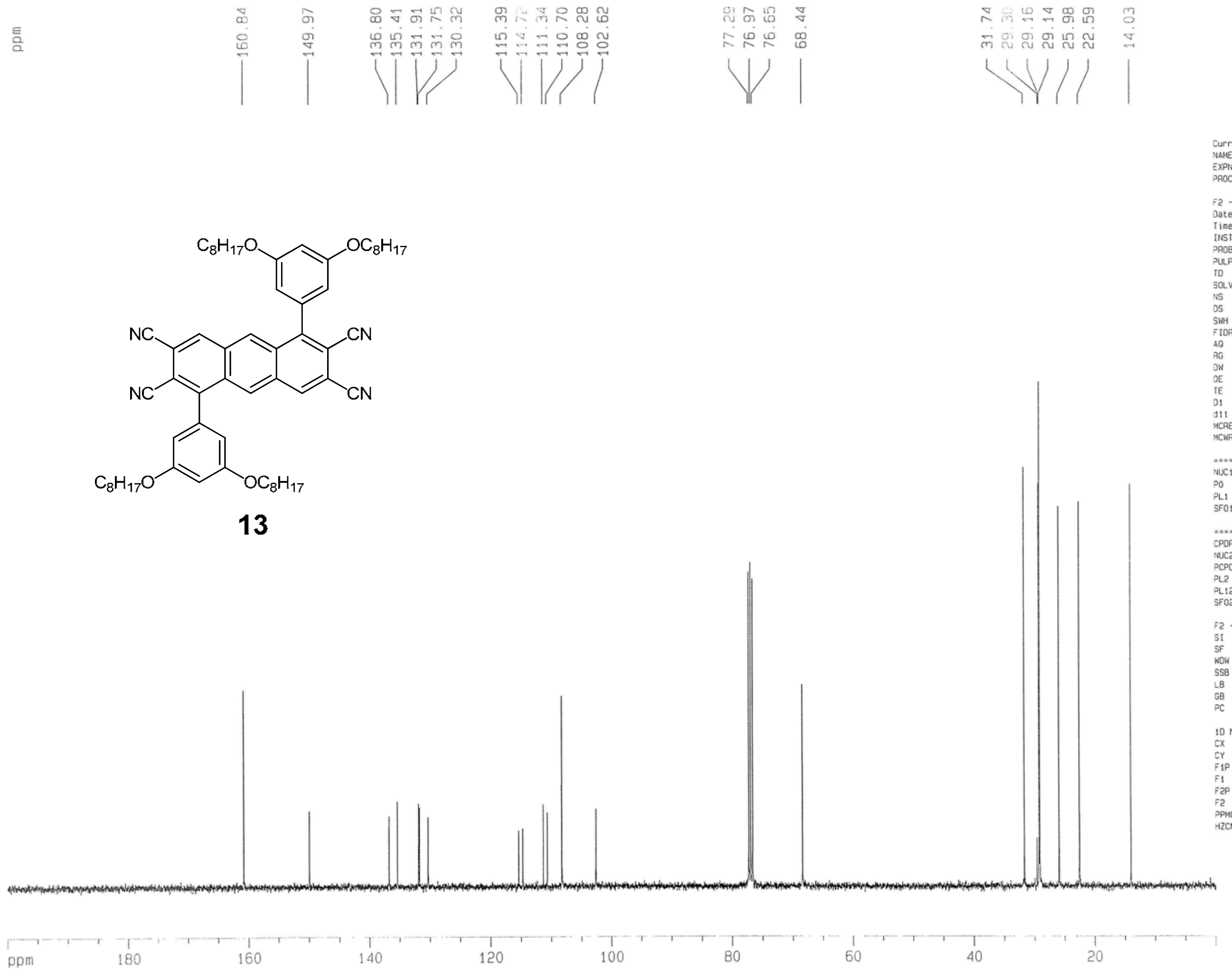

1h
10.061
8.119
7.241
6.876
6.873
6.703
5.280
3.962
3.949
3.936
1.770
1.755
1.741
1.552
1.424
1.409
1.299
1.286
1.273
1.262
0.874
0.862
0.848
0.835
O
CHO
OC8H17
C8H17O
OC8H17
OC8H17
CHO
O
12
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.10
2.35
1.25
5.14
6.39
6.77
25.53
10.44



**12**

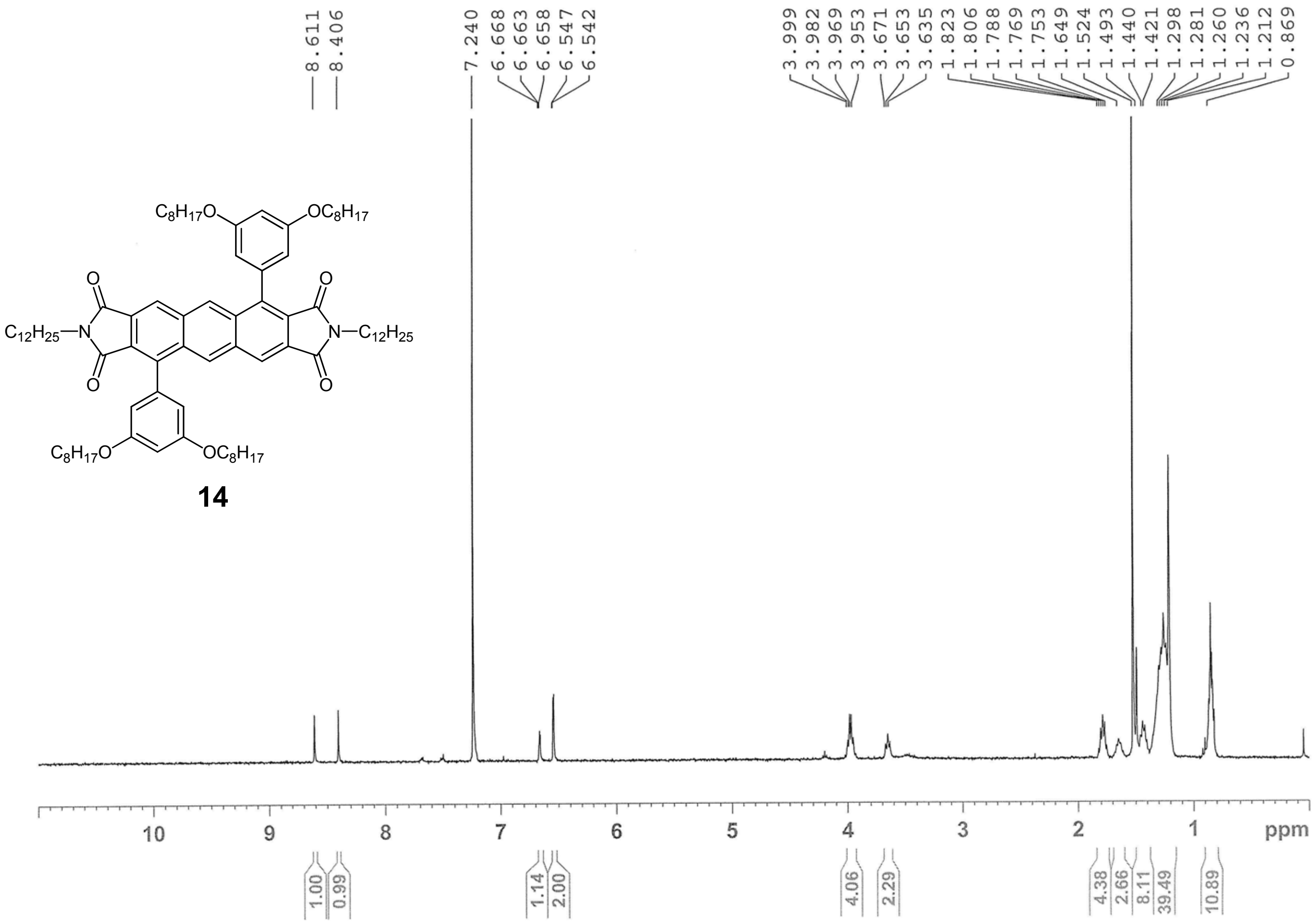
```
NAME              yi100624
EXPNO                    5
PROCNO                   1
Date_             20100624
Time                 16.05
INSTRUM              spect
PROBHD   5 mm QNP     1H/1
PULPROG             zg0dc
TD                   32768
SOLVENT              CDCl3
NS                     508
DS                       2
SWH              34013.605 Hz
FIDRES            1.038013 Hz
AQ               0.4817543 sec
RG                    6502
DW                  14.700 usec
DE                    6.00 usec
TE                   296.2 K
D1              3.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P0                    7.50 usec
PL1                   3.00 dB
PL1W           34.87223434 W
SFO1           125.7898571 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                   0.00 dB
PL12                 14.60 dB
PL2W           17.83439445 W
PL12W           0.61838412 W
SFO2           500.2020008 MHz
SI                   32768
SF             125.7753938 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.00
```


ppm
8.5408
8.4695
7.2399
6.6930
6.6879
6.6828
6.5343
6.5291
4.0067
3.9906
3.9765
3.9602
1.8317
1.8150
1.7975
1.7781
1.7615
1.5328
1.4658
1.4477
1.4285
1.4111
1.3087
1.2906
1.2685
1.2347
0.8781
0.8618
0.8444
C8H17O
OC8H17
NC
CN
NC
CN
C8H17O
OC8H17
13
Integral
1.000
0.992
1.055
2.065
4.520
4.580
4.828
20.568
7.816
ppm
10
9
8
7
6
5
4
3
2
1

