Supporting Information

Synthesis and Colour Tuning of Highly Efficient Fluorescent 9,10-Disubstituted-2,3,6,7-tetraphenyl-anthracene

Sheng-Hsun Lin, Fang-Iy Wu and Rai-Shung Liu*

Department of Chemistry, National Tsing-Hua University, Hsinchu, Taiwan, 30043, ROC. e-mail: rsliu@mx.nthu.edu.tw

Contents:

General Information.

All other reagents were used as received from commercial sources, unless otherwise stated. Unless otherwise noted, all experiments were carried out under N_2 atmosphere in oven-dried glassware using stander syringe, cannula and septa apparatus. Tetrahydrofuran, Toluene and hexane were dried with sodium and distilled before use. CH_2Cl_2 were dried over CaH_2, and distilled before use. All the ^1H NMR and ^{13}C NMR were recorded in $CDCl_3$ solution unless otherwise stated. Coupling constants (*J* values) are given in Hertz (Hz) and chemical shifts are expressed in parts per million (ppm). Substrate was prepared from the corresponding readily available 4,6-dibromoisophthalaldehyde after several steps. UV-Vis and PL spectra in diluted dichloromethane solution (10^{-5} M) were recorded using a Hitachi U-3300 spectrophotometer and a Hitachi F-4500 fluorescence spectrophotometer, respectively. Quantum yield was measured with reference to Coumarin-I (Φ_f = 0.99)[1]. The wavelength at the intersection point of the two absorption spectra between the sample and the standard was taken as the cxcitation wavelength for PL spectra and determining quantum yields. The HOMO energy level of the studied compound was calculated from the oxidation potential ($E^{1/2}$) obtained from the cyclic voltammetry (CV) measurement with Pt wire as counter electrode, glassy carbon electrode as working electrode. The potentials were measured against an Ag/Ag^+ (Ag/0.01 M $AgNO_3$) reference electrode. The final results were calibrated with the ferrocene/ferrocenium (Fc/Fc^+) couple. Under the assumption that the

energy level of ferrocene/ferrocenium is 4.8 eV below vacuum, the HOMO energy levels of **2c** and **4a-4g** were determined from the equation: 4.8 eV + $E^{1/2}$ (versus Fc/Fc^{+}).

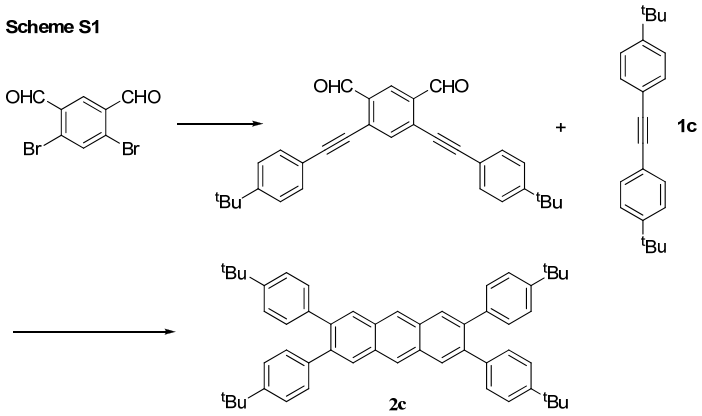
Device fabrication and characterization.

The EL devices with a configuration of ITO/TCTA (50 nm)/4a (3%) in DMPPP (30 nm)/BCP (10 nm)/TPBI(30 nm)/LiF(1 nm)/Al (100 nm) were fabricated by sequential thermal evaporation onto a clean glass precoated with a layer of indium tin oxide having a sheet resistance of 25 ohm/square. The effective area of the emitting diode is 9.00 mm^2. Current, voltage and light intensity measurements were recorded simultaneously using a Keithley 2400 source meter and a Newport 1835-C optical meter equipped with a Newport 818-ST silicon photodiode. EL spectra were measured on a Hitachi F-4500 fluorescence spectrophotometer. All the measurements were carried out at room temperature in the air.

A. Representative Synthetic procedures:

(I) Synthesis of 2,3,6,7-tetraphenylanthracene 2c

Scheme S1



(a) 4,6-Bis((4-tert-butylphenyl)ethynyl)isophthalaldehyde :

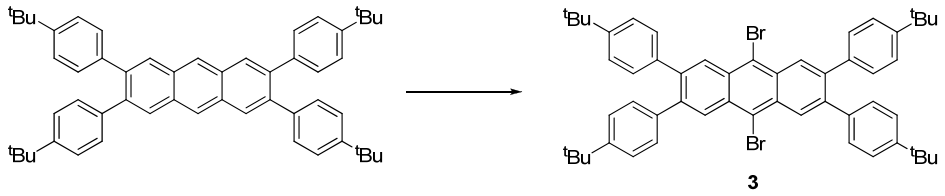
Nitrogen was bubbled through a mixture of THF (80 mL) and triethylamine (80 mL) for 30 min, and to this solution was added 4,6-dibromoisophthalaldehyde (5 g, 17.1 mmol), CuI (0.326 g, 1.71 mmol), $PdCl_2(PPh_3)_2$ (0.602 g, 0.86 mmol), and 1-*tert*-butyl-4-ethynylbenzene (6.23 g, 39.4 mmol). The resulting solution was stirred at 80 °C for 8 h before it was cooled to room temperature. Solvent was removed under reduced pressure, and the solution was filtered through a short silica bed with ethyl acetate/hexane (1:1 volume ratio). After concentration in vacuo, the crude material was eluted through a silica column with ethyl acetate/hexane(5/95) to afford the desired product (4.74 g, 62 %) as a yellow solid.

(b) Synthetic procedure for 2,3,6,7-tetraphenylanthracene (**2c**).

A mixture of compound **1c** (6.5 g, 22.4 mmol), $Cu(OTf)_2$ (0.081 g, 0.22 mmol) and CF_2HCO_2H (1.1 g , 11.2 mmol) in 1,2-dichloroethane (240 mL) was stirred for 10 min at 100 ℃ under Ar atmosphere. To this mixture was added a 1,2-dichloroethane (10 ml) solution of 4,6-bis((4-*tert*-butylphenyl)ethynyl)isophthalaldehyde (1.0 g, 2.2 mmol) drop-wise over a period of 2 h, and the mixture was stirred for additional 3 h. The solution was cooled to room temperature before it was treated with saturated $NaHCO_3$ aqueous solution. The organic layer was extracted with dichloromethane, dried over $MgSO_4$ and evaporated under reduced pressure. The crude product was eluted through a silica column using dichloromethane/hexane as an the eluent, giving **2c** (0.87 g) in a 55%

yield.

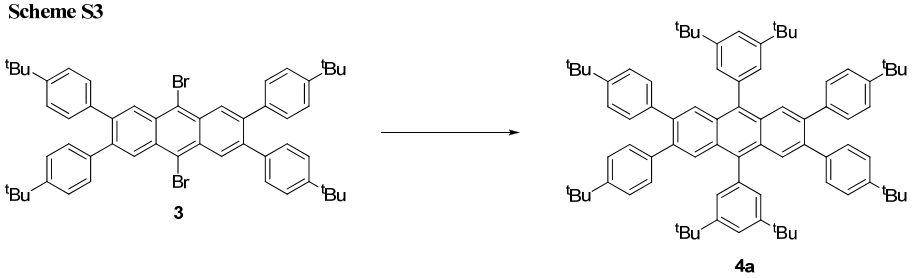
Scheme S2



(e) 9,10-Dibromo-2,3,6,7-tetrakis(4-tert-butylphenyl)anthracene (3).

A dichloromethane (70 mL) solution of **2c** (0.5 g, 0.71 mmol) was cooled to 0 °C, and to this solution was added dropwise a dichloromethane solution (2 ml) of Br_2 (0.25 g, 1.56 mmol) for a period of 5 min. The mixture was stirred for 0.5 h in dark. A saturated aqueous solution of Na_2SO_3 was added, and the resulting mixture was extracted with dichloromethane, dried over $MgSO_4$, and concentrated under reduced pressure. The residues were eluted with $CHCl_3$/hexane (5/95) through a silica column to afford compound **3** (0.495 g ,81%) as a yellow solid.

Scheme S3

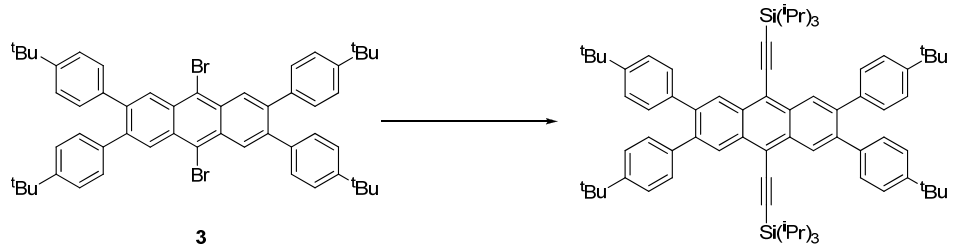


(c) Synthetic procedure for compound (4a):

The 3,5-di-*tert*-butylphenylboronic acid (0.108 g, 0.46 mmol), compound **3** (0.1 g, 0.12 mmol), $Pd(Ph_3P)_4$ (0.007 g , 0.06 mmol) and K_2CO_3 (0.064 g, 0.46 mmol) were dissolved in a mixing solvent of toluene (8 mL), ethanol (3 mL) and water (6 mL); the resulting mixture

was then heated to 80 □ for 8 h. The solution was cooled to room temperature, extracted with dichloromethane, dried over $MgSO_4$ and concentrated under reduced pressure. The residues were eluted through a silica column to afford compound **4a** (0.095 g, 76%).

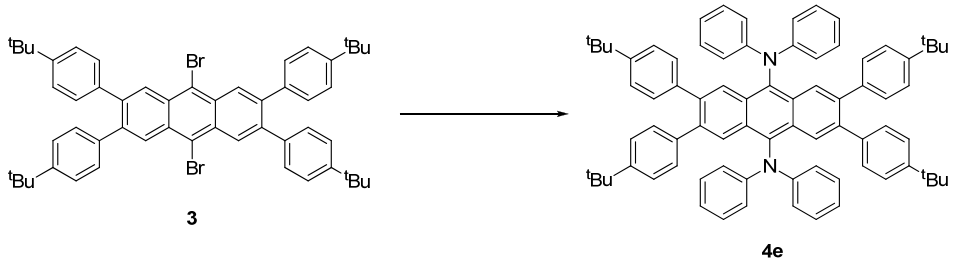
Scheme S4



(d) Synthetic procedure for compound (4c):

Compound **3** (0.10 g, 0.12 mmol), $Pd(Ph_3P)_4$ (0.007 g , 0.06 mmol) and CuI (0.003 g, 0.12 mmol) were dissolved in a solution of THF (7 ml) and triethylamine (7 ml), and the mixture was stirred for 5 min. To this mixture was added (triisopropylsilyl)acetylene (0.064g ,0.35 mmol) drop-wise under nitrogen atmosphere, and the resulting solution was heated to 80 □ for 8 h. The resulting solution was cooled to room temperature, and the solvent was removed under reduced pressure. The residues were eluted through a silica column to give compound **4c** (0.093 g , 75%).