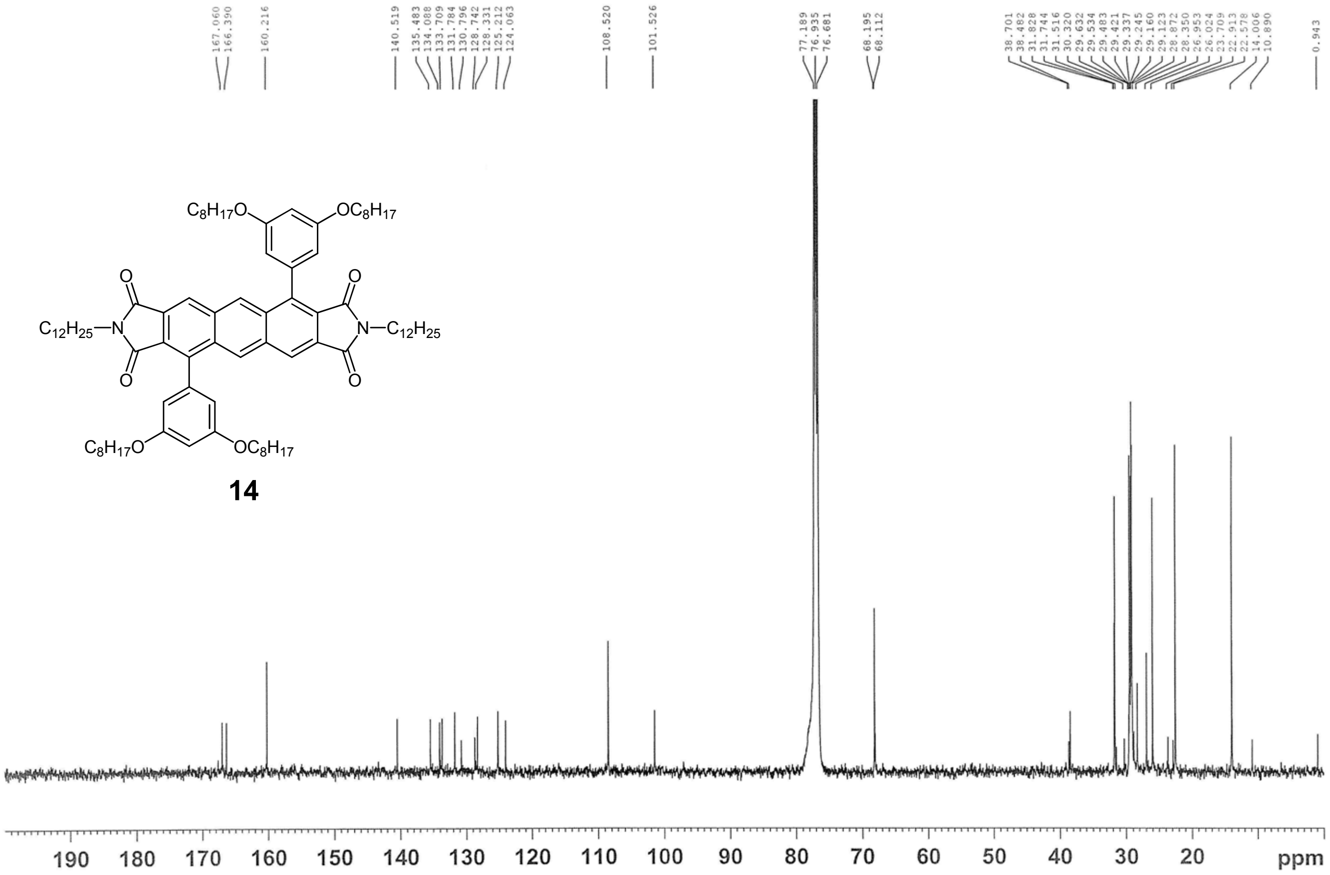


**13**

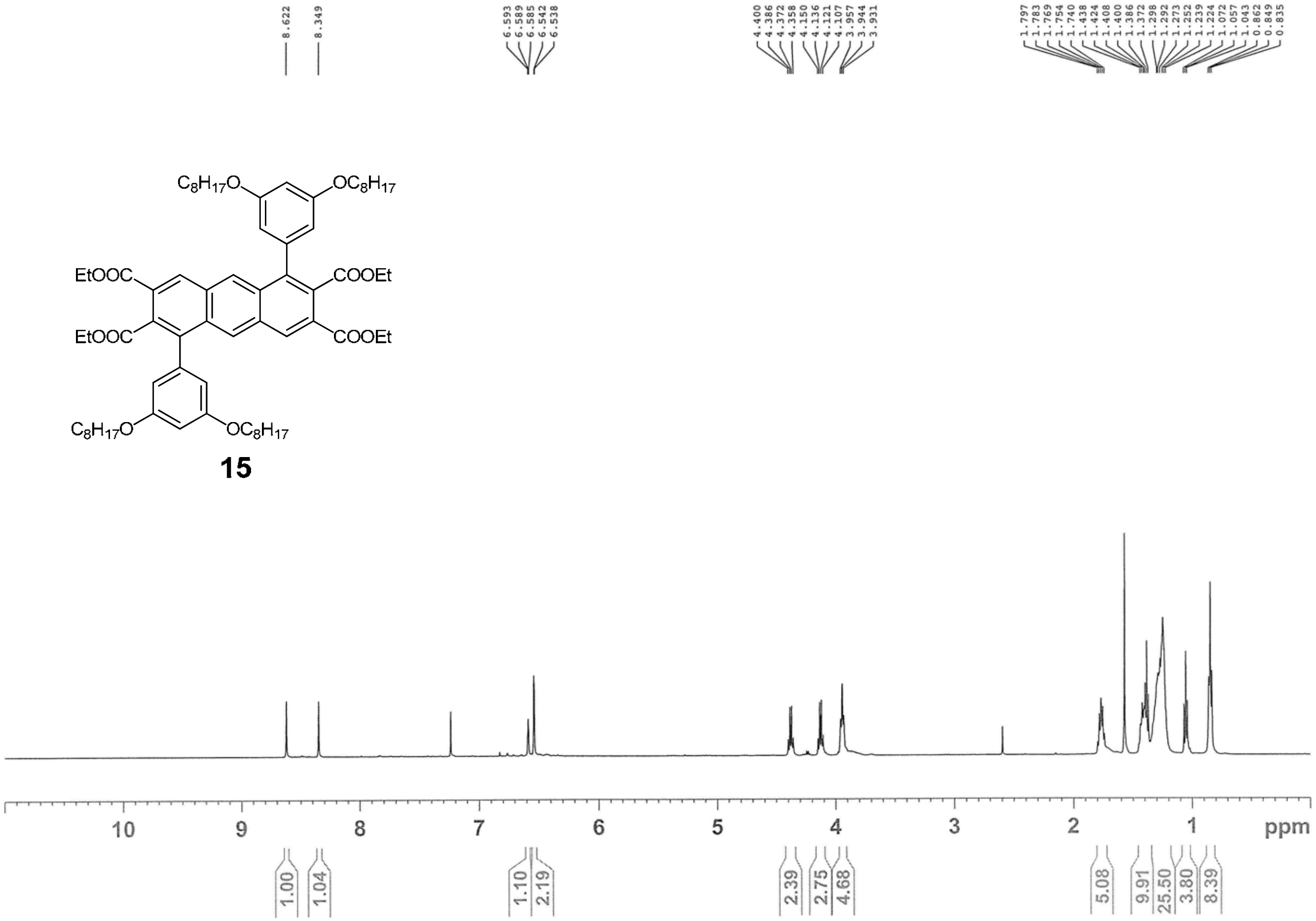
```
Current Data Parameters
NAME             yi081001
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20081001
Time                17.19
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg0dc
TD                  32768
SOLVENT             CDCl3
NS                    344
DS                      4
SWH             23980.814 Hz
FIDRES           0.731836 Hz
AQ              0.6832628 sec
RG                  574.7
DW                 20.850 usec
DE                   6.00 usec
TE                  298.0 K
D1             3.00000000 sec
d11            0.03000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P0                   5.73 usec
PL1                 -2.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               98.00 usec
PL2                 -2.00 dB
PL12                16.50 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF            100.6127759 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40

1D NMR plot parameters
CX                  24.00 cm
CY                  10.00 cm
F1P               200.000 ppm
F1               20122.55 Hz
F2P                -0.000 ppm
F2                  -0.00 Hz
PPMCM             8.33333 ppm/cm
HZCM            838.43982 Hz/cm
```


C8H17O
OC8H17
O
O
C12H25—N
N—C12H25
O
O
C8H17O
OC8H17
8.611
8.406
7.240
6.668
6.663
6.658
6.547
6.542
3.999
3.982
3.969
3.953
3.671
3.653
3.635
1.823
1.806
1.788
1.769
1.753
1.649
1.524
1.493
1.440
1.421
1.298
1.281
1.260
1.236
1.212
0.869
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.99
1.14
2.00
4.06
2.29
4.38
2.66
8.11
39.49
10.89

**14**

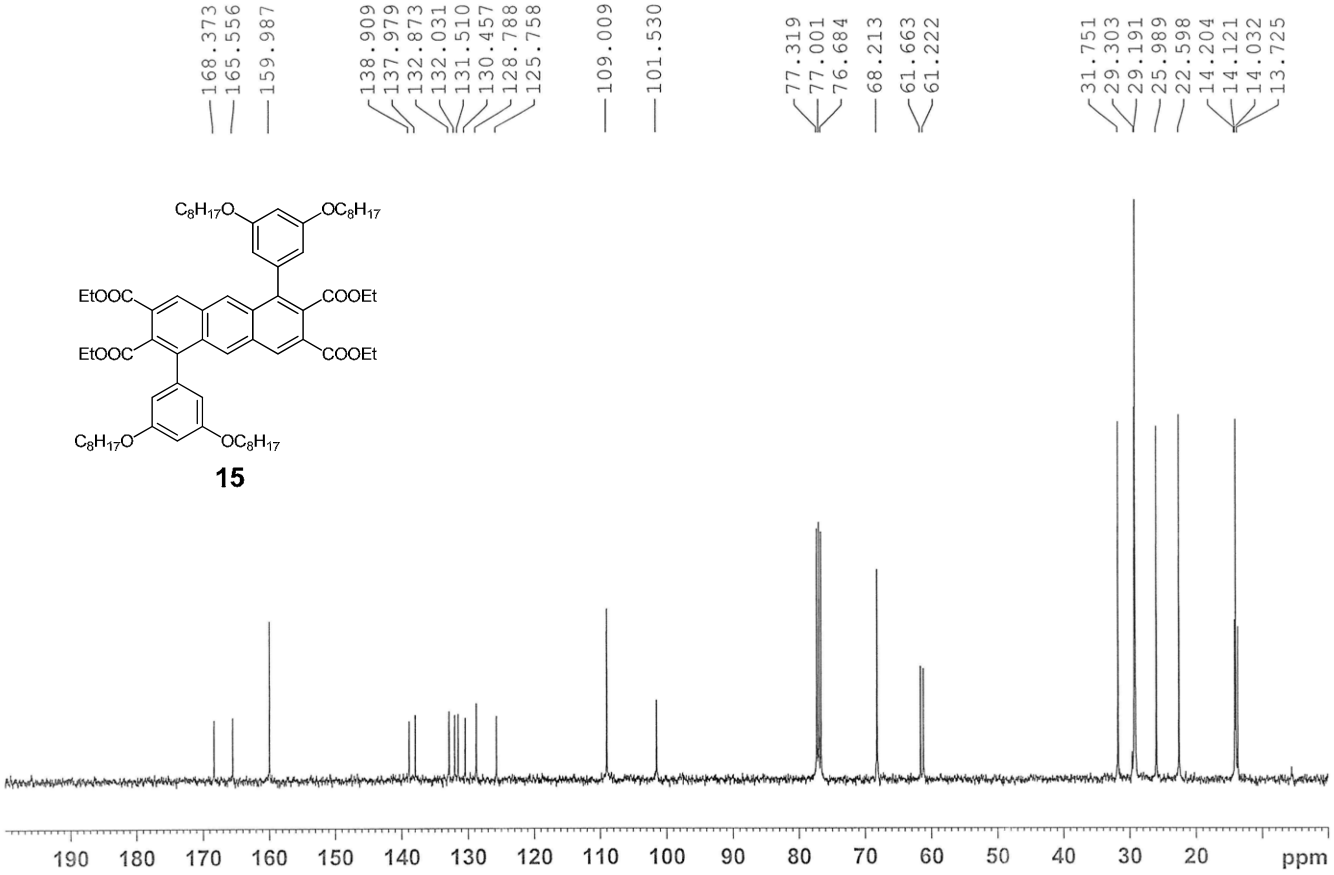

167.060
166.390
160.216
140.519
135.483
134.088
133.709
131.784
130.796
128.742
128.331
125.212
124.063
108.520
101.526
77.189
76.935
76.681
68.195
68.112
38.701
38.482
31.828
31.744
31.516
30.320
29.632
29.534
29.483
29.421
29.337
29.245
29.160
29.123
28.872
28.350
26.953
26.024
23.709
22.913
22.578
14.006
10.890
0.943
$C_8H_{17}O$
$OC_8H_{17}$
O
$C_{12}H_{25}$—N
N—$C_{12}H_{25}$
O
O
O
$C_8H_{17}O$
$OC_8H_{17}$
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

**14**


C8H17O
OC8H17
EtOOC
COOEt
EtOOC
COOEt
C8H17O
OC8H17

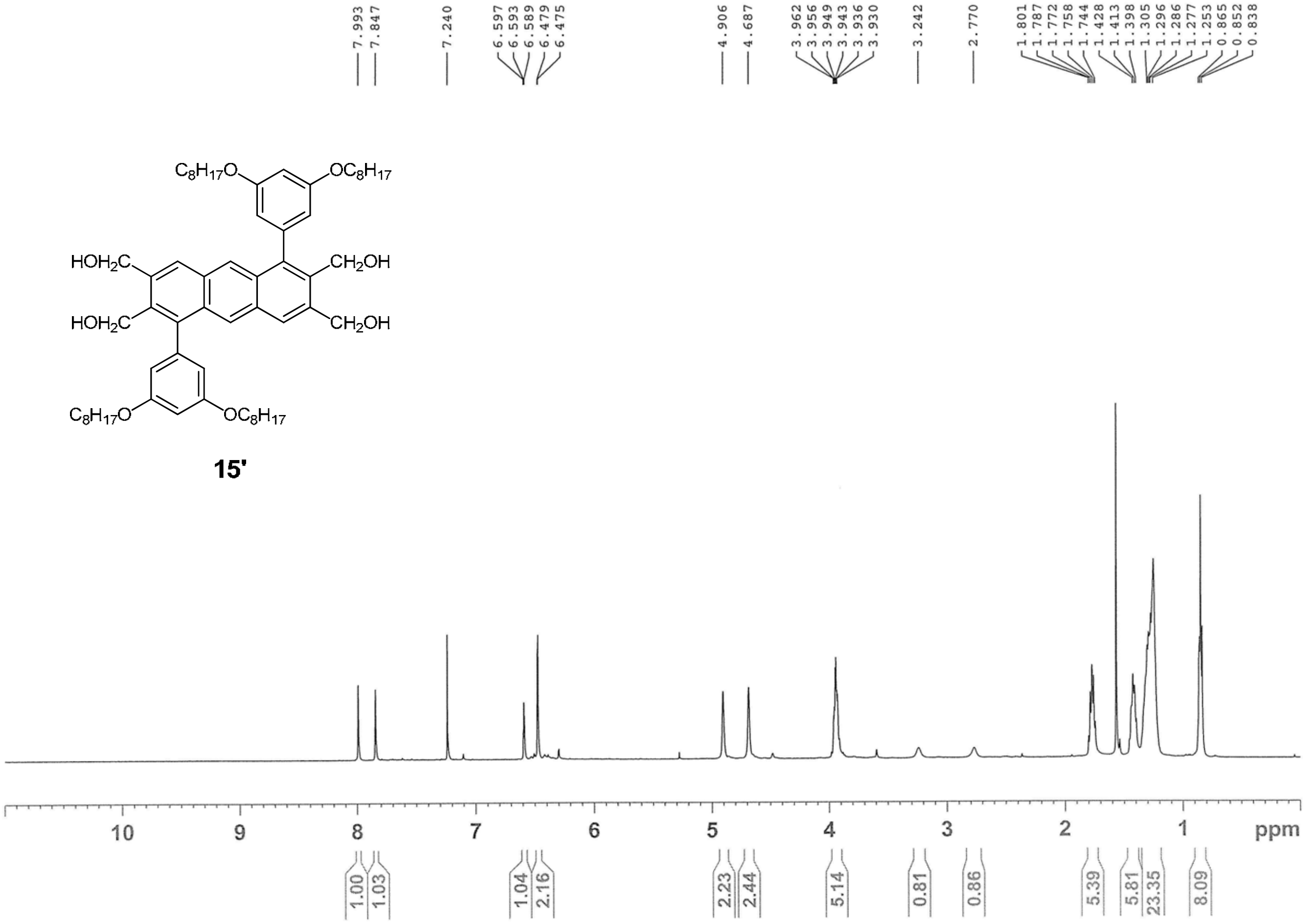
**15**

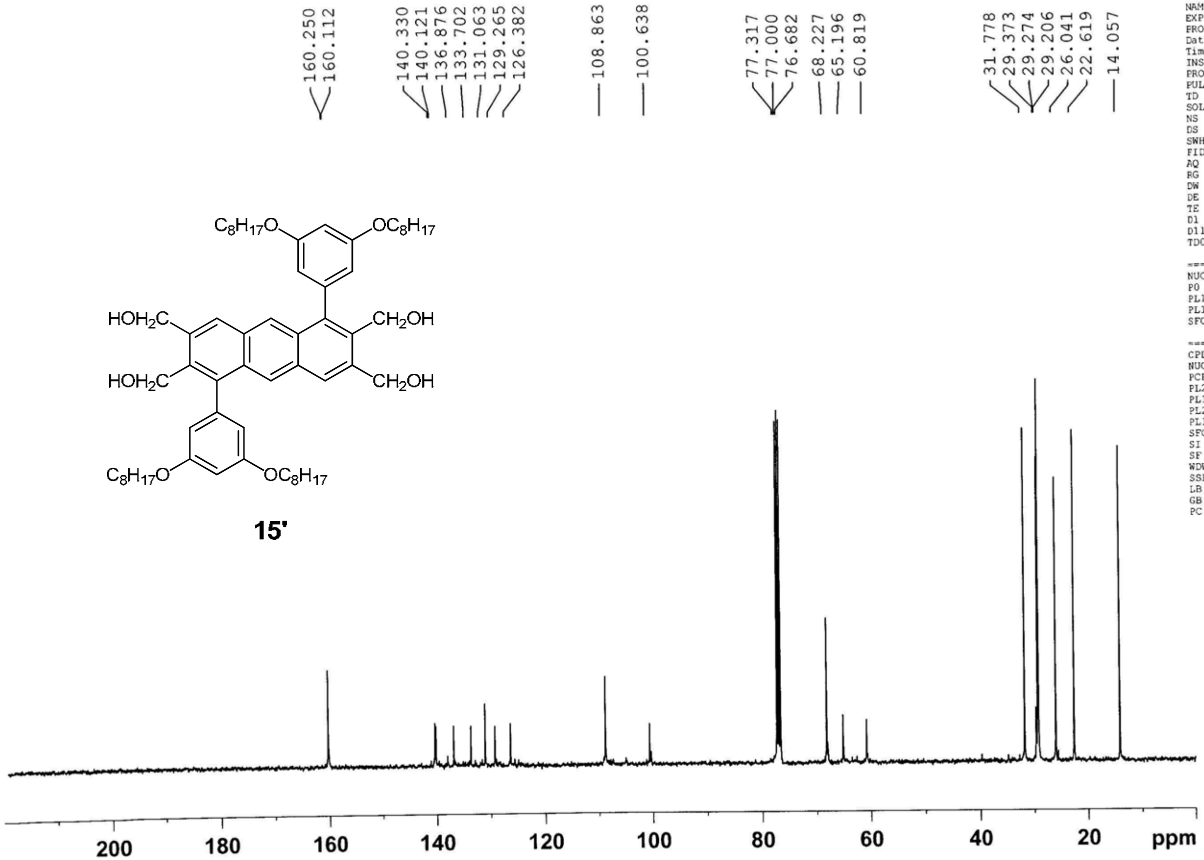
8.622
8.349
6.593
6.589
6.585
6.542
6.538
4.400
4.386
4.372
4.358
4.150
4.136
4.121
4.107
3.957
3.944
3.931
1.797
1.783
1.769
1.754
1.740
1.438
1.424
1.408
1.400
1.386
1.372
1.298
1.292
1.273
1.252
1.239
1.224
1.072
1.057
1.043
0.862
0.849
0.835
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.04
1.10
2.19
2.39
2.75
4.68
5.08
9.91
25.50
3.80
8.39