Scheme S5



(e) Synthetic procedure for compound (4e):

A mixture of compound **3 (0.**10 g, 0.12 mmol), diphenylamine (0.081g, 0.48 mmol), sodium *tert*-butoxide (0.097 g, 0.48 mmol), $Pd_2(dba)_3$ (0.01 g, 0.01 mmol) and $P(t\text{-}Bu)_3$ (0.005 g, 0.02 mmol) in dry toluene (15 ml) were stirred under nitrogen atmosphere at 100 °C for 12 h. The resulting solution was cooled to room temperature, and extracted with dichloromethane. The extract was dried over $MgSO_{4,}$ concentrated under reduced pressure, and purified by a silica column to afford **4e** (0.055 g, 46%)**.**

Reference:

1. (a) Y. S. Chen, P. Y. Kuo, T. L. Shie and D. Y. Yang, *Tetrahedron* .2006, **62**, 9410. (b) G. Jones II, W. R. Jackson, C. y. Choi, and W. R. Bergmark *J. Phys. Chem.* 1985, **89**, 294.

B. Electrochemical experiments for 2c, 4a-4g

Measurement:

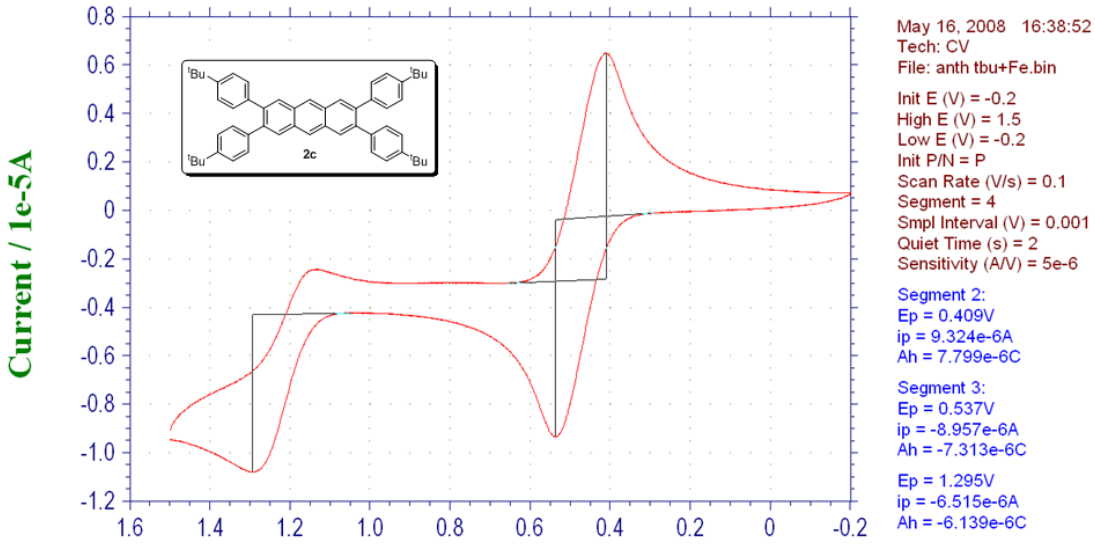


Figure 1. Cyclic voltammetry of 2c with ferrocene