168.373
165.556
159.987
138.909
137.979
132.873
132.031
131.510
130.457
128.788
125.758
109.009
101.530
77.319
77.001
76.684
68.213
61.663
61.222
31.751
29.303
29.191
25.989
22.598
14.204
14.121
14.032
13.725
C8H17O
OC8H17
EtOOC
COOEt
EtOOC
COOEt
C8H17O
OC8H17
15
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

C8H17O
OC8H17
HOH2C
HOH2C
CH2OH
CH2OH
C8H17O
OC8H17

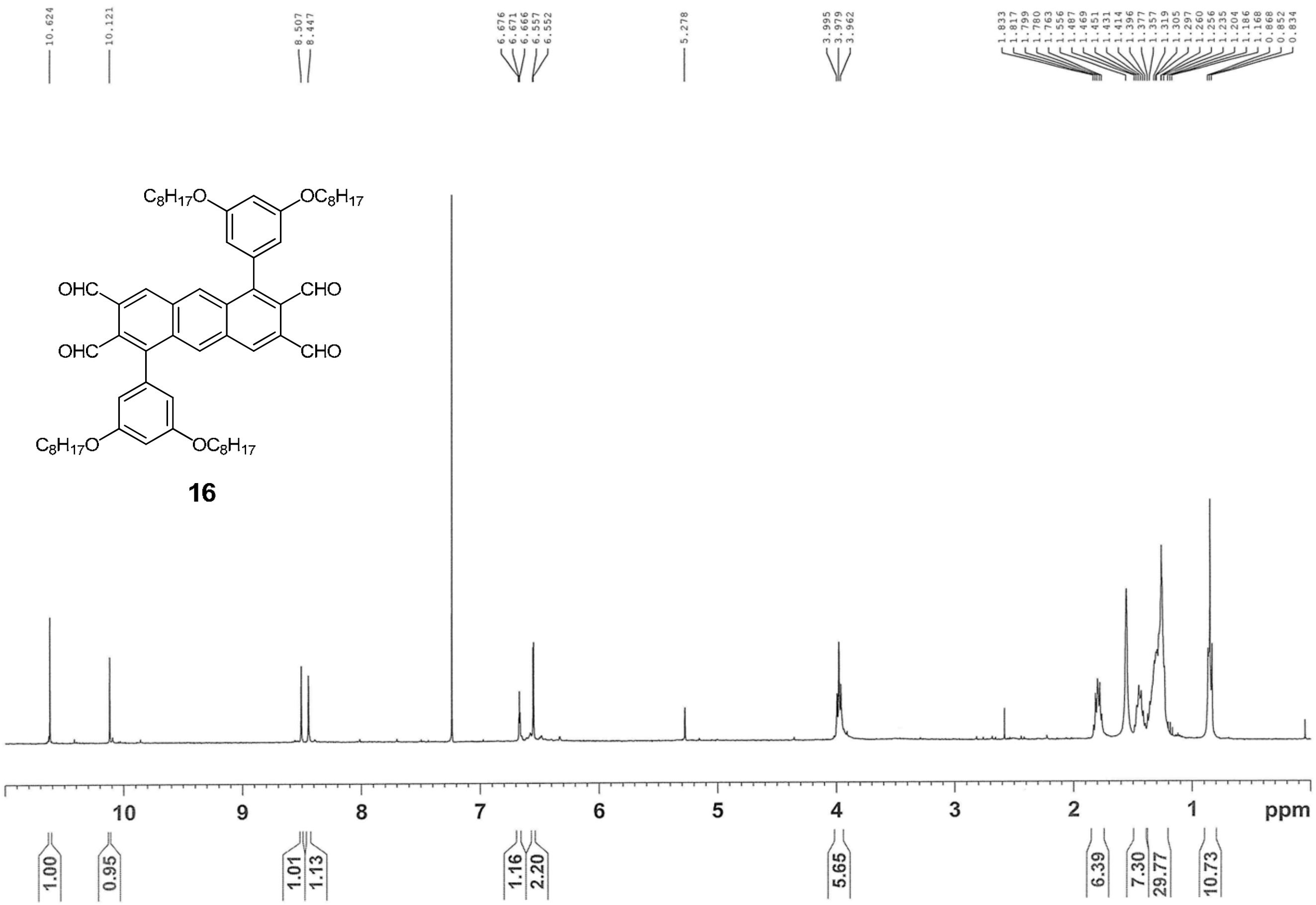
**15'**


7.993
7.847
7.240
6.597
6.593
6.589
6.479
6.475
4.906
4.687
3.962
3.956
3.949
3.943
3.936
3.930
3.242
2.770
1.801
1.787
1.772
1.758
1.744
1.428
1.413
1.398
1.305
1.296
1.286
1.277
1.253
0.865
0.852
0.838
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.03
1.04
2.16
2.23
2.44
5.14
0.81
0.86
5.39
5.81
23.35
8.09

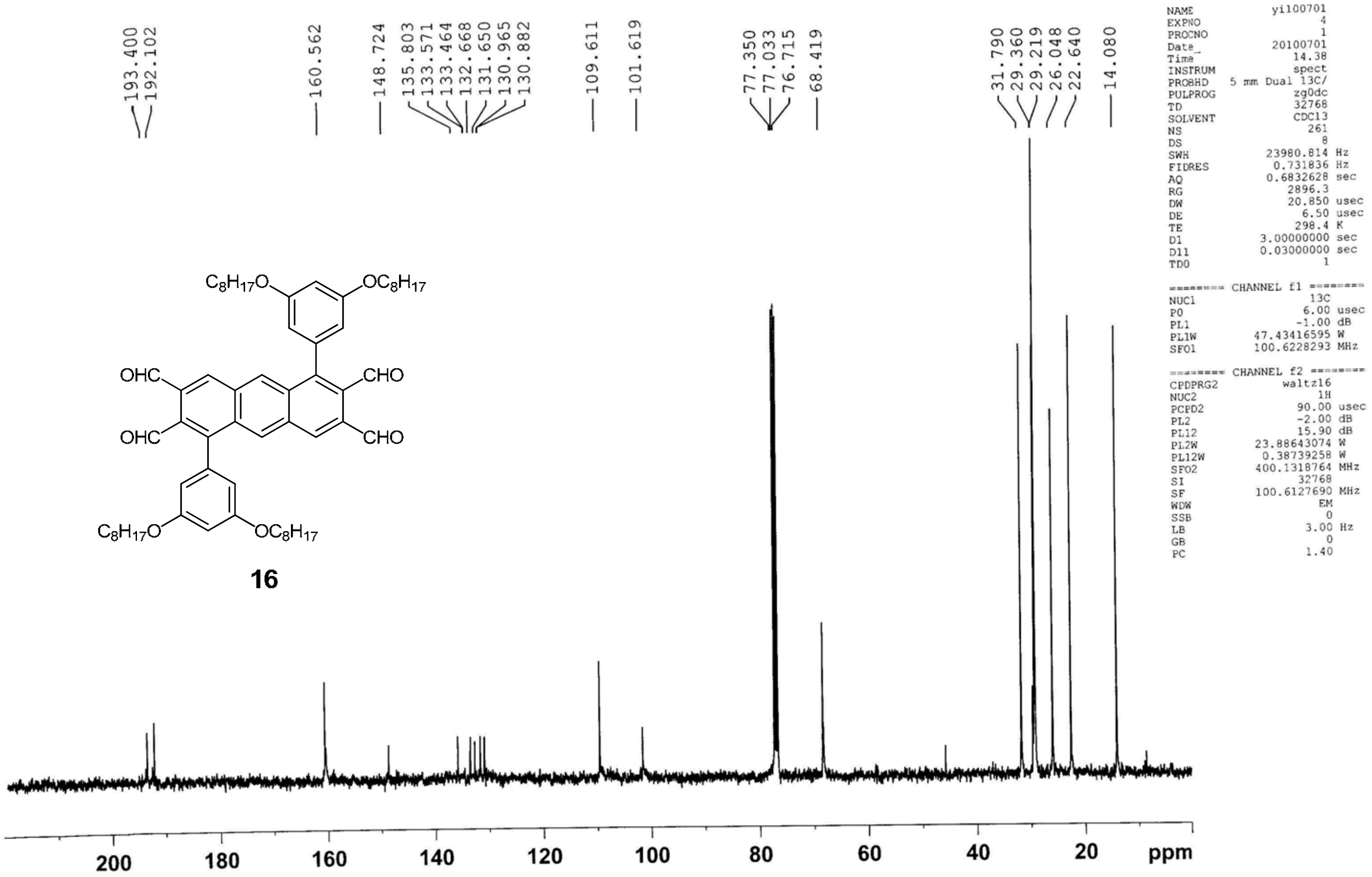


**15'**

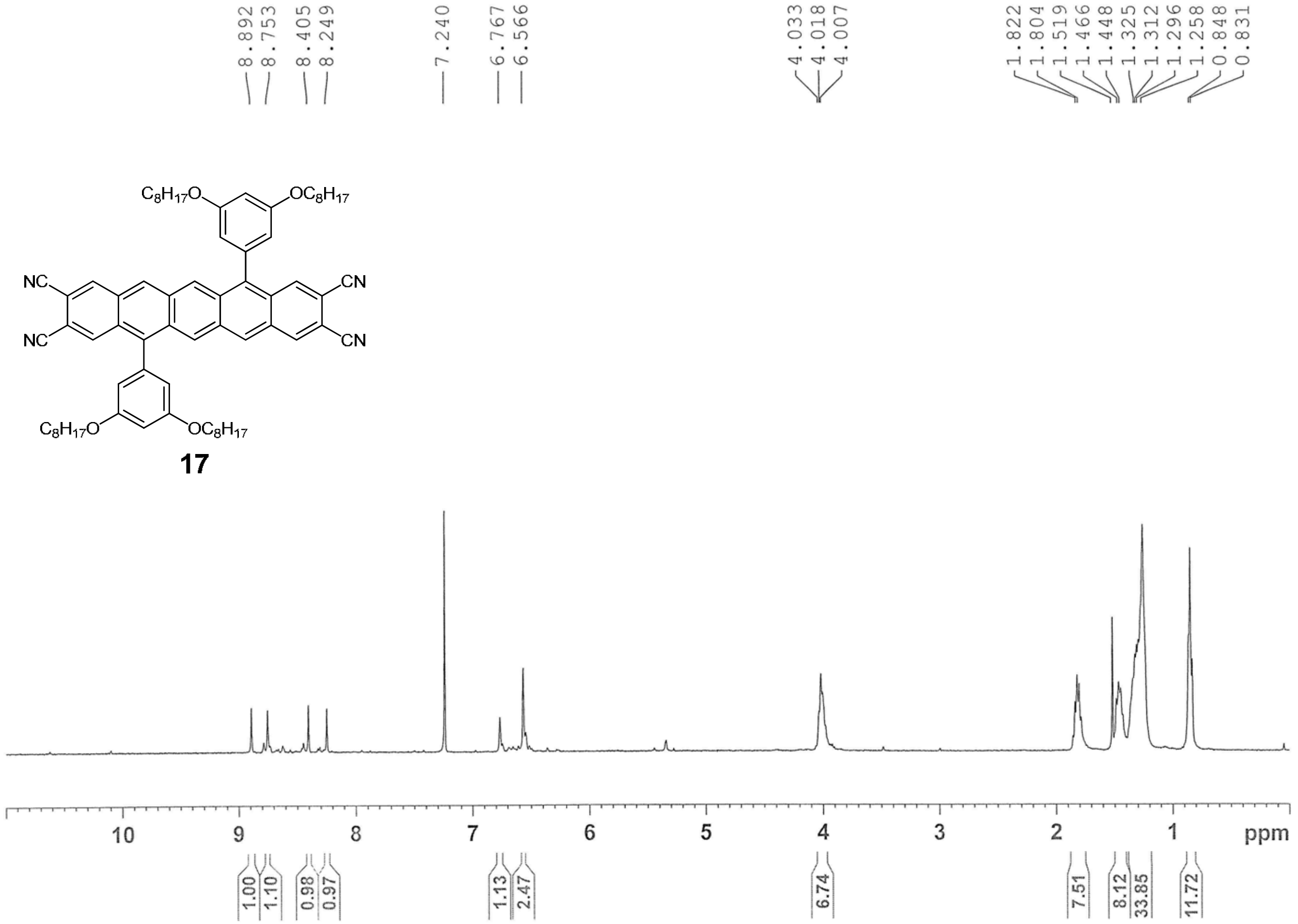
```
NAME            yi100630
EXPNO                  3
PROCNO                 1
Date_           20100630
Time               12.23
INSTRUM            spect
PROBHD   5 mm Dual 13C/
PULPROG           zg0dc
TD                 32768
SOLVENT            CDC13
NS                  1000
DS                     8
SWH            23980.814 Hz
FIDRES          0.731836 Hz
AQ             0.6832628 sec
RG                2896.3
DW                20.850 usec
DE                  6.50 usec
TE                 298.5 K
D1            3.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P0                  6.00 usec
PL1                -1.00 dB
PL1W         47.43416595 W
SFO1         100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                -2.00 dB
PL12               15.90 dB
PL2W         23.88643074 W
PL12W         0.38739258 W
SFO2         400.1318764 MHz
SI                 32768
SF           100.6127721 MHz
WDW                   EM
SSB                    0
LB                  3.00 Hz
GB                     0
PC                  1.40
```