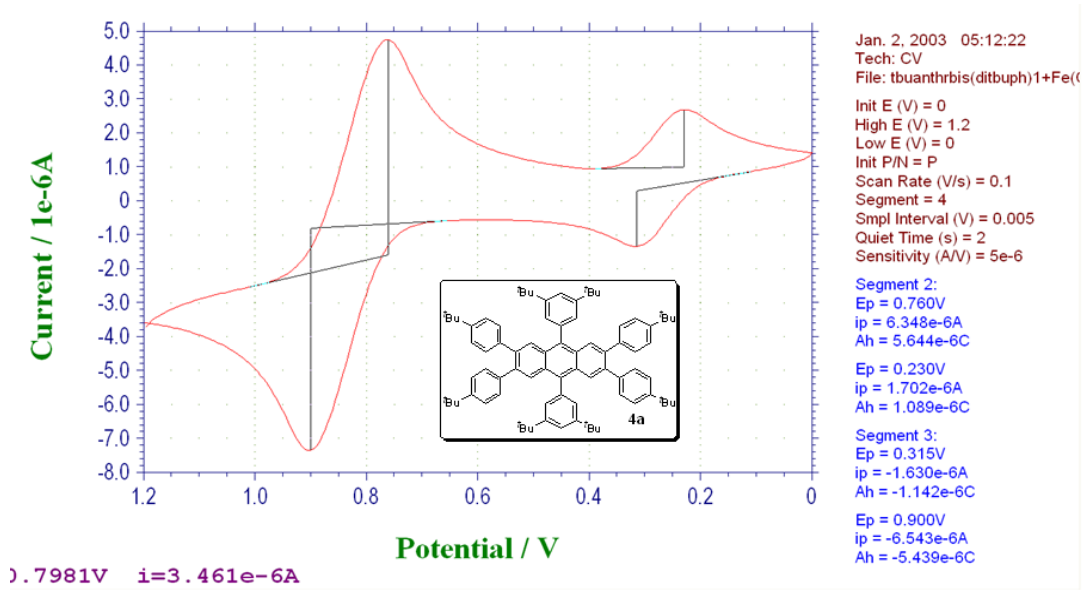


Figure 2. Cyclic voltammetry of 4a with ferrocene

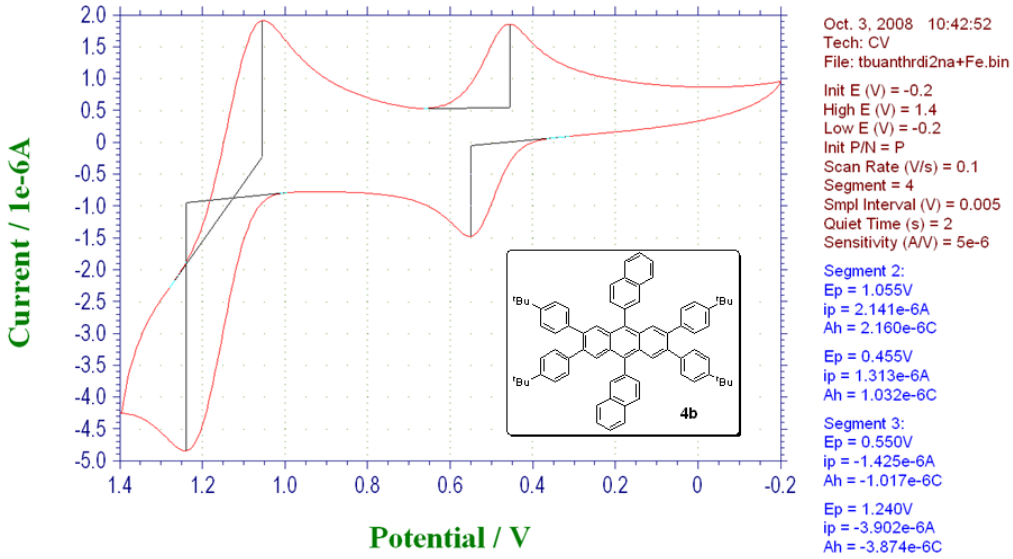


Figure 3. Cyclic voltammetry of 4b with ferrocene

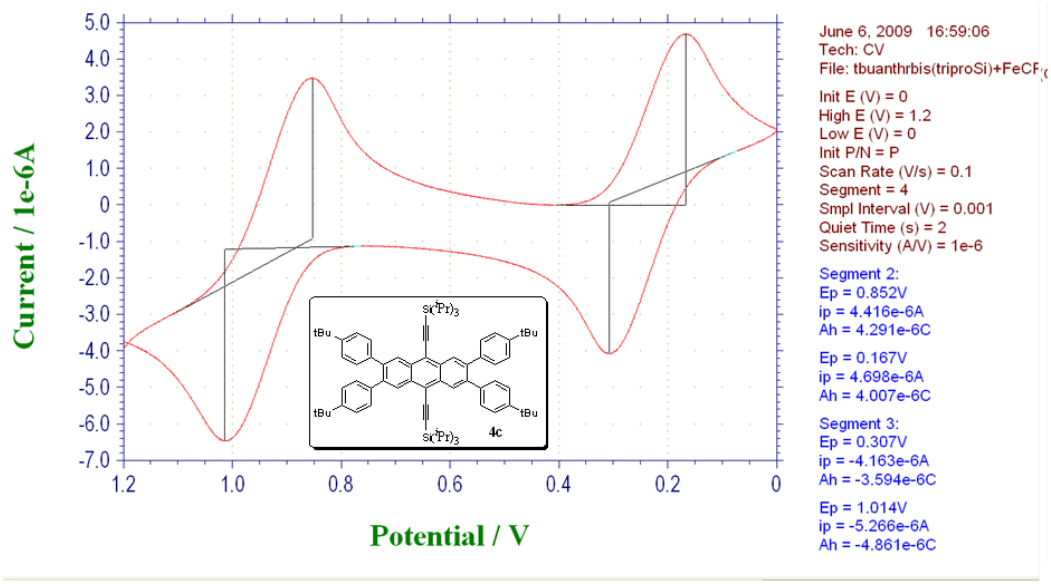


Figure 4. Cyclic voltammetry of 4c with ferrocene

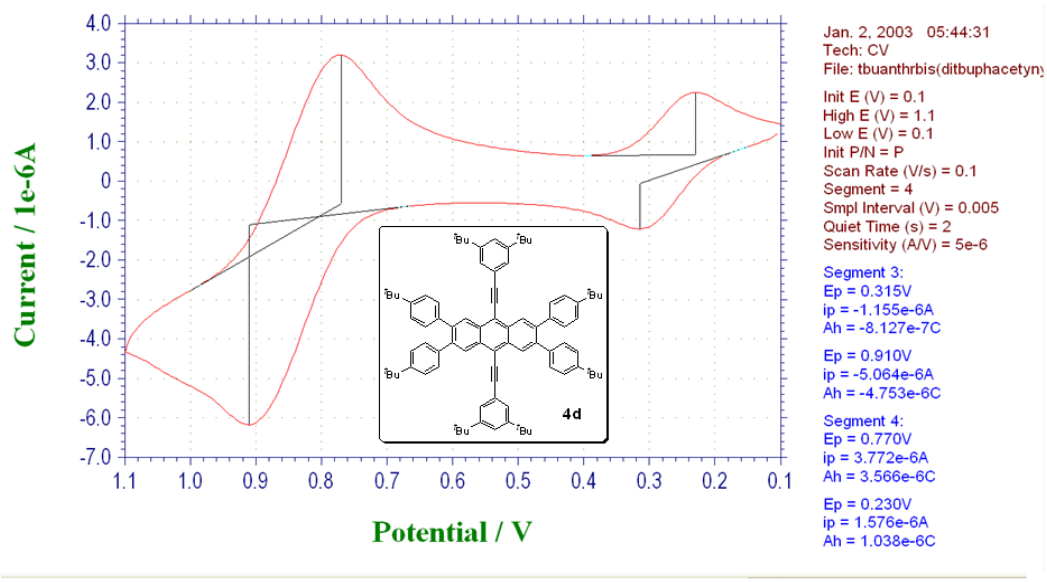


Figure 5. Cyclic voltammetry of 4d with ferrocene

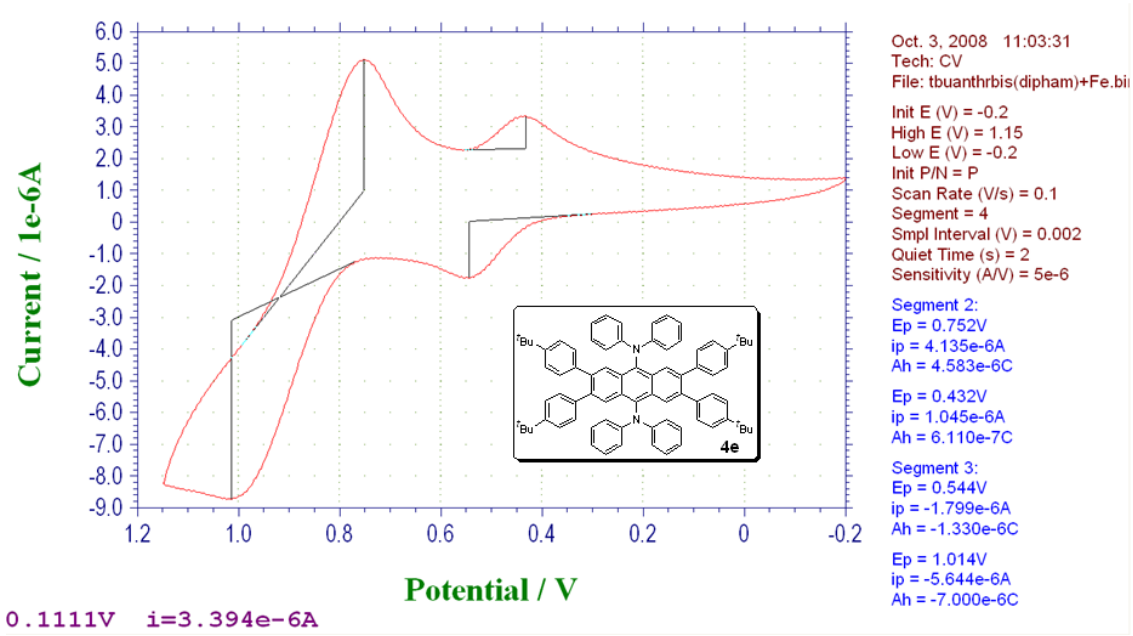


Figure 6. Cyclic voltammetry of 4e with ferrocene

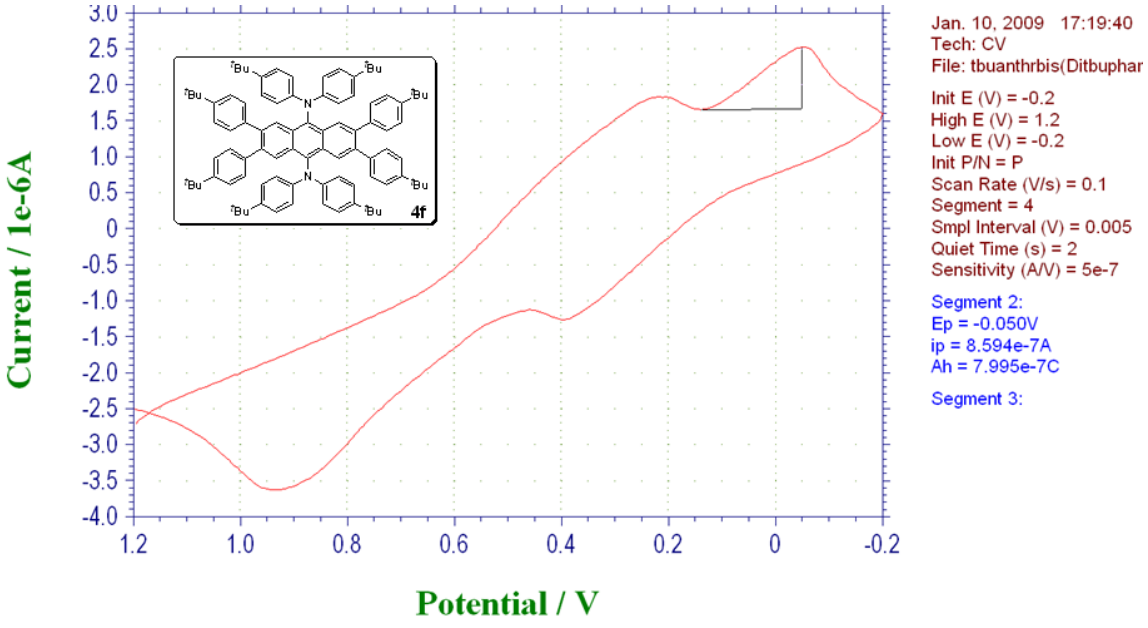


Figure 7. Cyclic voltammetry of 4f with ferrocene

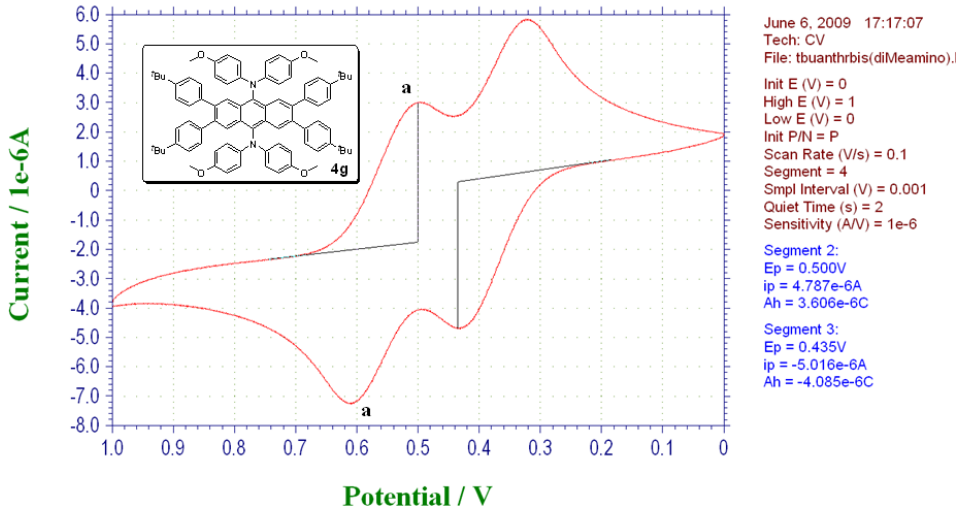


Figure 8. Cyclic voltammetry of 4g without ferrocene

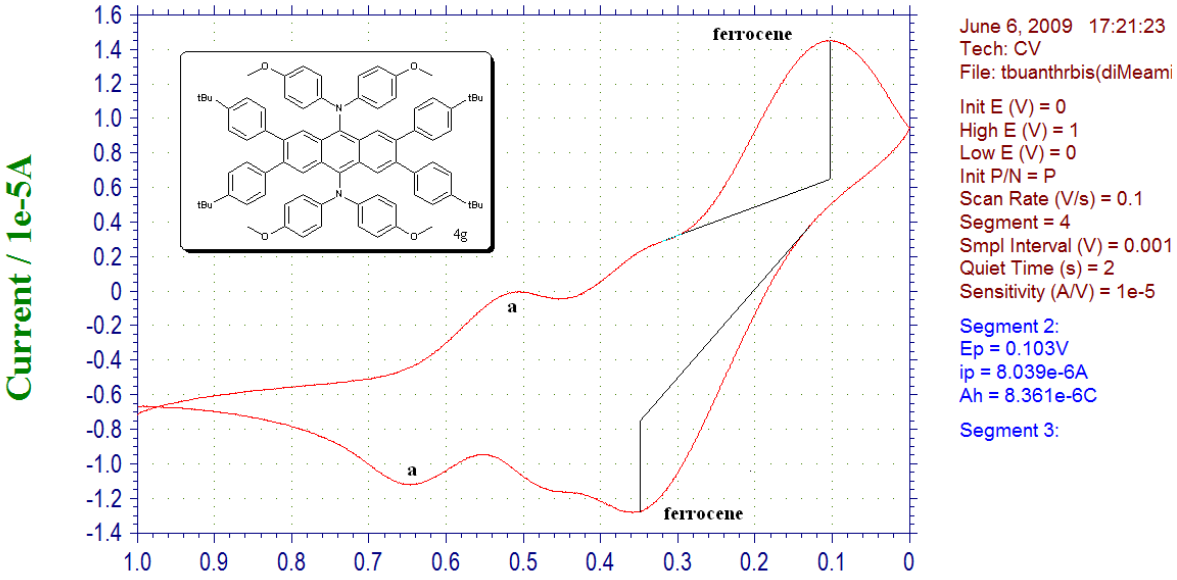


Figure 9. Cyclic voltammetry of 4g with ferrocene

C. EL performance of the device using compound **4a** as dopant (ITO/TCTA (50 nm)/**4a** (3%) in DMPPP (30 nm)/BCP (10 nm)/TPBI(30 nm)/LiF(1 nm)/Al).

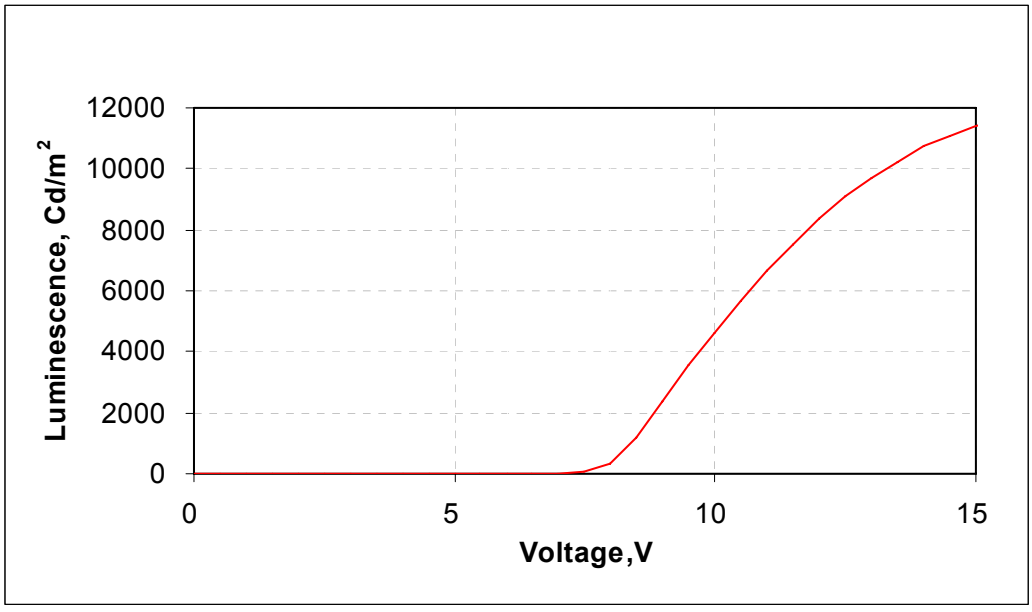


Figure 10. Luminescence spectra of compound 4a over various applied voltage

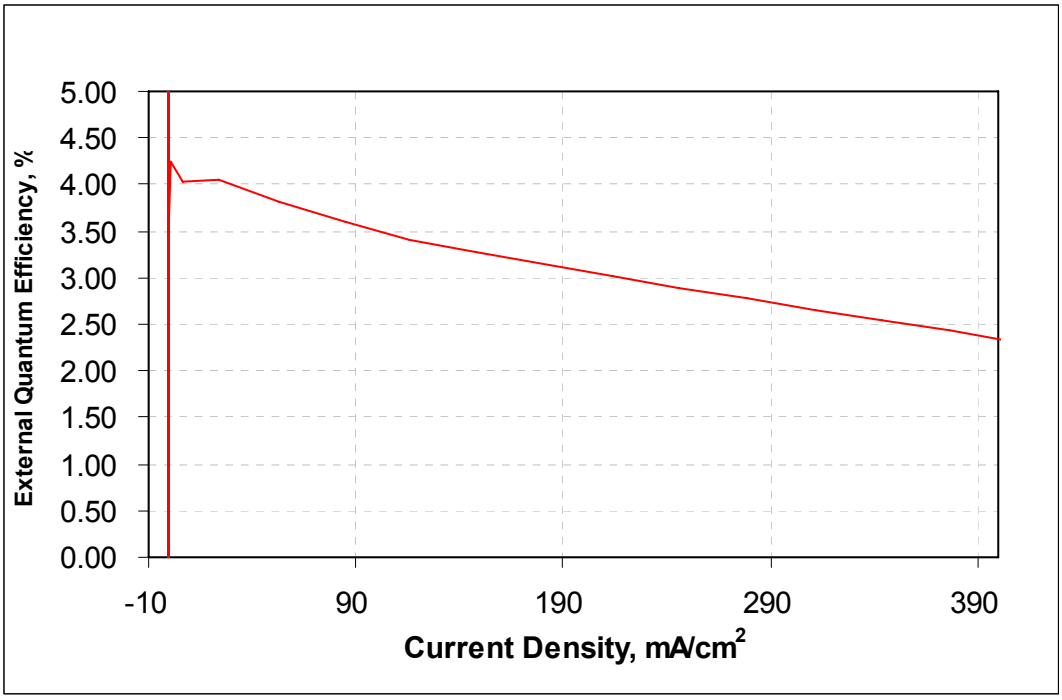
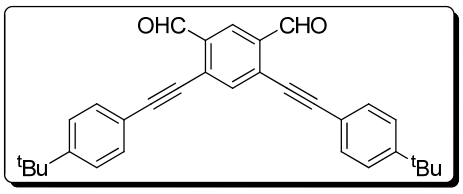


Figure 11. External Quantum Efficiency of compound 4a over various Current Density

D. Spectral data for key compounds:

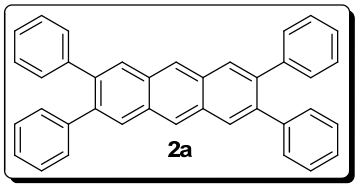
Spectral data for compound :



solid; IR (neat, cm^{-1}): 2780 (w), 2170 (w), 1705 (s), 1390(s), 1375 (m), 1372 (s); ^1H NMR (400 MHz, $CDCl_3$): δ 10.59 (s, 2 H), 8.45 (s, 1 H), 7.88 (s, 1H), 7.51 (m, 4H), 7.42 (m, 4H), 1.33 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.9, 153.3, 137.6, 134.34, 131.7, 131.1, 127.1, 125.6, 118.5, 100.9, 83.6, 34.9, 31.0; HRMS calcd for $C_{32}H_{30}O_2$: 446.2246,

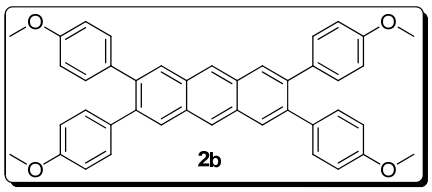
found 446.2241. Anal. calcd for $C_{32}H_{30}O_2$: C 86.06; H 6.77. Found: C 85.93; H 7.02.

Spectral data for compound (2a):



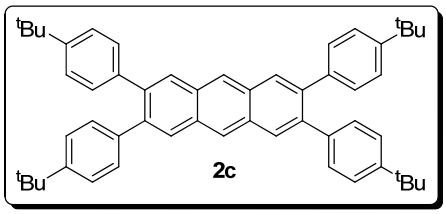
solid; IR (neat, cm^{-1}): 3058(s), 1658 (s),1492 (s) ; ^1H NMR (400 MHz, $CDCl_3$): δ 8.48 (s, 2 H), 8.05 (s, 4 H), 7.26 (m, 20H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.4, 139.0, 131.4, 129.9, 129.6, 127.9, 126.6, 126.0 ; HRMS calcd for $C_{38}H_{26}$: 482.2035, found 482.2058. Anal. calcd for $C_{38}H_{26}$: C 94.57; H 5.43. found: C 94.12; H 5.71.

Spectral data for compound (2b):



solid; IR (neat, cm^{-1}): 3120(s), 2989 (s), 1570 (m), 1450 (s), 1380(m), 1280 (s); ^1H NMR (400 MHz, $CDCl_3$): δ 8.40 (s, 2 H), 7.97(s, 4H), 7.18 (d, *J*= 6.8, 8.8 Hz, 8 H), 6.81 (d, *J*= 8.8 Hz, 8H), 3.80 (s , 12H) ; ^{13}C NMR (150 MHz, CD_2Cl_2): δ 158.9, 139.1, 134.3, 131.7, 131.3, 129.4, 125.8, 113.7, 55.5; HRMS calcd for $C_{42}H_{34}O_4$: 602.2457, found 602.2454. Anal. calcd for $C_{42}H_{34}O_4$: C 83.70; H 5.69. found: C 83.38; H 5.84.

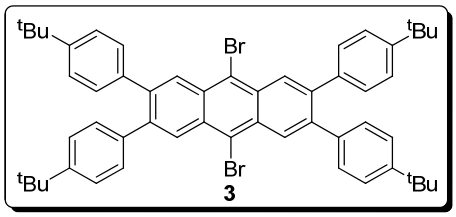
Spectral data for compound (2c):



2c

solid; IR (neat, cm^{-1}): 3280 (s), 2989 (s), 1650(m), 1395 (m), 1372 (s); ^1H NMR (600 MHz, $CDCl_3$): δ 8.42 (s, 2 H), 8.03 (s, 4H), 7.26 (m, 8H), 7.19 (m, 8H), 1.30 (s, 36H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 149.4, 139.0, 138.5, 131.3, 129.5, 129.3, 125.7, 124.6, 34.4, 31.3 ; HRMS calcd for $C_{54}H_{58}$: 706.4539, found 706.4540. Anal. calcd for $C_{54}H_{58}$: C 91.73; H 8.27. found: C 91.38; H 8.42.

Spectral data for compound (3) :



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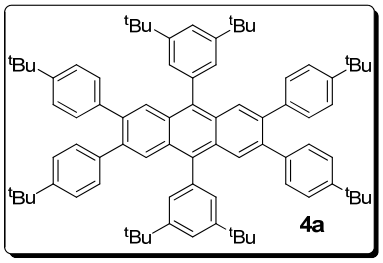
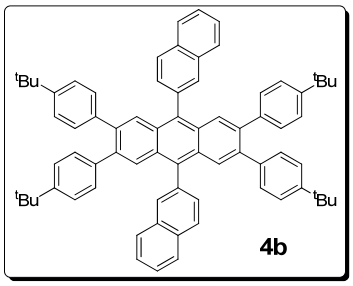
solid; IR (neat, cm^{-1}): 3290 (s), 2979 (s), 1460(s), 1394(m), 1371 (s), 706 (m); ^1H NMR (400 MHz, $CDCl_3$): δ 8.58 (s, 4H), 7.29 (d, J = 8.8 Hz, 8H), 7.22 (d, J = 8.8 Hz, 8H), 1.32 (s, 36H); ^{13}C NMR (100 MHz, $CDCl_3/CS_2$): δ 149.8, 140.9, 137.6, 130.4, 129.5, 124.8, 122.8, 34.3, 31.3 ; MALDITOF-MS calcd for $C_{54}H_{56}Br_2$: 862.2749, found m/z = 864.831. Anal. calcd for $C_{54}H_{56}Br_2$: C 74.99; H 6.53. Found: C 74.58; H 6.62.

Spectral data for compound (4a) :



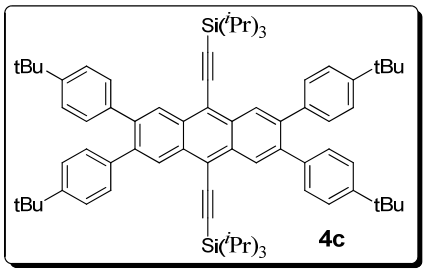
solid; IR (neat, cm^{-1}): 3280 (s), 2970(s), 1673 (s), 1310(s), 1395 (m), 1371 (s); ^1H NMR (400 MHz, CD_2Cl_2): δ 7.91. (s, 4H), 7.56 (s, 2H), 7.54 (s, 4H), 7.20 (d, *J*= 8.4 Hz, 8H), 7.09 (d, *J*= 8.4 Hz, 8H), 1.46 (s, 36H), 1.27 (s, 36H) ; ^{13}C NMR (100 MHz, CD_2Cl_2): δ 151.1, 150.0, 139.3, 138.7, 138.2, 137.7, 129.9, 129.3, 127.0, 125.1, 121.6, 35.4, 34.8, 31.9, 31.5 ;MALDITOF-MS calcd for $C_{82}H_{98}$: 1082.7669, found m/z = 1082.531. Anal. calcd for $C_{82}H_{98}$: C, 90.88; H, 9.12. Found: C, 90.81; H, 9.08.

Spectral data for compound (4b) :



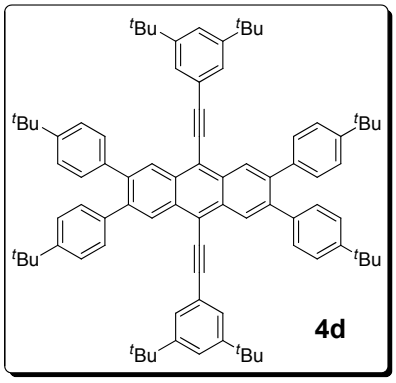
solid; IR (neat, cm^{-1}): 3238 (s), 2989 (s), 1393 (m), 1370(s); ^1H NMR (400 MHz, $CDCl_3$): δ 8.06-8.04 (m, 4H), 7.99-7.97 (m, 2H), 7.94-7.91 (m, 2H), 7.76 (d, *J*=0.4, 4H), 7.71-7.69 (m, 2H), 7.58-7.55 (m, 4H), 7.07 (m, 8H), 6.93 (m, 8H), 1.20 (s, 36H); ^{13}C NMR (100 MHz, $CDCl_3$); δ 149.2, 138.8, 138.5, 136.9, 136.5, 133.6, 132.9, 130.3, 129.9, 129.6, 129.5, 128.3, 128.2, 127.94, 127.90, 126.2, 126.1, 124.5, 34.3, 31.3 ; MALDITOF-MS calcd for $C_{74}H_{70}$: 958.5478, found m/z = 958.133. Anal. calcd for $C_{74}H_{70}$: C, 92.65; H, 7.35. Found: C, 92.60; H, 7.38.