16

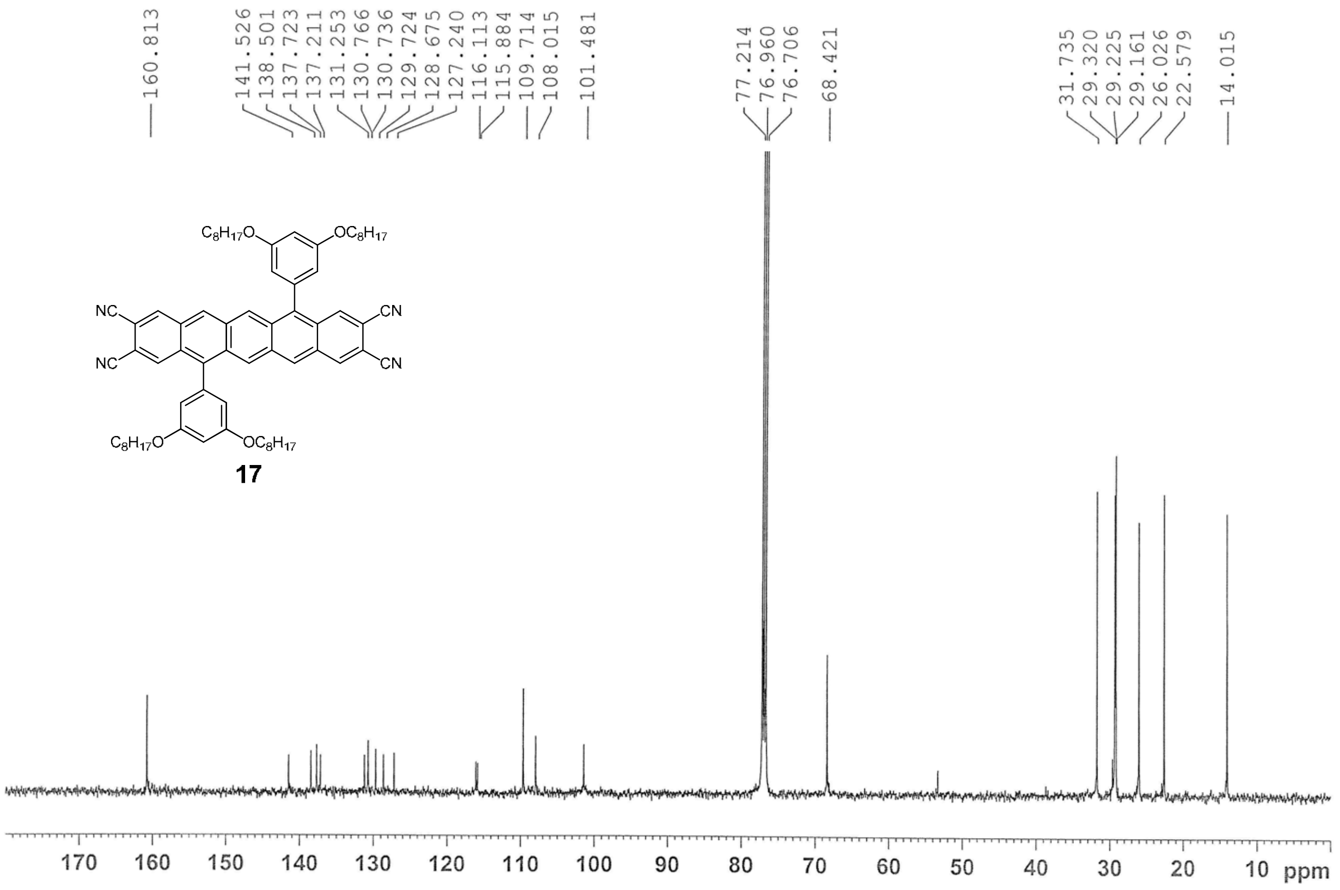
10.624
10.121
8.507
8.447
6.676
6.671
6.666
6.557
6.552
5.278
3.995
3.979
3.962
1.833
1.817
1.799
1.780
1.763
1.556
1.487
1.469
1.451
1.431
1.414
1.396
1.377
1.357
1.319
1.305
1.297
1.260
1.256
1.235
1.204
1.186
1.168
0.868
0.852
0.834
C8H17O
OC8H17
OHC
CHO
OHC
CHO
C8H17O
OC8H17
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.95
1.01
1.13
1.16
2.20
5.65
6.39
7.30
29.77
10.73



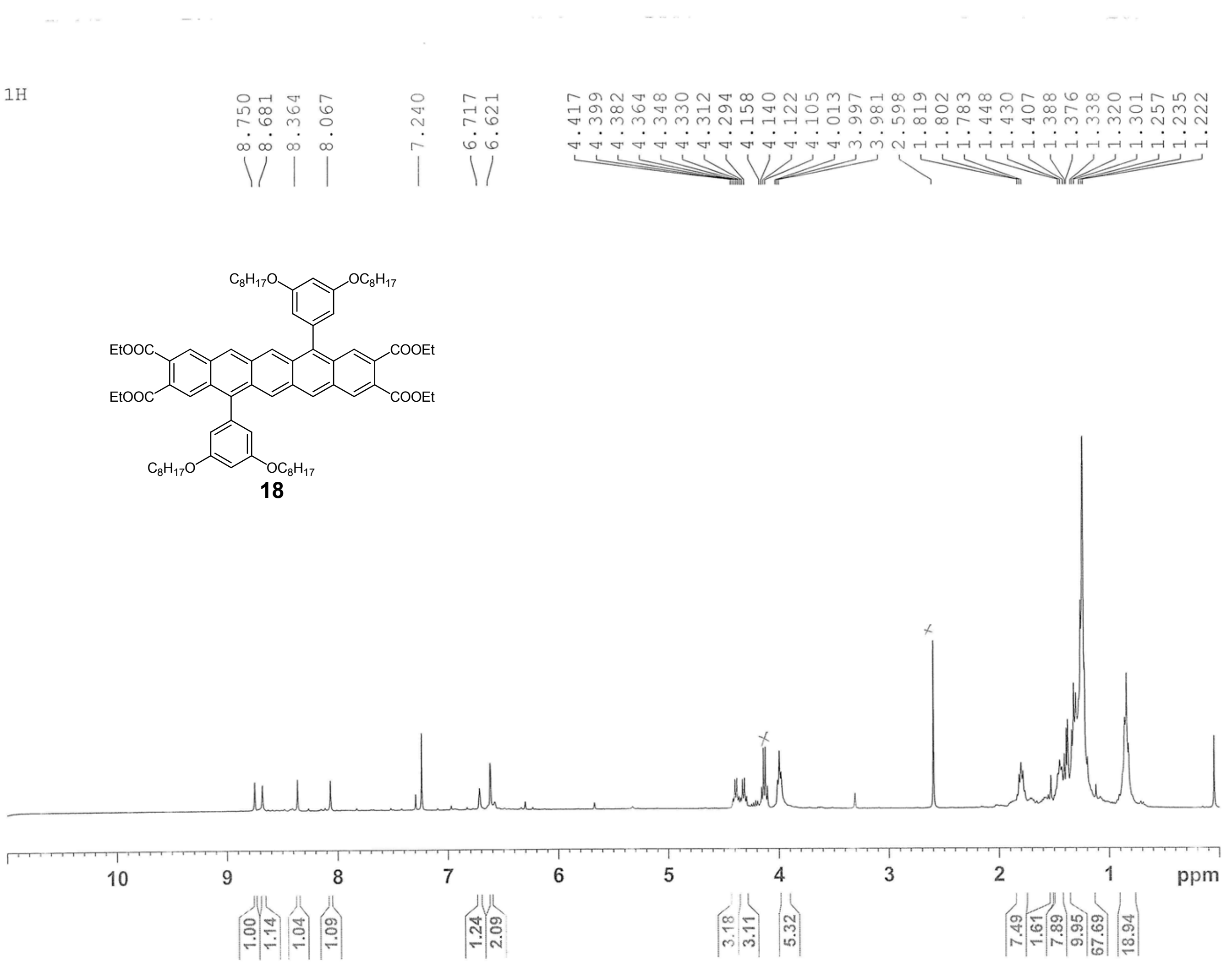
```
NAME              yi100701
EXPNO                    4
PROCNO                   1
Date_             20100701
Time                 14.38
INSTRUM              spect
PROBHD   5 mm Dual 13C/
PULPROG             zg0dc
TD                   32768
SOLVENT              CDCl3
NS                     261
DS                       8
SWH             23980.814 Hz
FIDRES           0.731836 Hz
AQ              0.6832628 sec
RG                 2896.3
DW                 20.850 usec
DE                   6.50 usec
TE                  298.4 K
D1             3.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P0                    6.00 usec
PL1                  -1.00 dB
PL1W           47.43416595 W
SFO1           100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  -2.00 dB
PL12                 15.90 dB
PL2W           23.88643074 W
PL12W           0.38739258 W
SFO2           400.1318764 MHz
SI                   32768
SF             100.6127690 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.40
```

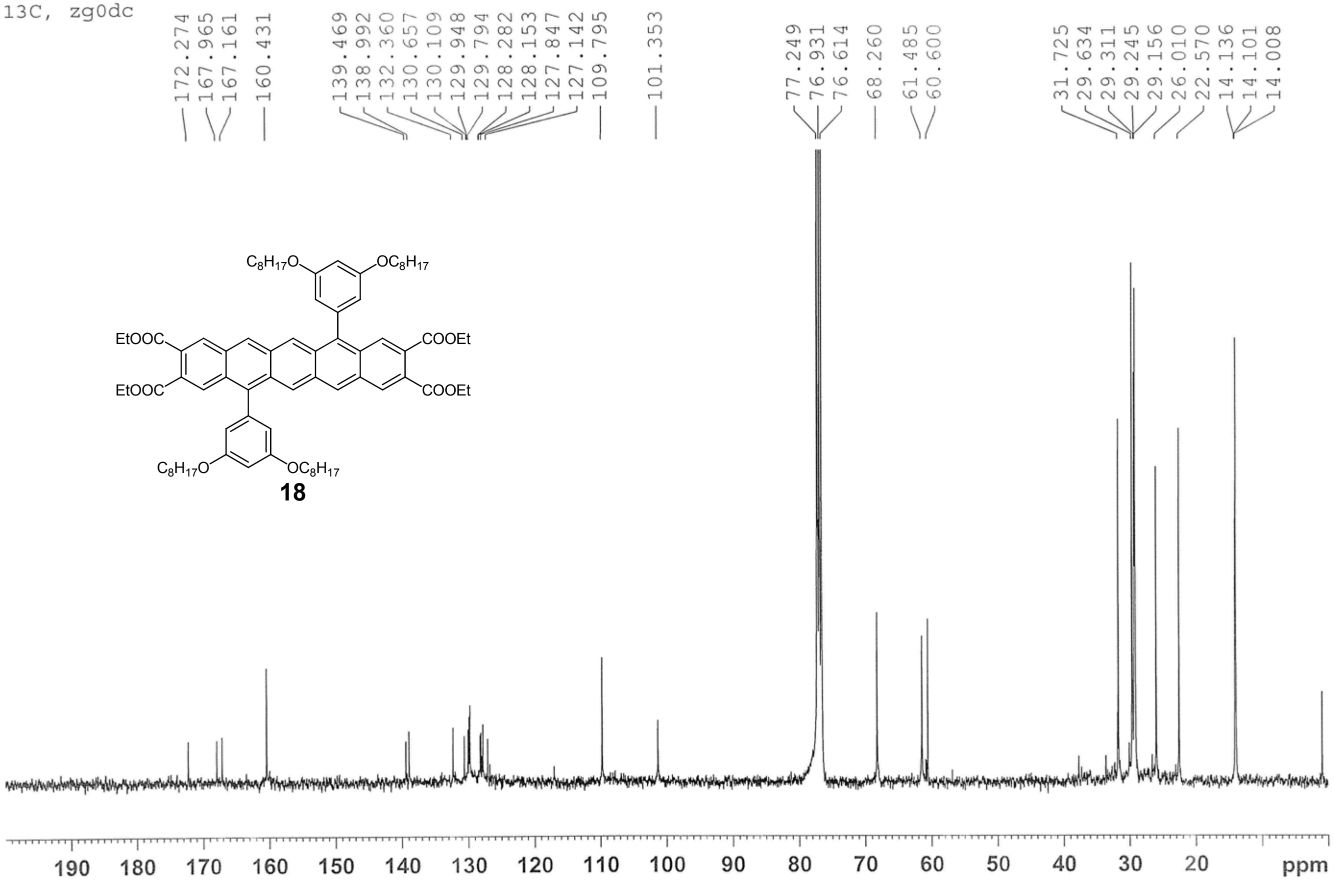

8.892
8.753
8.405
8.249
7.240
6.767
6.566
4.033
4.018
4.007
1.822
1.804
1.519
1.466
1.448
1.325
1.312
1.296
1.258
0.848
0.831
NC
NC
CN
CN
$C_8H_{17}O$
$OC_8H_{17}$
$C_8H_{17}O$
$OC_8H_{17}$
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.10
0.98
0.97
1.13
2.47
6.74
7.51
8.12
33.85
11.72