Spectral data for compound (4c):



solid; IR (neat, cm^{-1}): 3240 (s), 2940(s), 2890 (m), 2130(w), 1385(s), 1370(s); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.69 (s, 4H), 7.27 (s, 16H), 1.33 (s, 36H), 1.23 (m, 42H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.6, 139.9, 138.2, 132.0, 129.6, 129.0, 124.7, 118.0, 104.9, 103.6, 34.5, 31.4, 18.9, 11.5 ; MALDITOF-MS calcd for $C_{76}H_{98}Si_2$: 1066.7207, found m/z = 1066.605. Anal. calcd for $C_{76}H_{98}Si_2$: C, 85.49; H, 9.25. Found: C, 85.00; H, 9.40.

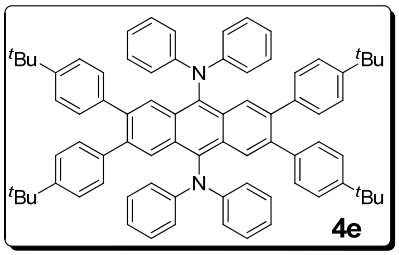
Spectral data for compound (4d):



solid; IR (neat, cm^{-1}): 3280 (s), 2960(s), 2845 (m), 2090(w), 1396(m), 1370(s); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.74 (s, 4H), 7.56 (d, *J*= 1.6Hz, 4H), 7.44 (d, *J* = 1.6Hz, 2H), 7.29 (s, 16H) 1.36 (s, 36H), 1.31 (s, 36H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.0, 149.7, 140.1, 138.6, 131.8, 129.7, 128.8, 126.1, 124.8, 123.2, 122.7, 118.0, 104.1, 86.0, 34.9, 34.5, 31.4; MALDITOF-MS calcd for $C_{86}H_{98}$: 1130.7669, found m/z = 1130.592.

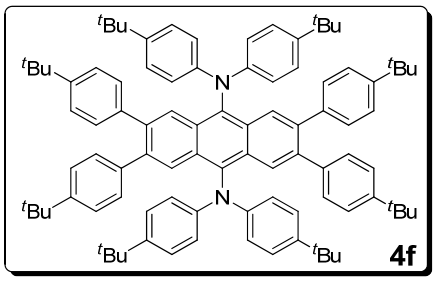
Anal. calcd for $C_{86}H_{98}$: C, 91.27; H, 8.73. Found: C, 91.01; H, 8.75.

Spectral data for compound (4e):



solid; IR (neat, cm^{-1}): 3230 (s), 2900(s), 2840 (m), 1560(s), 1397(m), 1370(s), 1243 (s); ^1H NMR (400 MHz, $CDCl_3$): δ 8.20 (s, 4H), 7.26-7.16(m, 16H), 7.10 (d, J = 8.4 Hz, 8H), 6.95 (t, J = 7.2 Hz, 4H), 6.70 (d , J = 8.4 Hz, 8H), 1.25 (s, 36H) ; ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.5, 148.1, 139.7, 138.1, 130.9, 129.5, 129.3, 126.4, 124.5, 121.4, 120.9, 34.4, 31.3; MALDITOF-MS calcd for $C_{78}H_{76}N_2$: 1040.6009, found m/z = 1040.528. Anal. calcd for $C_{78}H_{76}N_2$: C, 89.95; H, 7.36; N, 2.69. Found: C, 89.63; H, 7.28; N, 2.80.

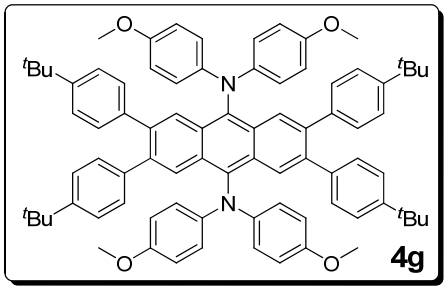
.**Spectral data for compound (4f):**



solid; IR (neat, cm^{-1}): 3238 (s), 2910 (m), 1396(m), 1370(s) ; ^1H NMR (400 MHz, $CDCl_3$): δ 8.15 (s, 4H), 7.25 (d, J = 8 Hz, 8H), 7.09 (d, J = 8.4 Hz, 8H), 7.06 (d, J = 8.4Hz, 8H), 6.71 (d, J = 8 Hz, 8H), 1.33 (s, 36H), 1.24 (s, 36H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.4, 146.1, 143.8, 139.2, 138.2, 137.4, 130.7, 129.6, 126.9, 126.1, 124.4, 120.5, 34.4, 34.3, 31.6, 31.4; MALDITOF-MS calcd for $C_{94}H_{108}N_2$: 1264.8513, found m/z

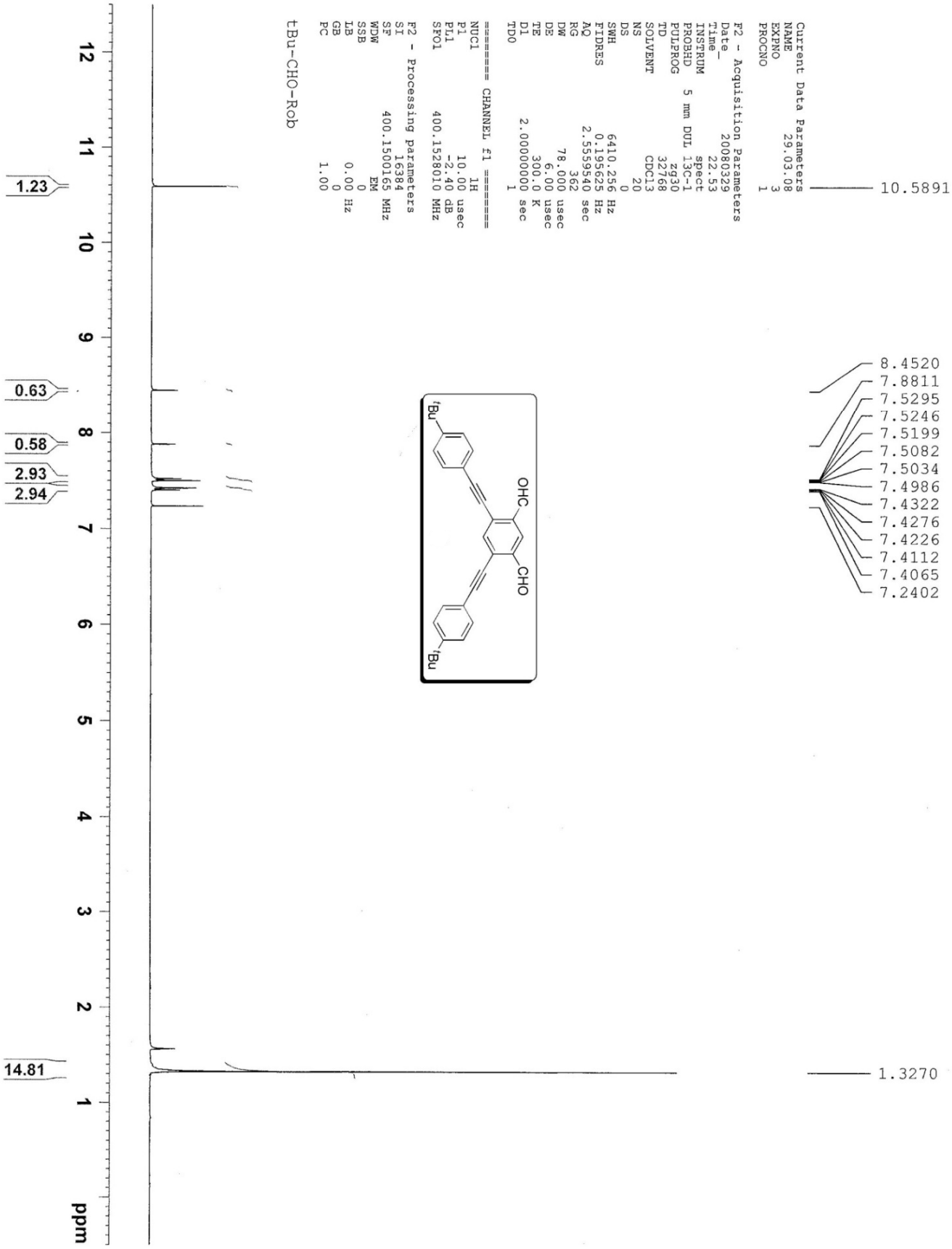
= 1264.727. Anal. calcd for $C_{94}H_{108}N_2$: C, 89.19; H, 8.60; N, 2.21. Found: C, 88.72; H, 8.73; N, 2.34.

Spectral data for compound (4g):



solid; IR (neat, cm^{-1}): 3200 (s), 2910 (s), 2860 (m), 1397 (m), 1372 (s); ^1H NMR (400 MHz, $CDCl_3$): δ 8.21 (s, 4H), 7.11 (d, *J*=8.4, 8H), 7.06 (d, *J* = 9.2 Hz, 8H), 6.81(d, *J* = 6.4 Hz, 8H), 6.79 (d, J= 6.8Hz, 8H), 3.77(s, 12H), 1.25 (s, 36H) ; ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.0, 149.4, 142.4, 139.5, 138.2, 137.3, 131.0, 129.6, 126.6, 124.5, 121.8, 114.7, 55.7, 34.4, 31.4; MALDITOF-MS calcd for $C_{82}H_{84}N_2O_4$: 1160.6431, found m/z = 1160.451. Anal. calcd for $C_{82}H_{84}N_2O_4$: C, 84.79; H, 7.29; N, 2.41. Found: C, 84.57. H, 7.38; N, 2.29.