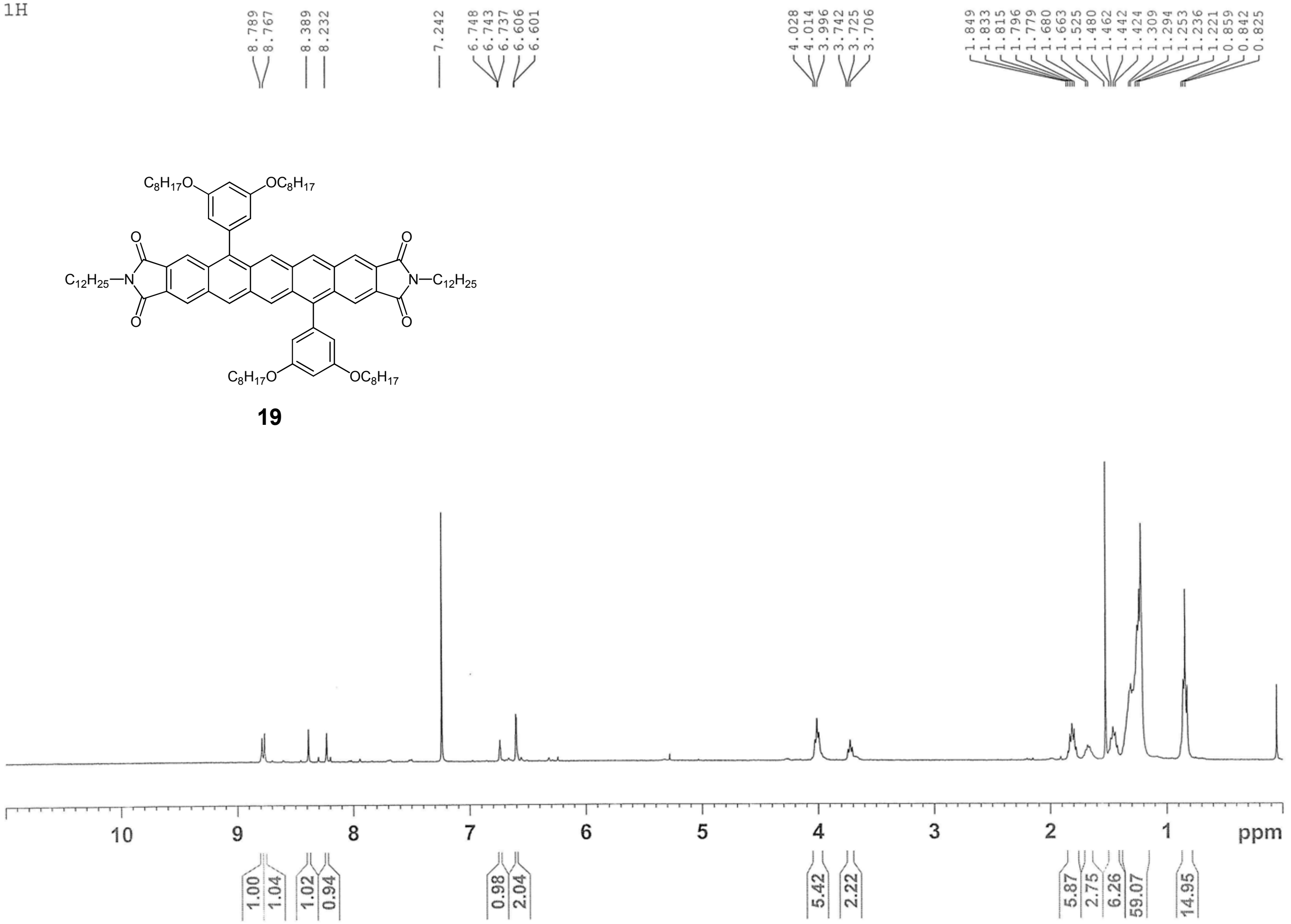
**17**

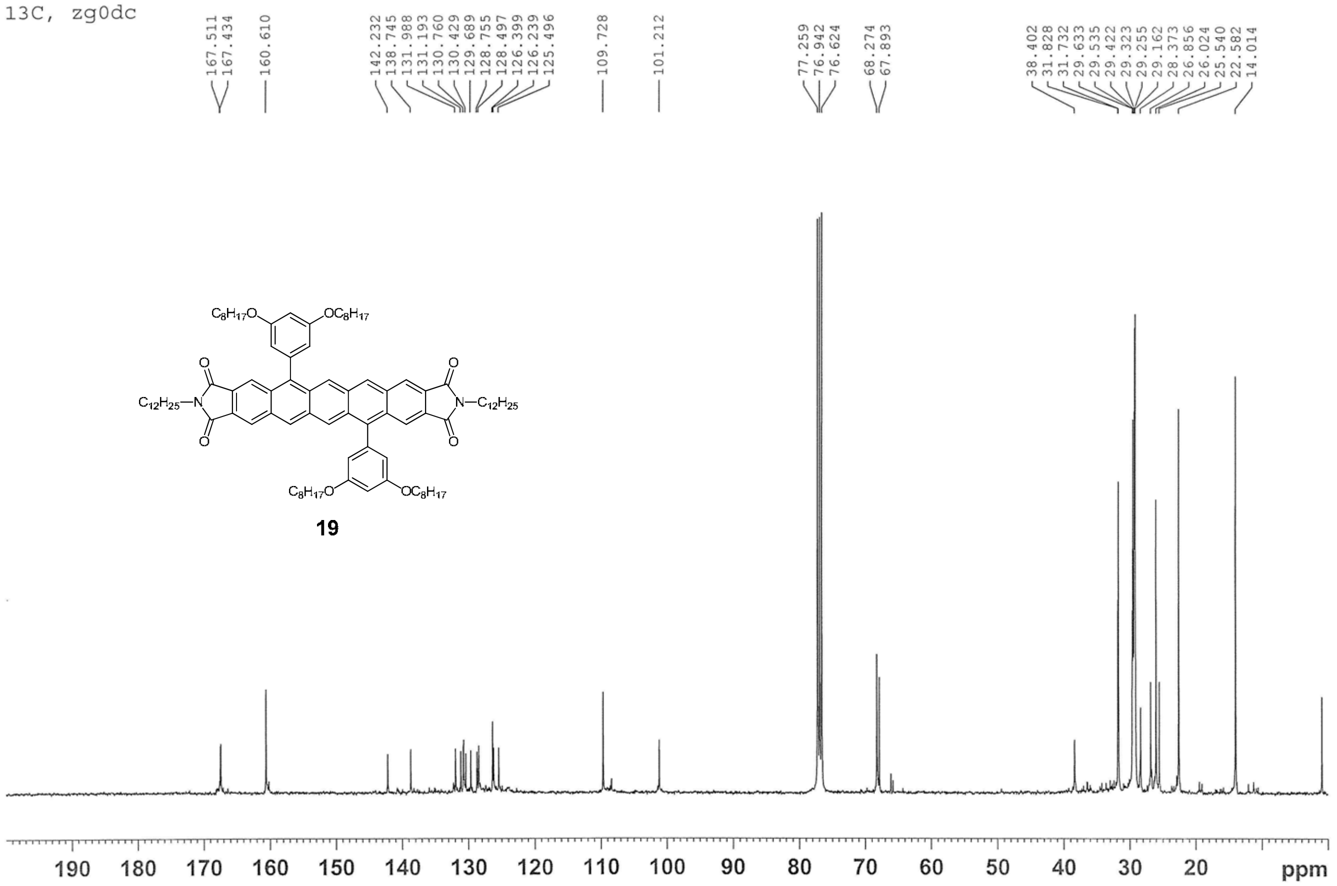

160.813
141.526
138.501
137.723
137.211
131.253
130.766
130.736
129.724
128.675
127.240
116.113
115.884
109.714
108.015
101.481
77.214
76.960
76.706
68.421
31.735
29.320
29.225
29.161
26.026
22.579
14.015
$C_8H_{17}O$
$OC_8H_{17}$
NC
NC
CN
CN
$C_8H_{17}O$
$OC_8H_{17}$
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

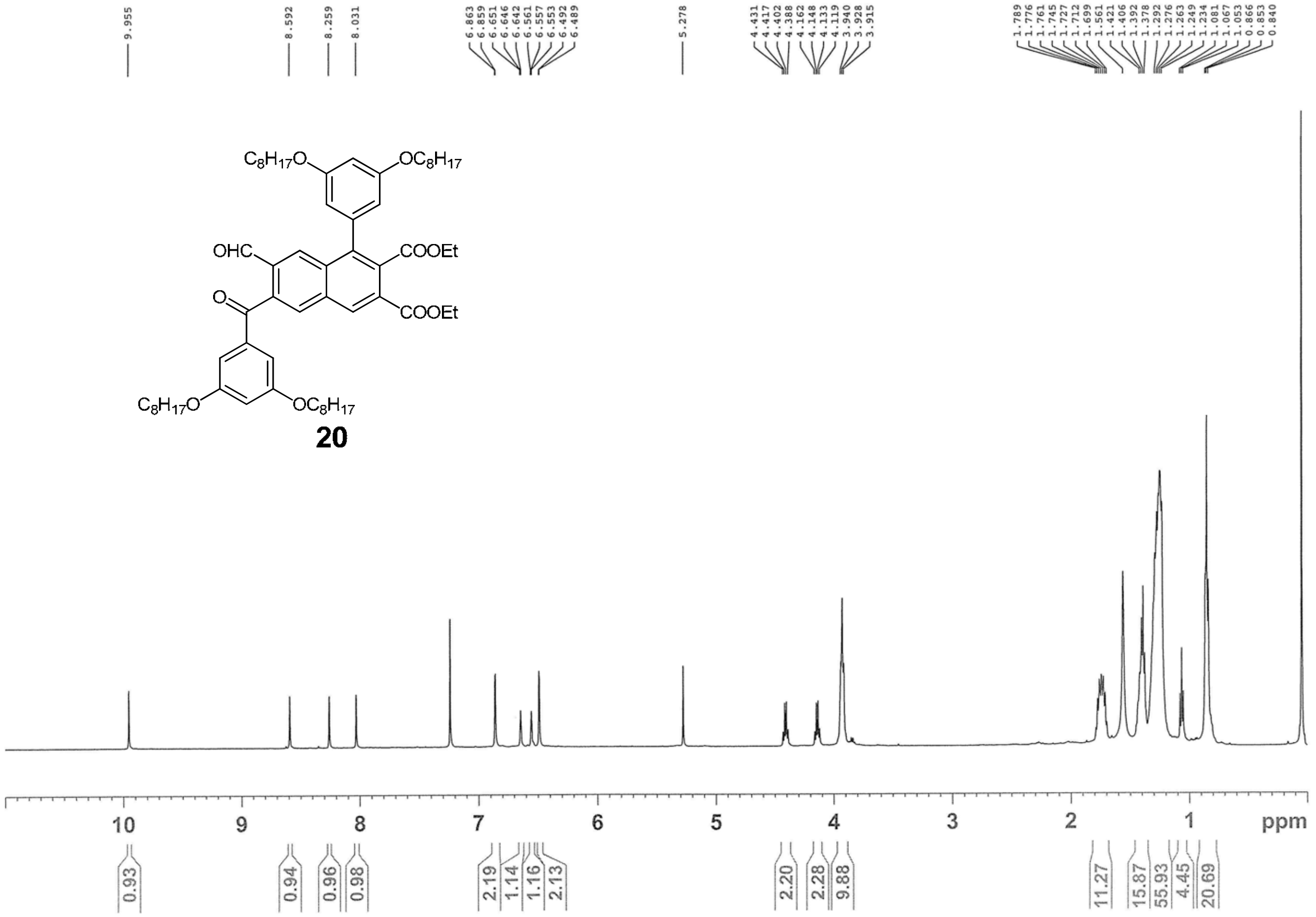
**17**

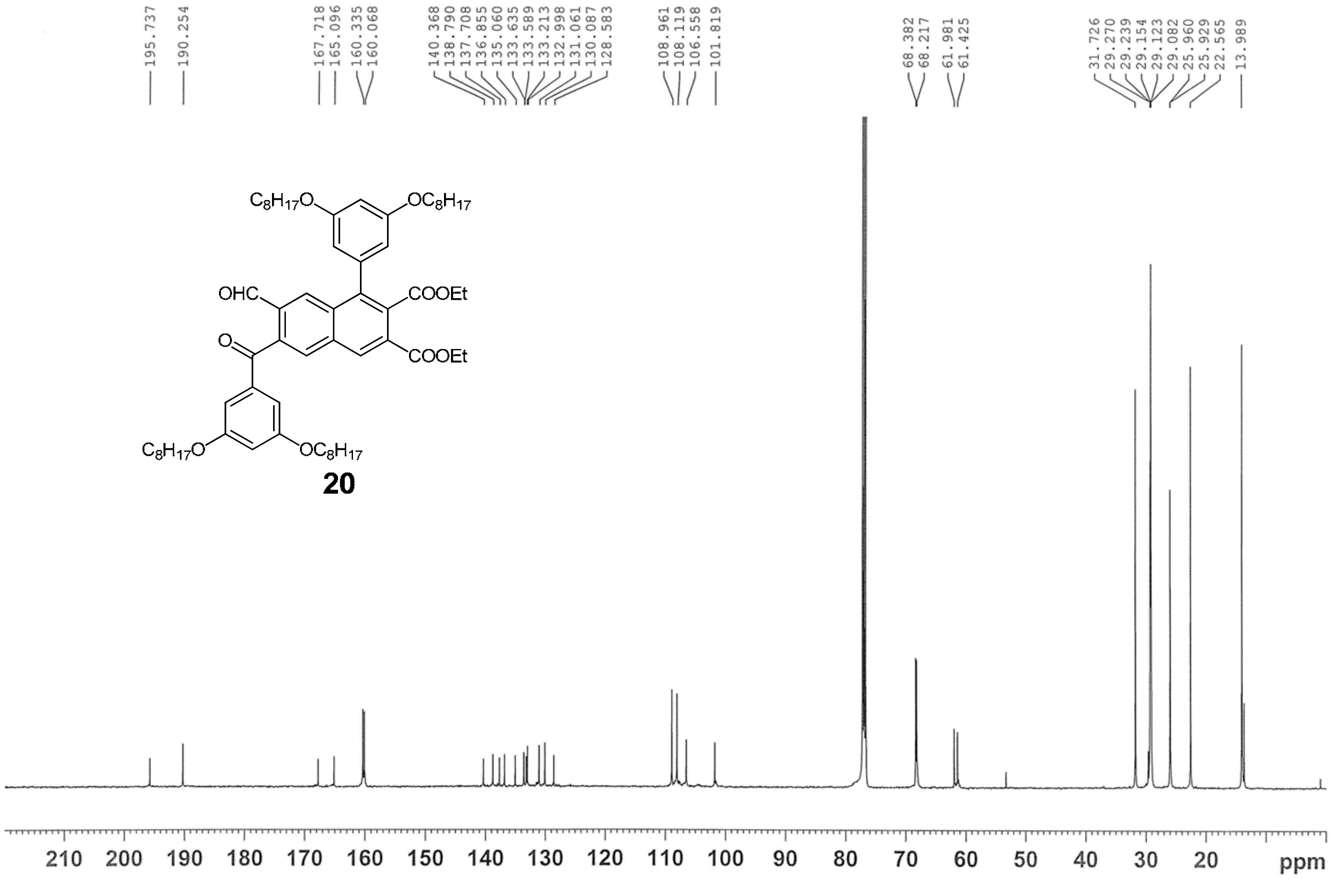

1H
8.750
8.681
8.364
8.067
7.240
6.717
6.621
4.417
4.399
4.382
4.364
4.348
4.330
4.312
4.294
4.158
4.140
4.122
4.105
4.013
3.997
3.981
2.598
1.819
1.802
1.783
1.448
1.430
1.407
1.388
1.376
1.338
1.320
1.301
1.257
1.235
1.222
$C_8H_{17}O$
$OC_8H_{17}$
EtOOC
EtOOC
COOEt
COOEt
$C_8H_{17}O$
$OC_8H_{17}$
18
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.14
1.04
1.09
1.24
2.09
3.18
3.11
5.32
7.49
1.61
7.89
9.95
67.69
18.94