E. NMR spectral- data for key compounds: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PROCNO 1
F2 - Acquisition Parameters
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Time_ 22.53
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PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 20
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 362
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
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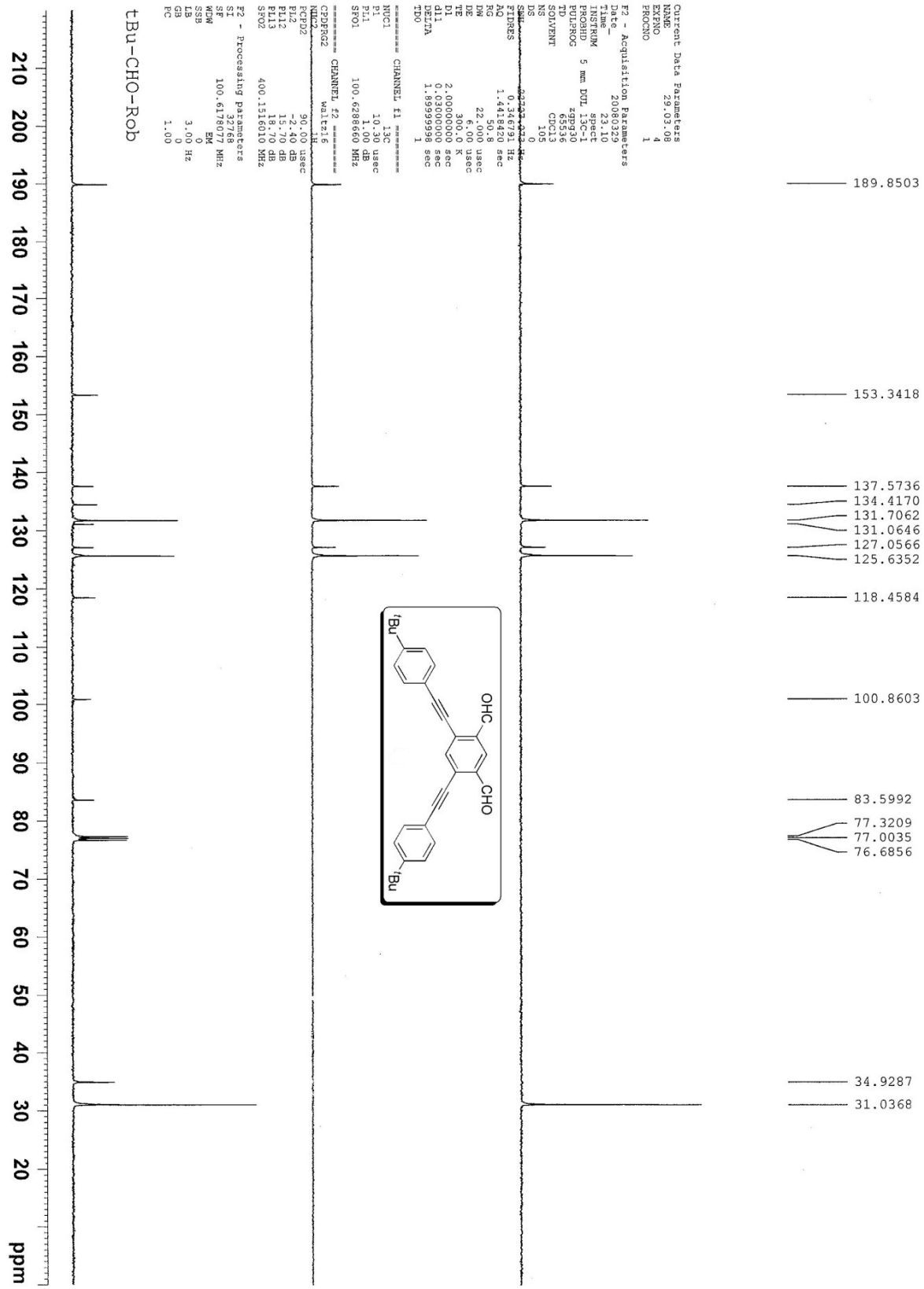
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500165 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
tBu-CHO-Rob
OHC
CHO
tBu
tBu
10.5891
8.4520
7.8811
7.5295
7.5246
7.5199
7.5082
7.5034
7.4986
7.4322
7.4276
7.4226
7.4112
7.4065
7.2402
1.3270
1.23
0.63
0.58
2.93
2.94
14.81
12
11
10
9
8
7
6
5
4
3
2
1
ppm


tBu-CHO-Rob
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NAME
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
d11
DELTA
TD0
======== CHANNEL f1 ========
NUC1
P1
PL1
SFO1
======== CHANNEL f2 ========
CPDPRG2
NUC2
PCPD2
PL2
PL12
PL13
SFO2
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC
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153.3418
137.5736
134.4170
131.7062
131.0646
127.0566
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118.4584
100.8603
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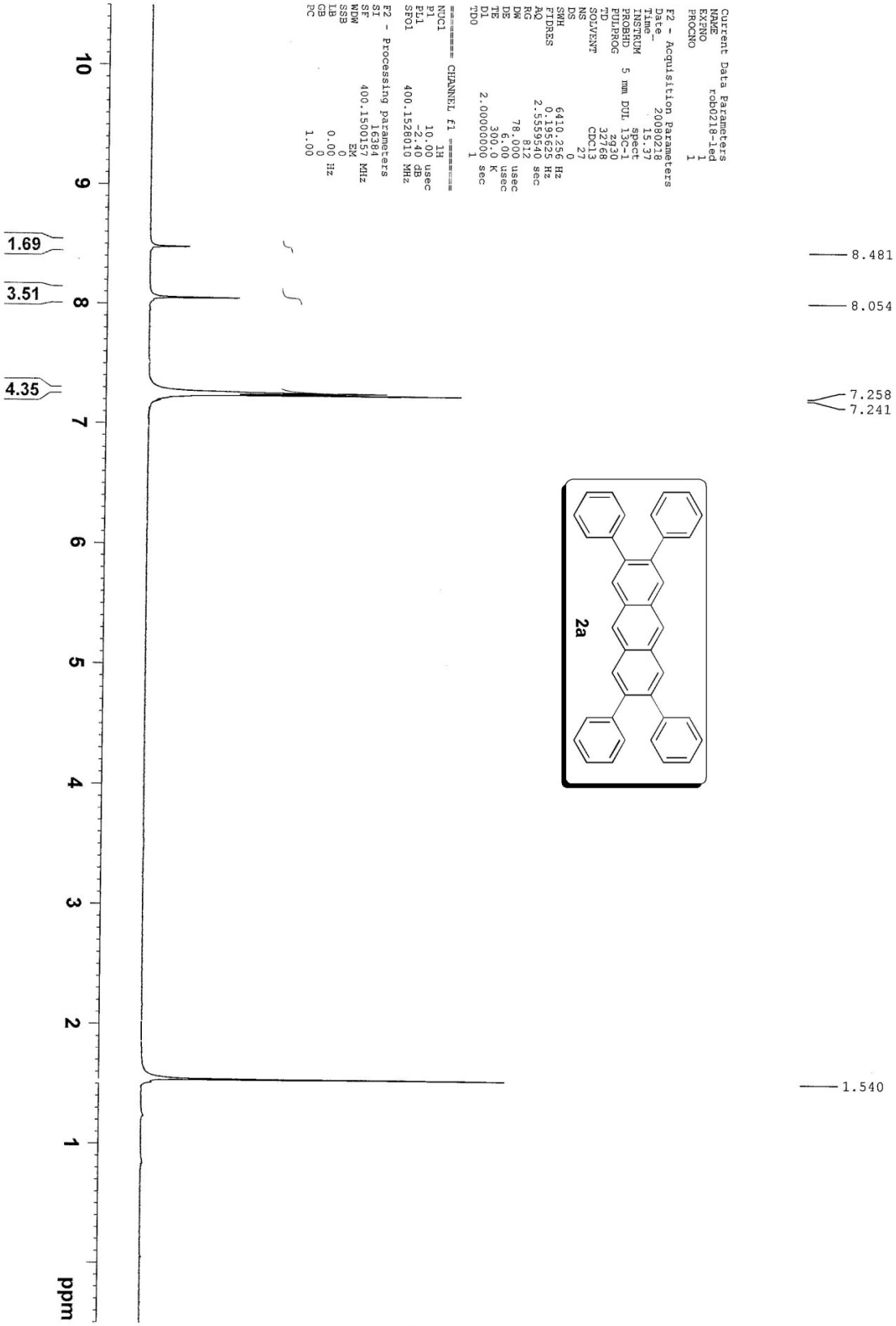
77.3209
77.0035
76.6856
34.9287
31.0368
OHC
CHO
tBu
tBu
ppm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NAME robd218-1ed
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090218
Time 15.37
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 27
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559940 sec
RG 8192
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500157 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
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3.51
4.35
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7.241
1.540
2a
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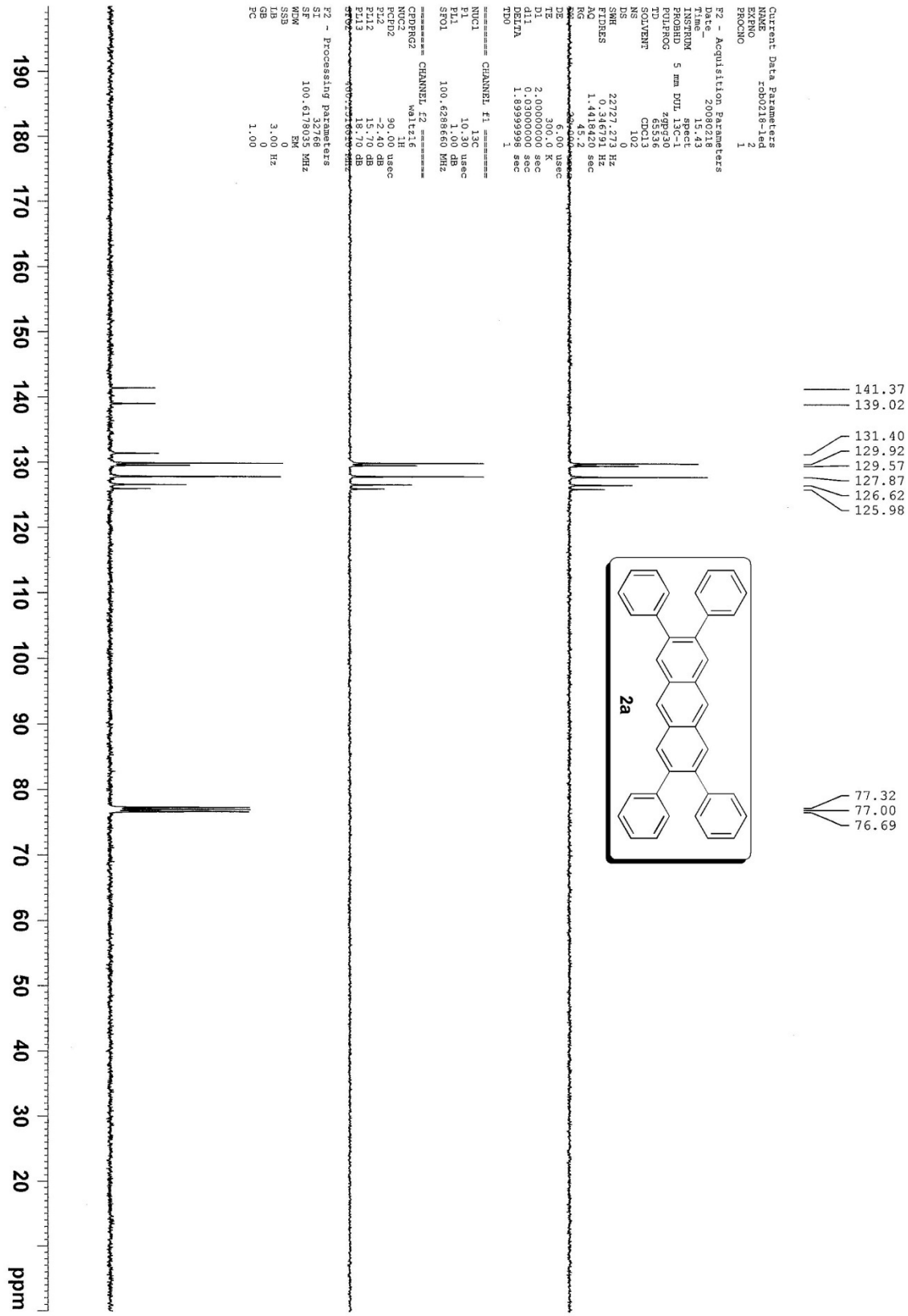
9
8
7
6
5
4
3
2
1
ppm