13C, zg0dc
172.274
167.965
167.161
160.431
139.469
138.992
132.360
130.657
130.109
129.948
129.794
128.282
128.153
127.847
127.142
109.795
101.353
77.249
76.931
76.614
68.260
61.485
60.600
31.725
29.634
29.311
29.245
29.156
26.010
22.570
14.136
14.101
14.008
$C_8H_{17}O$
$OC_8H_{17}$
EtOOC
EtOOC
COOEt
COOEt
$C_8H_{17}O$
$OC_8H_{17}$
18
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

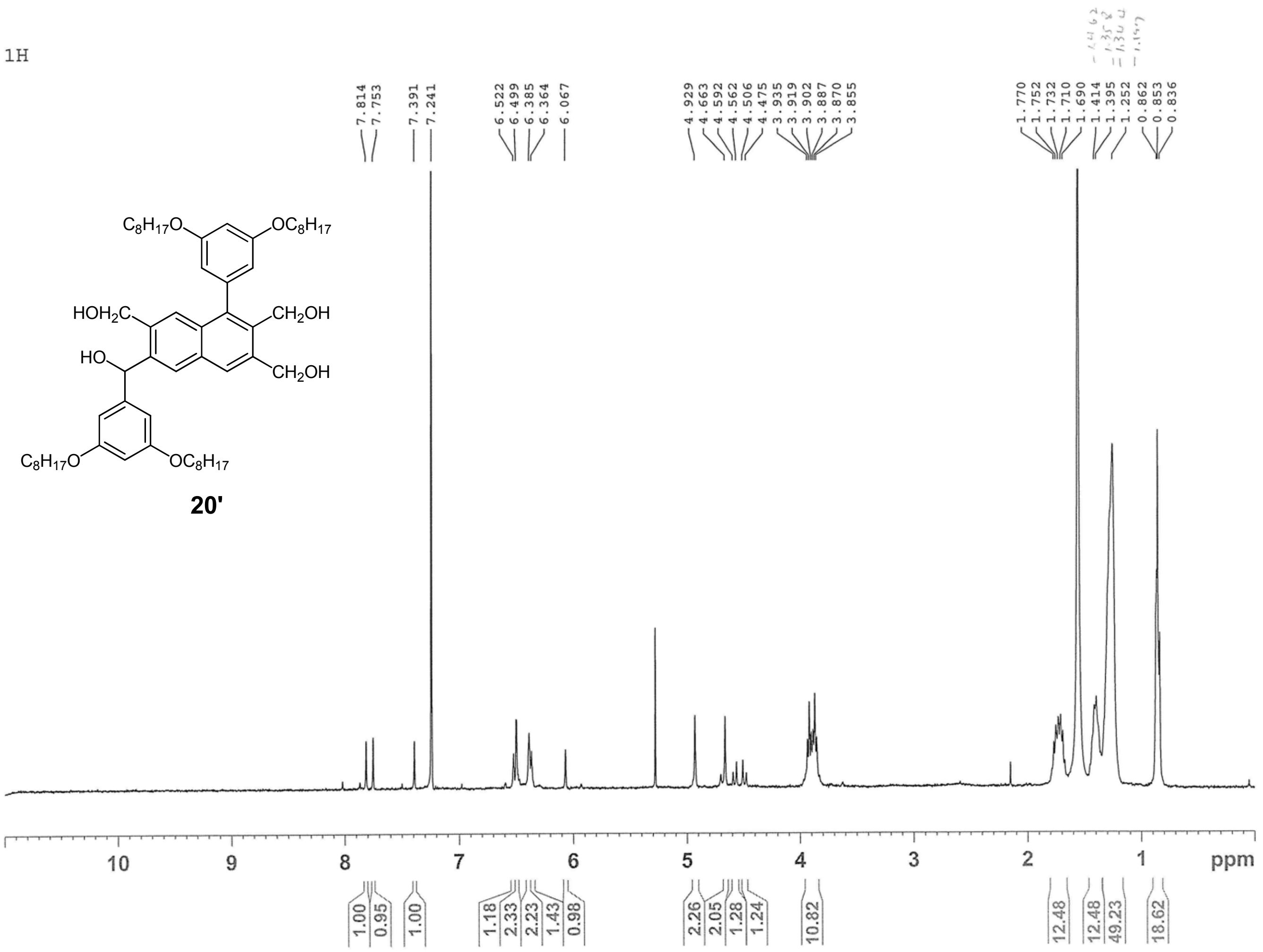

1H
8.789
8.767
8.389
8.232
7.242
6.748
6.743
6.737
6.606
6.601
4.028
4.014
3.996
3.742
3.725
3.706
1.849
1.833
1.815
1.796
1.779
1.680
1.663
1.525
1.480
1.462
1.442
1.424
1.309
1.294
1.253
1.236
1.221
0.859
0.842
0.825
$C_8H_{17}O$
$OC_8H_{17}$
$C_{12}H_{25}$—N
N—$C_{12}H_{25}$
O
19
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.04
1.02
0.94
0.98
2.04
5.42
2.22
5.87
2.75
6.26
59.07
14.95


13C, zg0dc
167.511
167.434
160.610
142.232
138.745
131.988
131.193
130.760
130.429
129.689
128.755
128.497
126.399
126.239
125.496
109.728
101.212
77.259
76.942
76.624
68.274
67.893
38.402
31.828
31.732
29.633
29.535
29.422
29.323
29.255
29.162
28.373
26.856
26.024
25.540
22.582
14.014
C8H17O
OC8H17
O
C12H25—N
N—C12H25
19
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

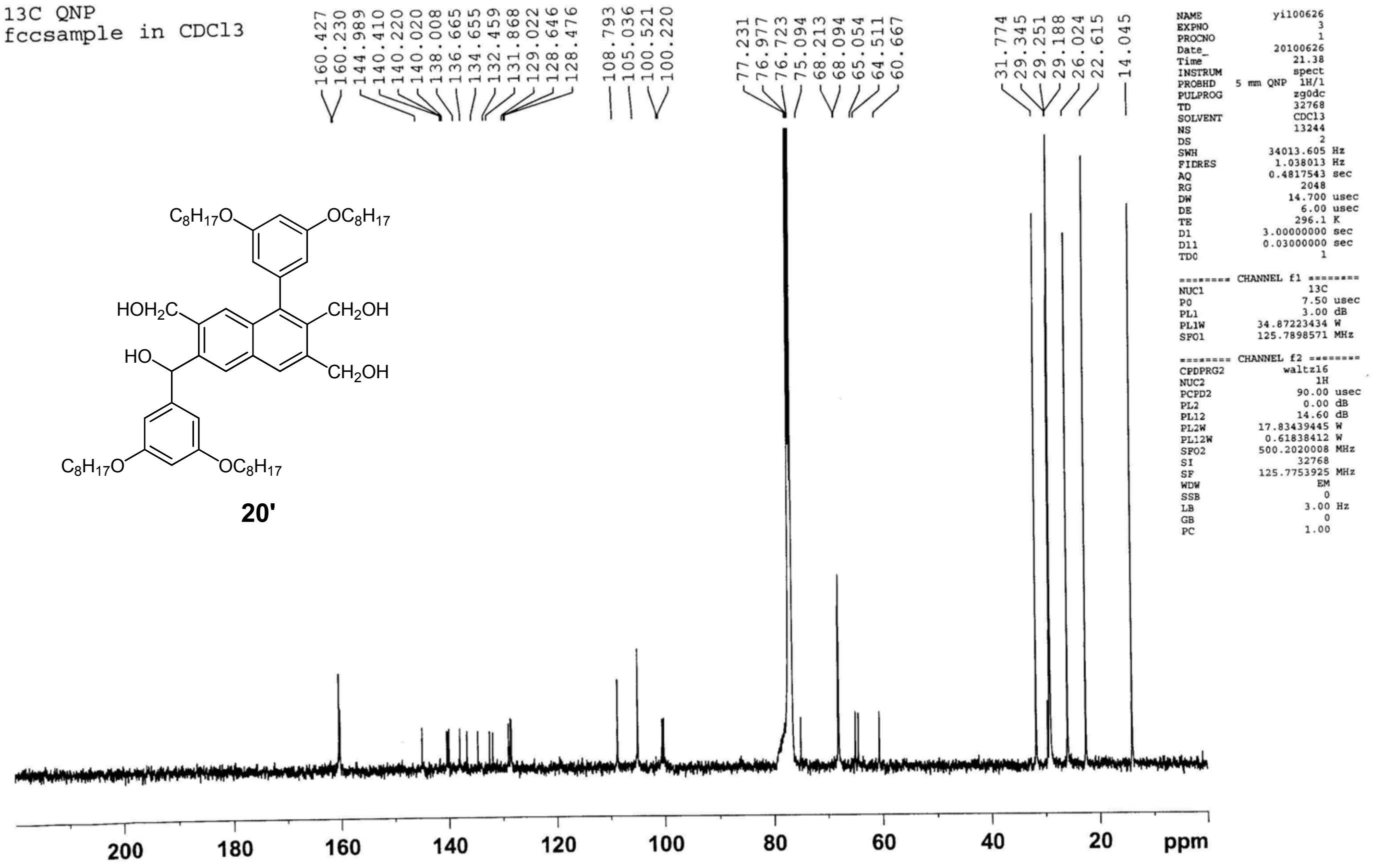

9.955
8.592
8.259
8.031
6.863
6.859
6.651
6.646
6.642
6.561
6.557
6.553
6.492
6.489
5.278
4.431
4.417
4.402
4.388
4.162
4.148
4.133
4.119
3.940
3.928
3.915
1.789
1.776
1.761
1.745
1.727
1.712
1.699
1.561
1.421
1.406
1.392
1.378
1.292
1.276
1.263
1.249
1.234
1.081
1.067
1.053
0.866
0.853
0.840
C8H17O
OC8H17
OHC
COOEt
COOEt
O
C8H17O
OC8H17
20
10
9
8
7
6
5
4
3
2
1
ppm
0.93
0.94
0.96
0.98
2.19
1.14
1.16
2.13
2.20
2.28
9.88
11.27
15.87
55.93
4.45
20.69


195.737
190.254
167.718
165.096
160.335
160.068
140.368
138.790
137.708
136.855
135.060
133.635
133.589
133.213
132.998
131.061
130.087
128.583
108.961
108.119
106.558
101.819
68.382
68.217
61.981
61.425
31.726
29.270
29.239
29.154
29.123
29.082
25.960
25.929
22.565
13.989
$C_8H_{17}O$
$OC_8H_{17}$
OHC
COOEt
COOEt
O
$C_8H_{17}O$
$OC_8H_{17}$
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

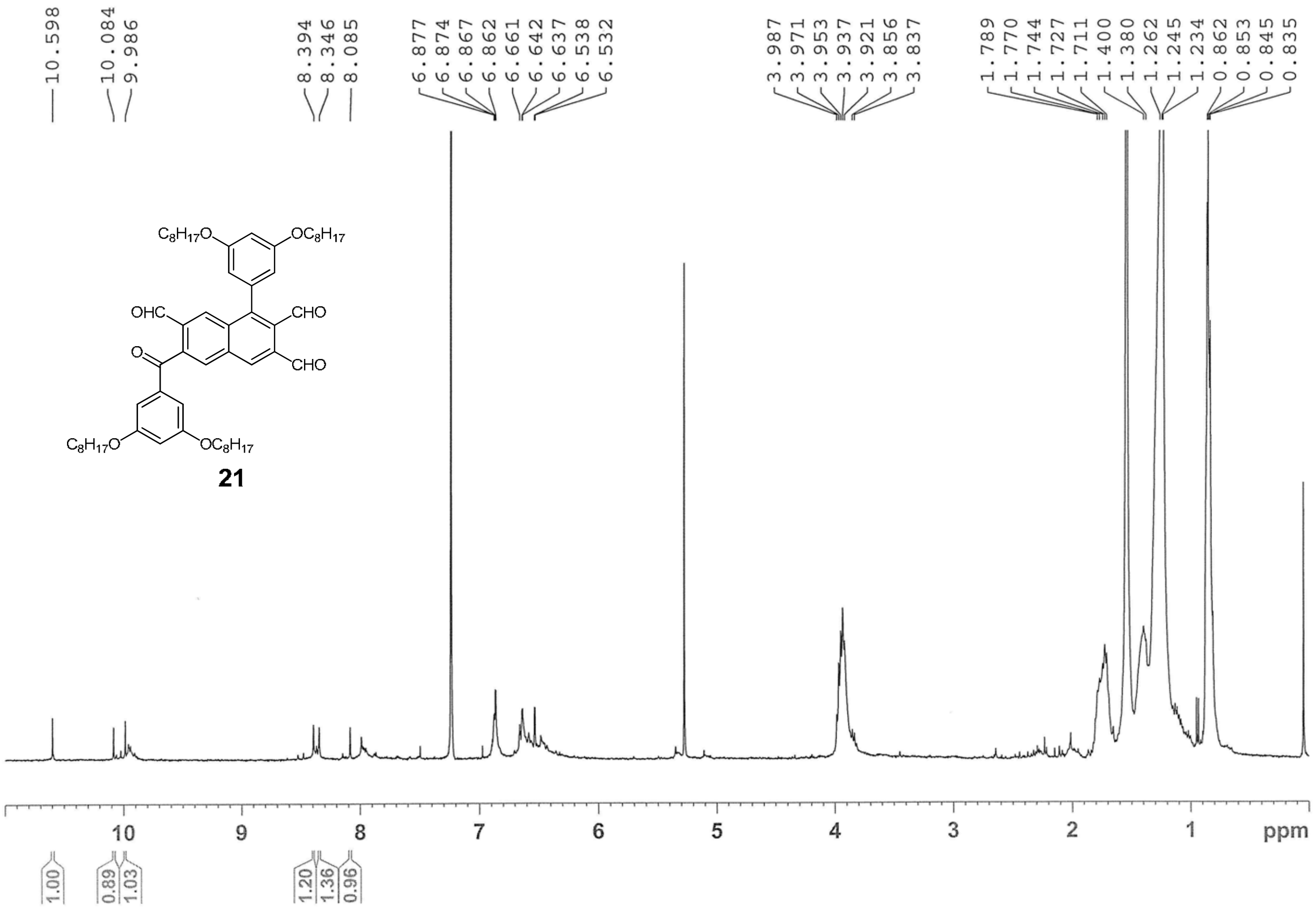
**20**


1H
7.814
7.753
7.391
7.241
6.522
6.499
6.385
6.364
6.067
4.929
4.663
4.592
4.562
4.506
4.475
3.935
3.919
3.902
3.887
3.870
3.855
1.770
1.752
1.732
1.710
1.690
1.414
1.395
1.252
0.862
0.853
0.836
1.463
1.358
1.344
1.197
$C_8H_{17}O$
$OC_8H_{17}$
$HOH_2C$
$CH_2OH$
HO
$CH_2OH$
$C_8H_{17}O$
$OC_8H_{17}$
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.95
1.00
1.18
2.33
2.23
1.43
0.98
2.26
2.05
1.28
1.24
10.82
12.48
12.48
49.23
18.62