Current Data Parameters
NAME rob0218-1ed
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080218
Time 15.43
INSTRUM spect
PROBHD 5 mm BUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 102
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 45.2
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.8999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.30 usec
PL1 1.00 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.70 dB
PL13 18.70 dB
SFO2 400.1316010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178035 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
141.37
139.02
131.40
129.92
129.57
127.87
126.62
125.98
77.32
77.00
76.69
2a
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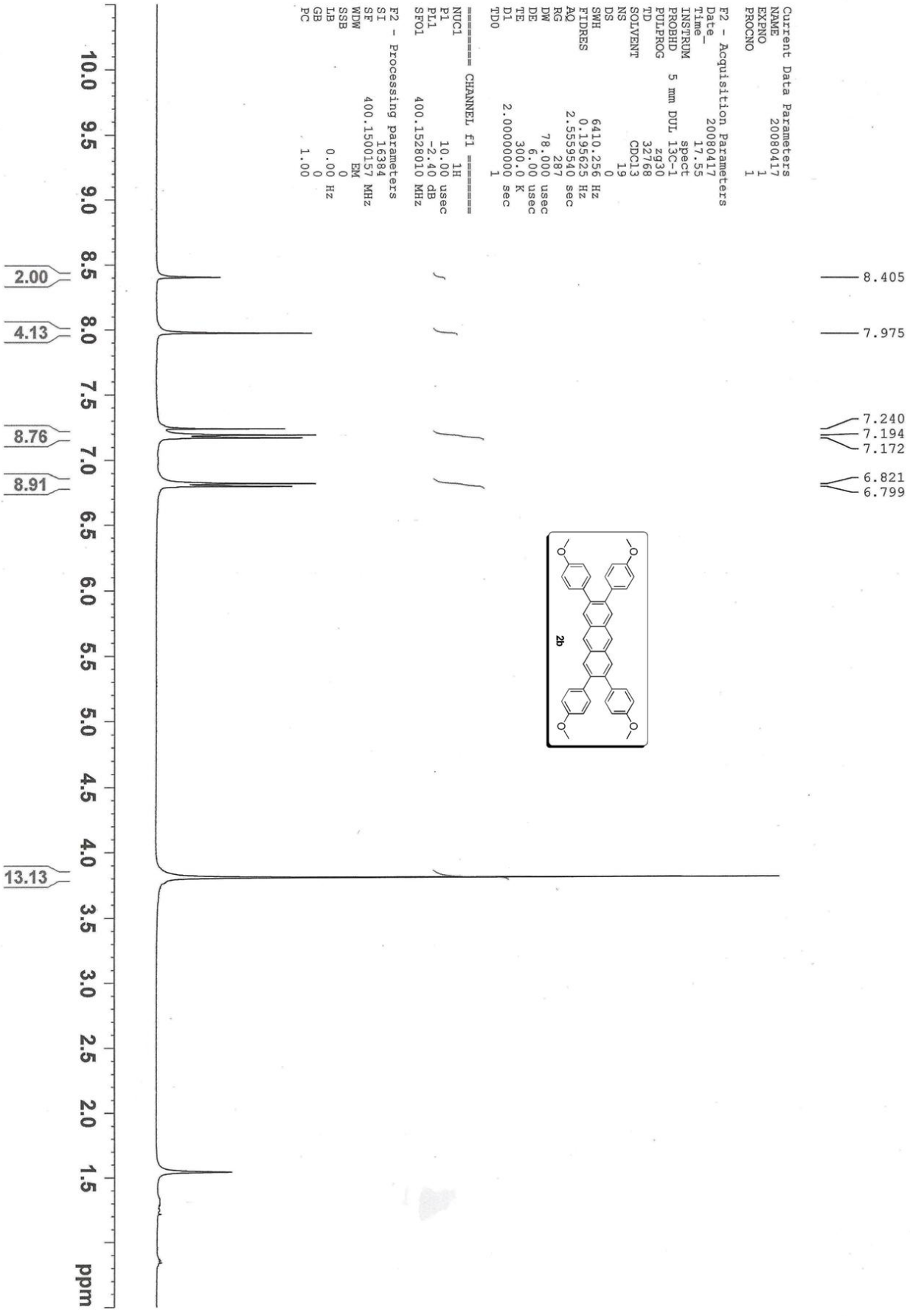
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NAME 20080417
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080417
Time 17.55
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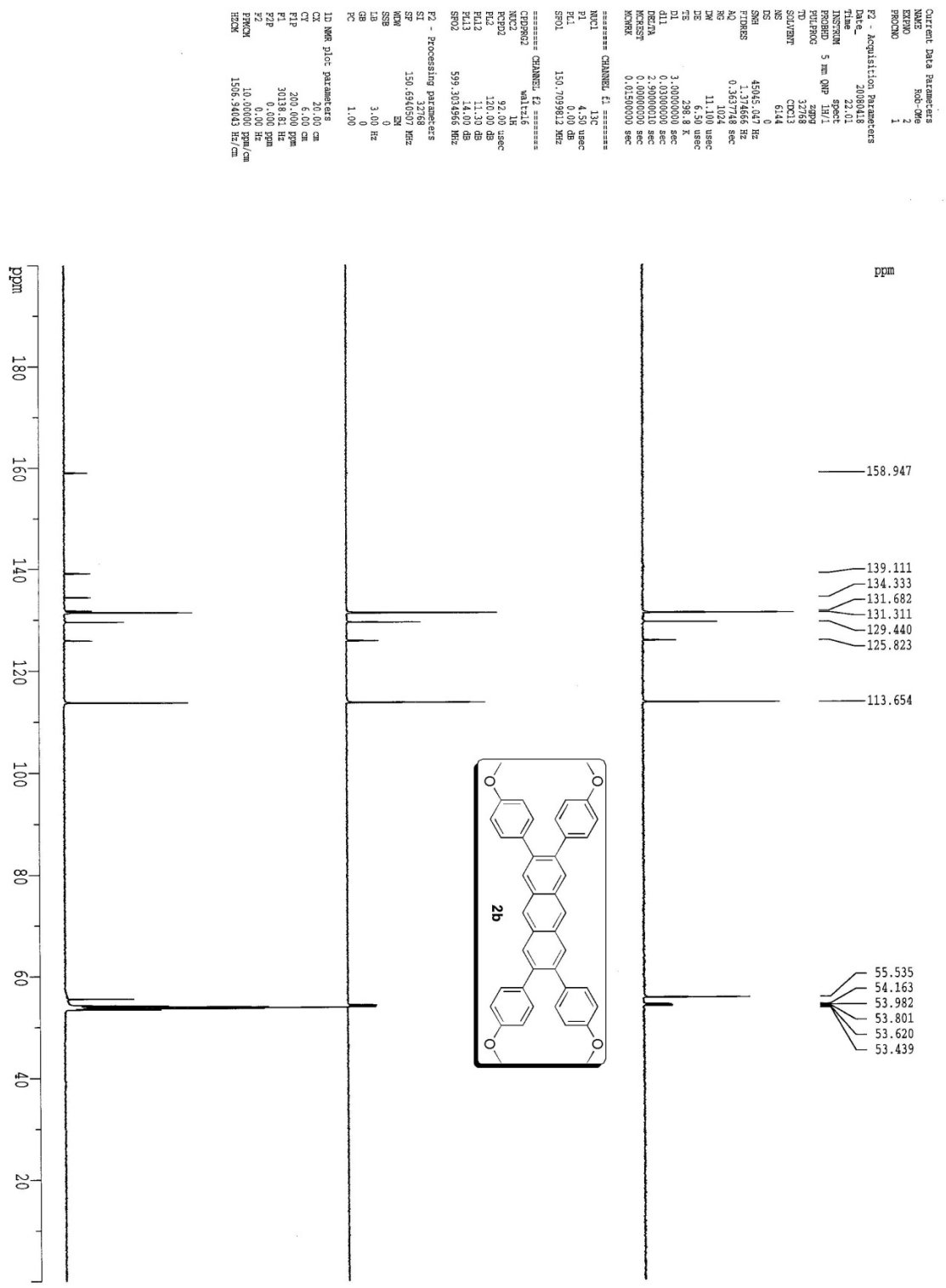
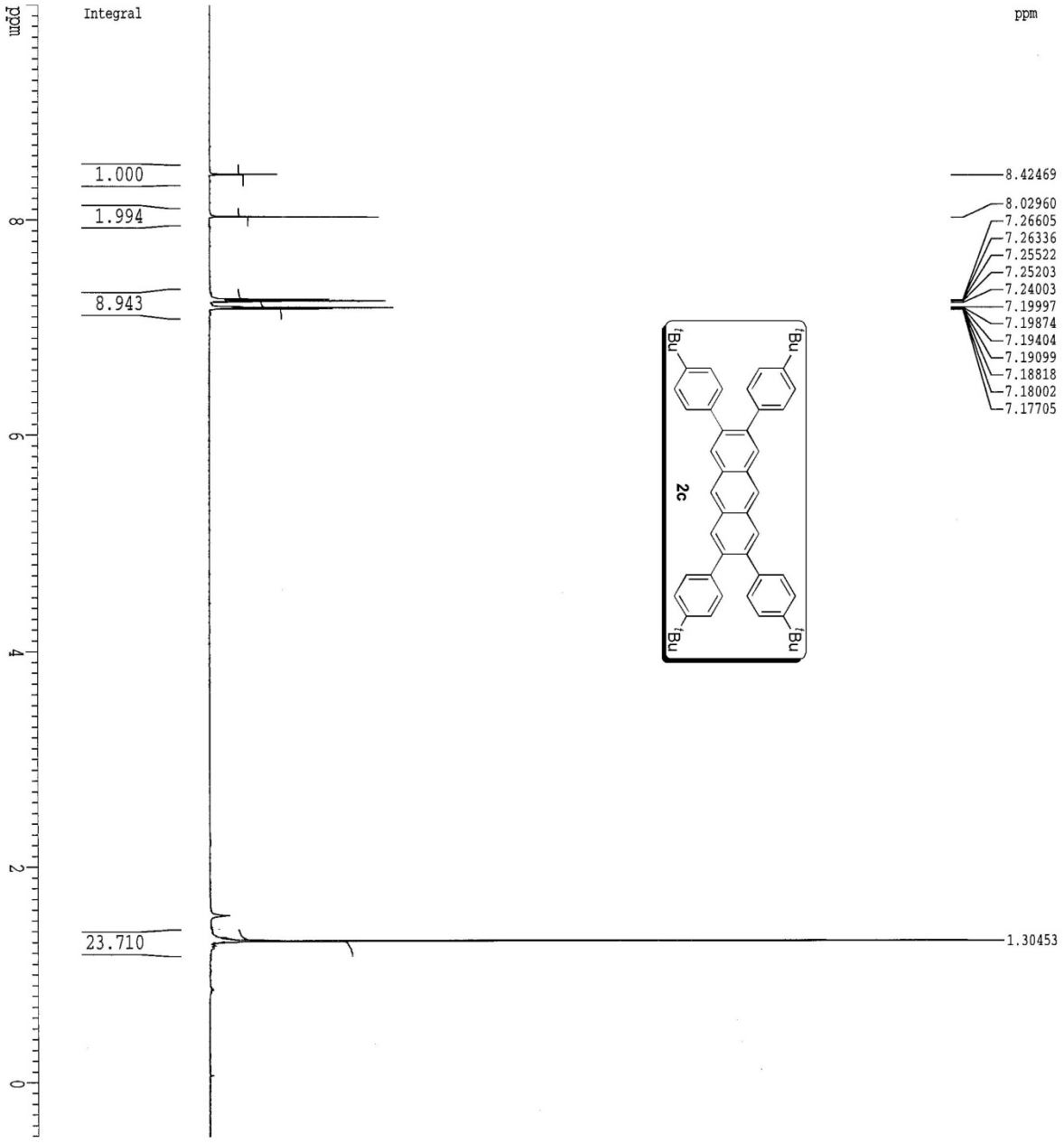
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 19
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 287
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500157 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
2b
8.405
7.975
7.240
7.194
7.172
6.821
6.799
2.00
4.13
8.76
8.91
13.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm