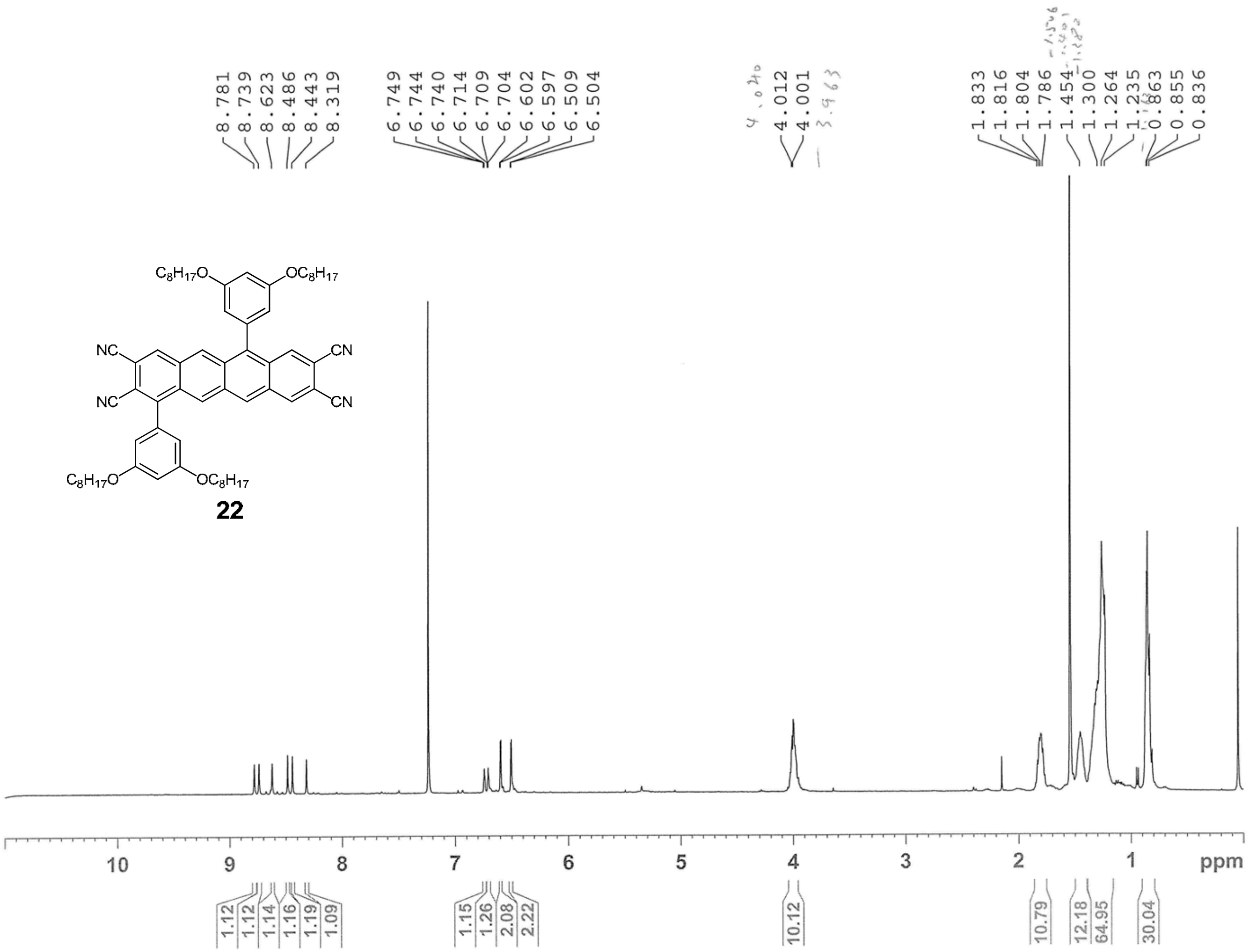
**20'**


13C QNP
fccsample in CDCl3
160.427
160.230
144.989
140.410
140.220
140.020
138.008
136.665
134.655
132.459
131.868
129.022
128.646
128.476
108.793
105.036
100.521
100.220
77.231
76.977
76.723
75.094
68.213
68.094
65.054
64.511
60.667
31.774
29.345
29.251
29.188
26.024
22.615
14.045
NAME yi100626
EXPNO 3
PROCNO 1
Date_ 20100626
Time 21.38
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg0dc
TD 32768
SOLVENT CDCl3
NS 13244
DS 2
SWH 34013.605 Hz
FIDRES 1.038013 Hz
AQ 0.4817543 sec
RG 2048
DW 14.700 usec
DE 6.00 usec
TE 296.1 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P0 7.50 usec
PL1 3.00 dB
PL1W 34.87223434 W
SFO1 125.7898571 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 14.60 dB
PL2W 17.83439445 W
PL12W 0.61838412 W
SFO2 500.2020008 MHz
SI 32768
SF 125.7753925 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
C8H17O
OC8H17
HOH2C
CH2OH
HO
CH2OH
C8H17O
OC8H17
200
180
160
140
120
100
80
60
40
20
ppm

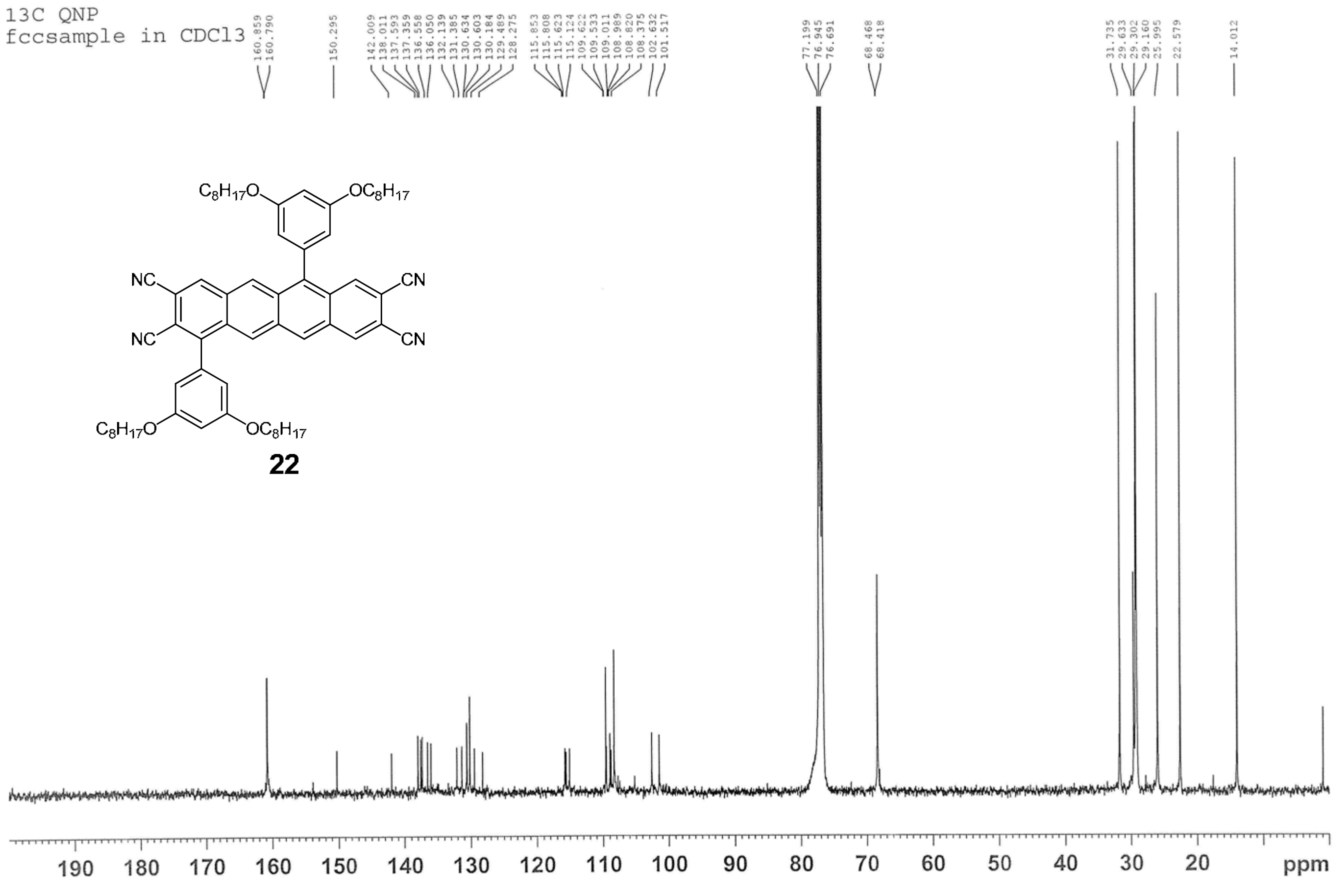
20'


10.598
10.084
9.986
8.394
8.346
8.085
6.877
6.874
6.867
6.862
6.661
6.642
6.637
6.538
6.532
3.987
3.971
3.953
3.937
3.921
3.856
3.837
1.789
1.770
1.744
1.727
1.711
1.400
1.380
1.262
1.245
1.234
0.862
0.853
0.845
0.835
C8H17O
OC8H17
OHC
CHO
CHO
O
C8H17O
OC8H17
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.89
1.03
1.20
1.36
0.96

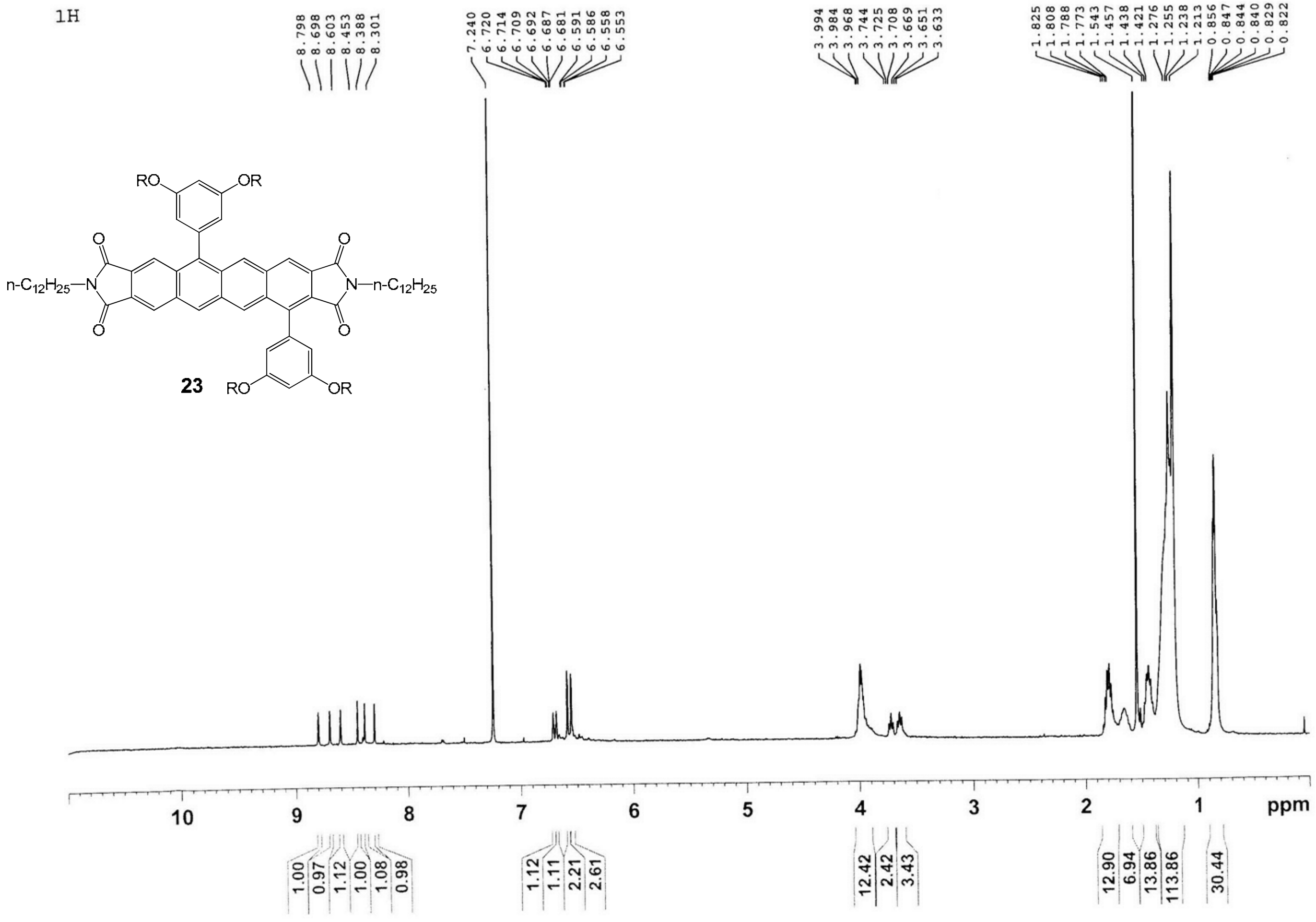
**21**

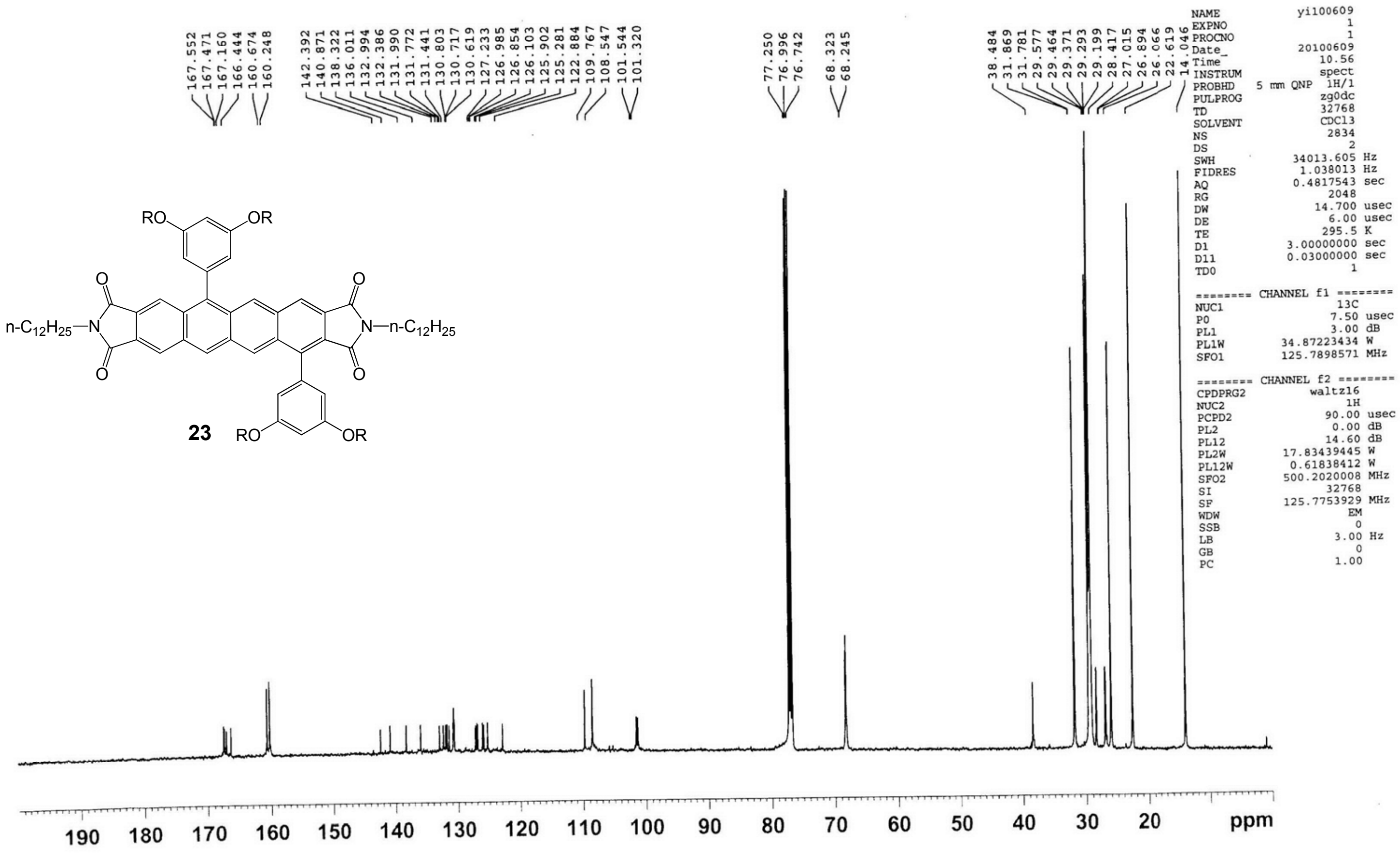

8.781
8.739
8.623
8.486
8.443
8.319
6.749
6.744
6.740
6.714
6.709
6.704
6.602
6.597
6.509
6.504
4.040
4.012
4.001
3.963
1.833
1.816
1.804
1.786
1.5506
1.4401
1.454
1.2822
1.300
1.264
1.235
1.163
0.863
0.855
0.836
$C_8H_{17}O$
$OC_8H_{17}$
NC
NC
CN
CN
$C_8H_{17}O$
$OC_8H_{17}$
10
9
8
7
6
5
4
3
2
1
ppm
1.12
1.12
1.14
1.16
1.19
1.09
1.15
1.26
2.08
2.22
10.12
10.79
12.18
64.95
30.04

**22**


13C QNP
fccsample in CDCl3
160.859
160.790
150.295
142.009
138.011
137.593
137.359
136.558
136.050
132.139
131.385
130.634
130.603
130.184
129.489
128.275
115.853
115.808
115.623
115.124
109.622
109.533
109.011
108.989
108.820
108.375
102.632
101.517
77.199
76.945
76.691
68.468
68.418
31.735
29.633
29.302
29.160
25.995
22.579
14.012
C8H17O
OC8H17
NC
NC
CN
CN
C8H17O
OC8H17
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

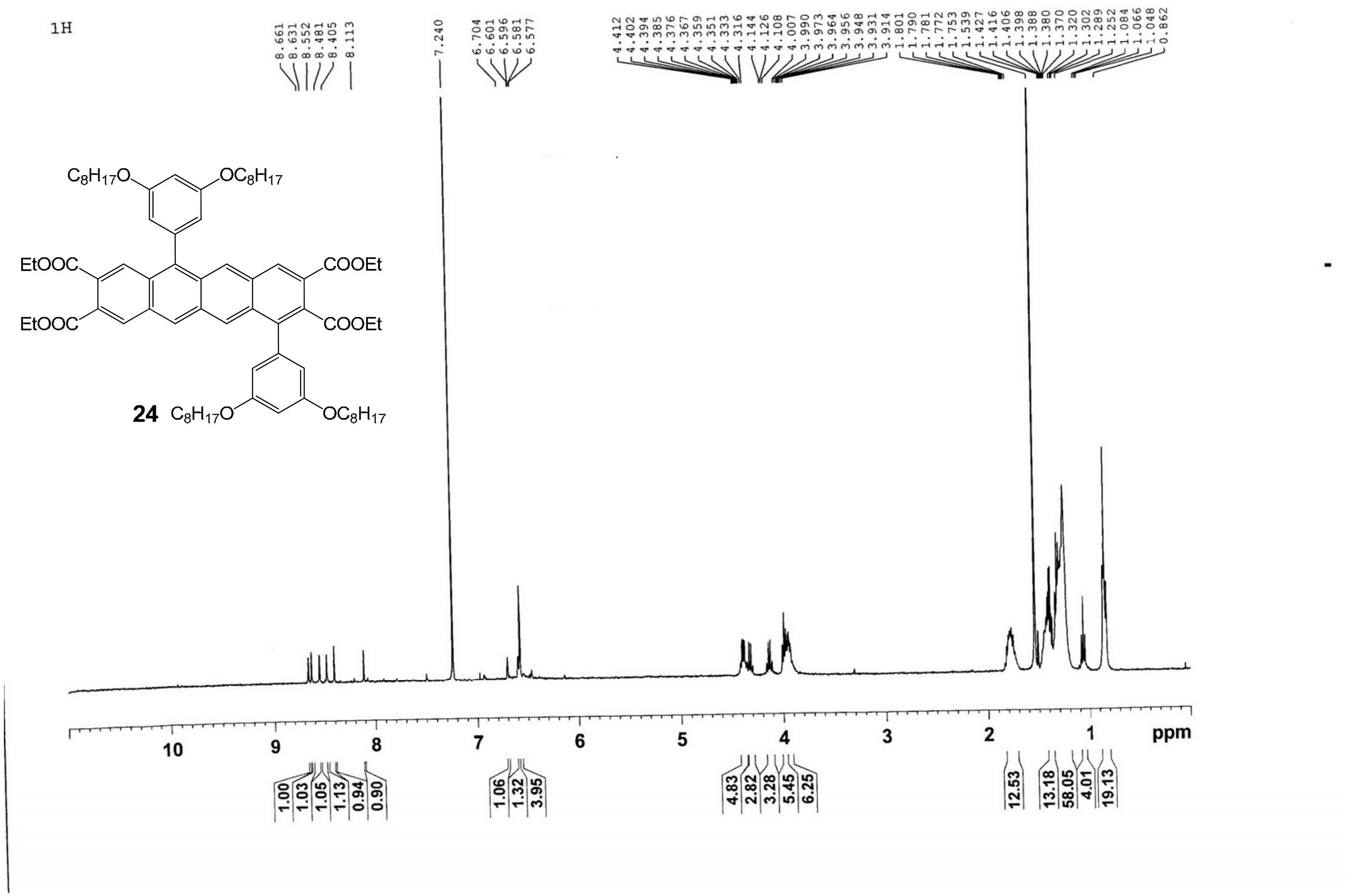
**22**

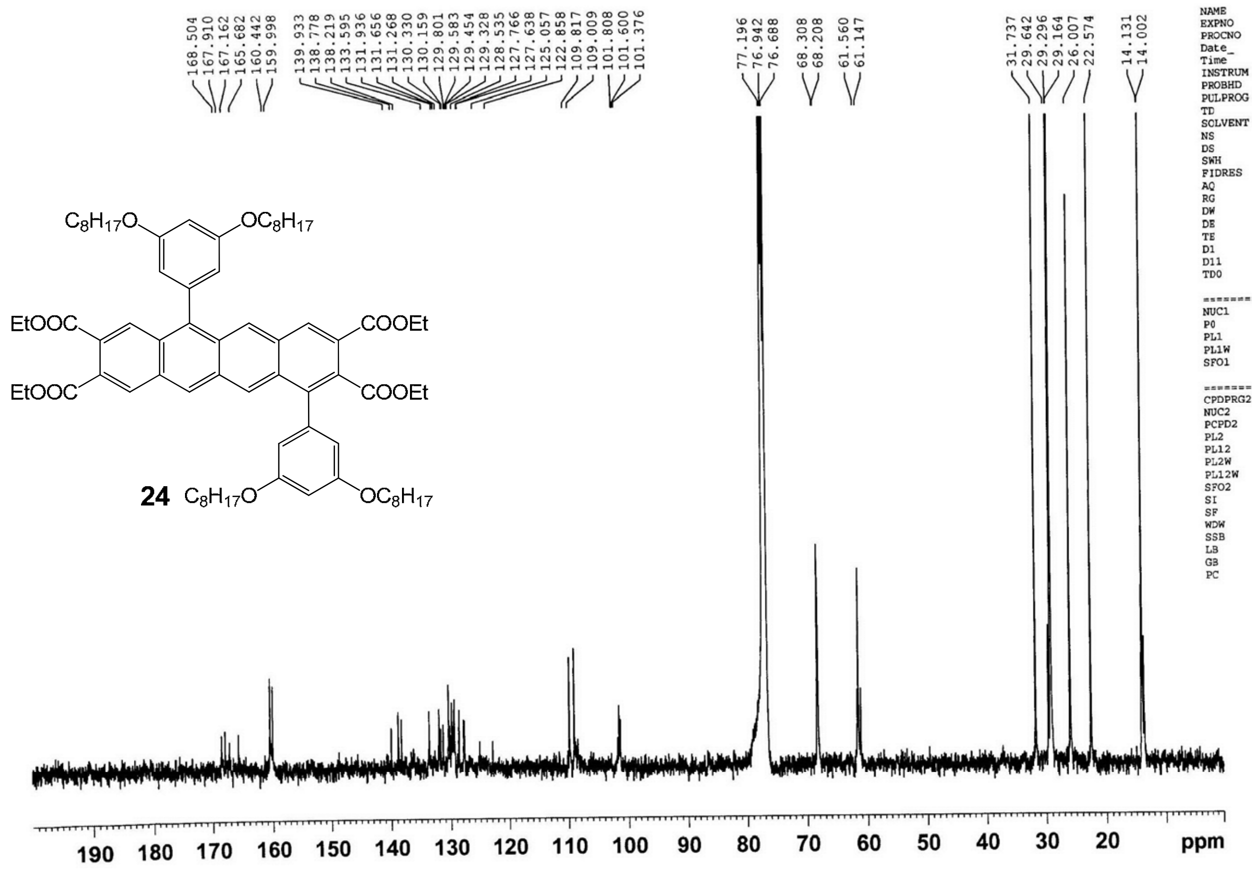

1H
8.798
8.698
8.603
8.453
8.388
8.301
7.240
6.720
6.714
6.709
6.692
6.687
6.681
6.591
6.586
6.558
6.553
3.994
3.984
3.968
3.744
3.725
3.708
3.669
3.651
3.633
1.825
1.808
1.788
1.773
1.543
1.457
1.438
1.421
1.276
1.255
1.238
1.213
0.856
0.847
0.844
0.840
0.829
0.822
RO
OR
O
n-C12H25
N
23
ppm
10
9
8
7
6
5
4
3
2
1
1.00
0.97
1.12
1.00
1.08
0.98
1.12
1.11
2.21
2.61
12.42
2.42
3.43
12.90
6.94
13.86
113.86
30.44



**23**

```
NAME           yi100609
EXPNO                 1
PROCNO                1
Date_          20100609
Time              10.56
INSTRUM           spect
PROBHD   5 mm QNP  1H/1
PULPROG          zg0dc
TD                32768
SOLVENT           CDCl3
NS                 2834
DS                    2
SWH           34013.605 Hz
FIDRES         1.038013 Hz
AQ            0.4817543 sec
RG                 2048
DW               14.700 usec
DE                 6.00 usec
TE                295.5 K
D1           3.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P0                 7.50 usec
PL1                3.00 dB
PL1W        34.87223434 W
SFO1        125.7898571 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                0.00 dB
PL12              14.60 dB
PL2W        17.83439445 W
PL12W        0.61838412 W
SFO2        500.2020008 MHz
SI                32768
SF          125.7753929 MHz
WDW                  EM
SSB                   0
LB                 3.00 Hz
GB                    0
PC                 1.00
```


1H
8.661
8.631
8.552
8.481
8.405
8.113
7.240
6.704
6.601
6.596
6.581
6.577
4.412
4.402
4.394
4.385
4.376
4.367
4.359
4.351
4.333
4.316
4.144
4.126
4.108
4.007
3.990
3.973
3.964
3.956
3.948
3.931
3.914
1.801
1.790
1.781
1.772
1.753
1.539
1.427
1.416
1.406
1.398
1.388
1.380
1.370
1.320
1.302
1.289
1.252
1.084
1.066
1.048
0.862
C8H17O
OC8H17
EtOOC
EtOOC
COOEt
COOEt
24
C8H17O
OC8H17
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.03
1.05
1.13
0.94
0.90
1.06
1.32
3.95
4.83
2.82
3.28
5.45
6.25
12.53
13.18
58.05
4.01
19.13



**24**

```
NAME              yi100610
EXPNO                    6
PROCNO                   1
Date_             20100610
Time                 22.23
INSTRUM              spect
PROBHD   5 mm QNP  1H/1
PULPROG             zg0dc
TD                   32768
SOLVENT              CDCl3
NS                   12000
DS                       2
SWH              34013.605 Hz
FIDRES            1.038013 Hz
AQ               0.4817543 sec
RG                   13004
DW                  14.700 usec
DE                    6.00 usec
TE                   296.9 K
D1              3.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P0                    7.50 usec
PL1                   3.00 dB
PL1W           34.87223434 W
SFO1           125.7898571 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                   0.00 dB
PL12                 14.60 dB
PL2W           17.83439445 W
PL12W           0.61838412 W
SFO2           500.2020008 MHz
SI                   32768
SF             125.7753975 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.00
```