Current Data Parameters
NAME Rob-CMe
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080418
Time 22.01
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 1024
DW 11.100 usec
DE 6.50 usec
TE 298.8 K
D1 3.00000000 sec
d11 0.03000000 sec
DELTA 2.90000010 sec
MCREST 0.00000000 sec
MCWRK 0.02500000 sec
======== CHANNEL f1 ========
NUC1 13c
P1 4.50 usec
PL1 0.00 dB
SFO1 150.7099812 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 11.30 dB
PL13 14.00 dB
SFO2 599.3034966 MHz
F2 - Processing parameters
SI 32768
SF 150.6940507 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 200.000 ppm
F1 30138.81 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1506.94043 Hz/cm
ppm
158.947
139.111
134.333
131.682
131.311
129.440
125.823
113.654
55.535
54.163
53.982
53.801
53.620
53.439
2b



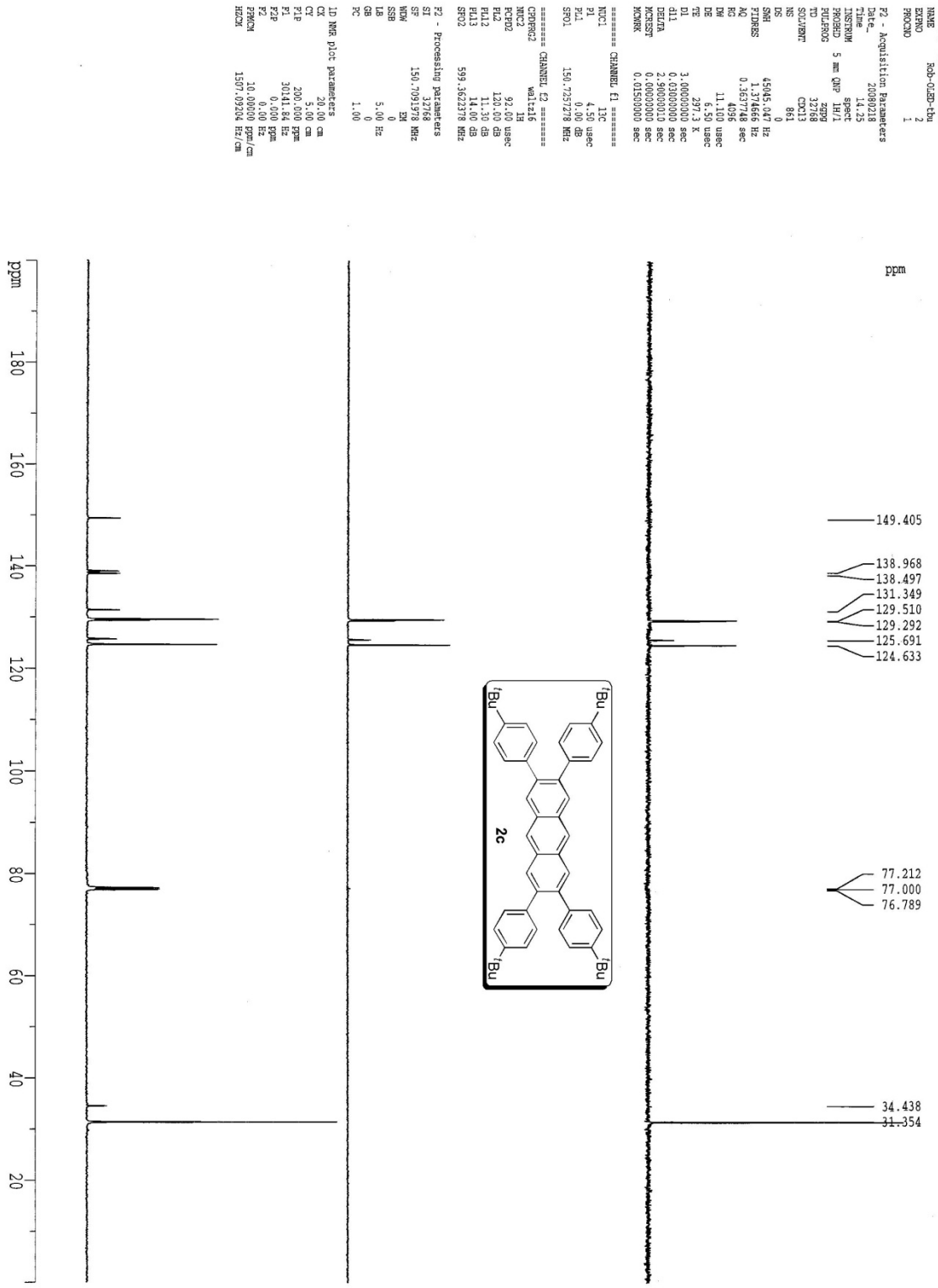
Current Data Parameters
NAME Rob-OLED-tbu
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080218
Time 15.59
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CD2Cl2
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 8
DW 41.600 usec
DE 6.50 usec
TE 297.7 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 9.80 usec
PL1 0.00 dB
SFO1 599.3626894 MHz

F2 - Processing parameters
SI 32768
SF 599.3600263 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.10

1D NMR plot parameters
CX 20.00 cm
CY 40.00 cm
F1P 10.000 ppm
F1 5993.60 Hz
F2P -0.500 ppm
F2 -299.68 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.66403 Hz/cm


Current Data Parameters
NAME Rob-OLED-tbu
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080218
Time 14.25
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 861
DS 0
SWH 45045.047 Hz
FIDRES 1.374466 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 297.3 K
D1 3.00000000 sec
d11 0.03000000 sec
DELTA 2.90000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.50 usec
PL1 0.00 dB
SFO1 150.725728 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 11.30 dB
PL13 14.00 dB
SFO2 599.362378 MHz
F2 - Processing parameters
SI 32768
SF 150.709178 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 200.000 ppm
F1 30114.84 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1507.09204 Hz/cm
ppm
149.405
138.968
138.497
131.349
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129.292
125.691
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77.000
76.789
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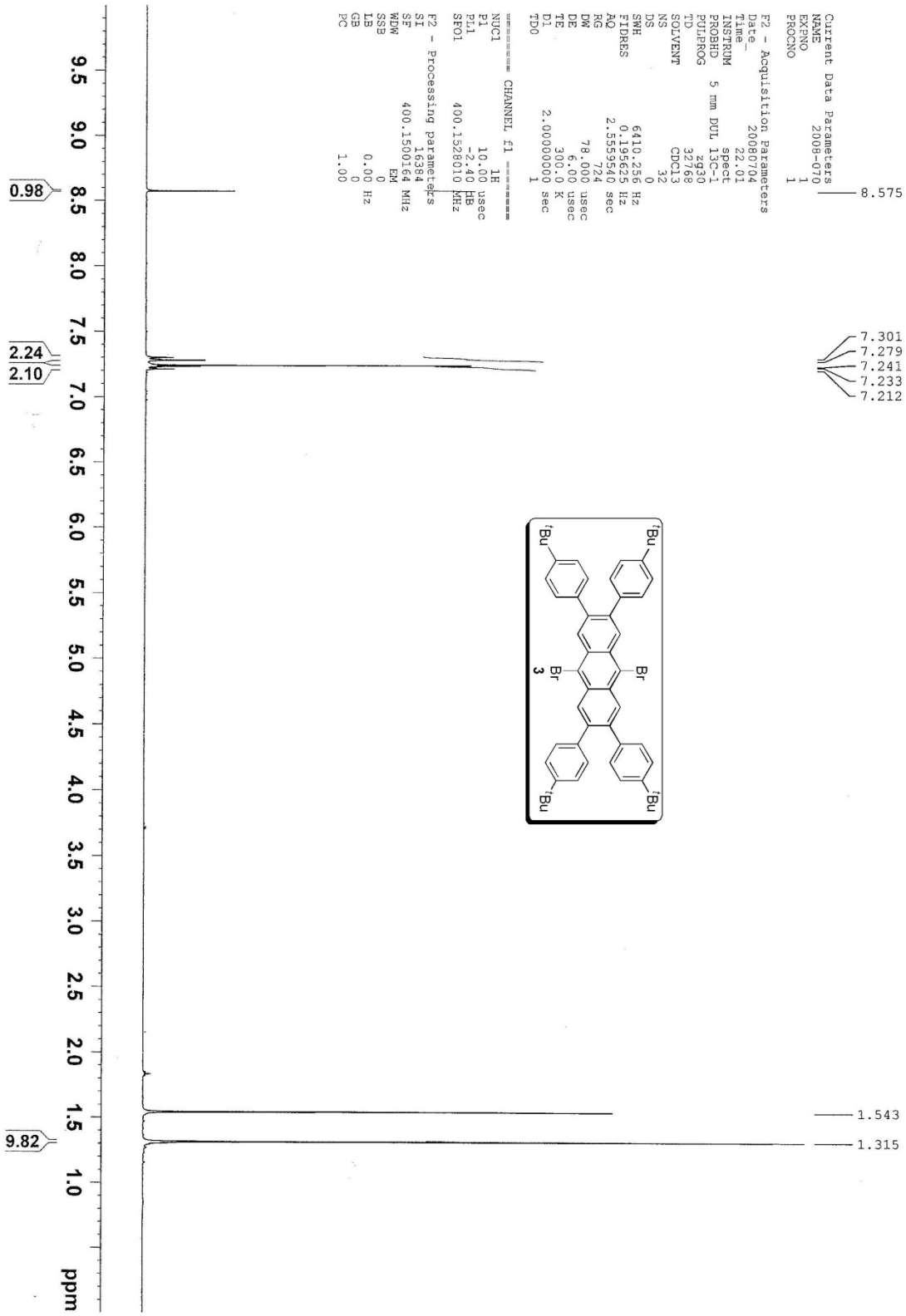
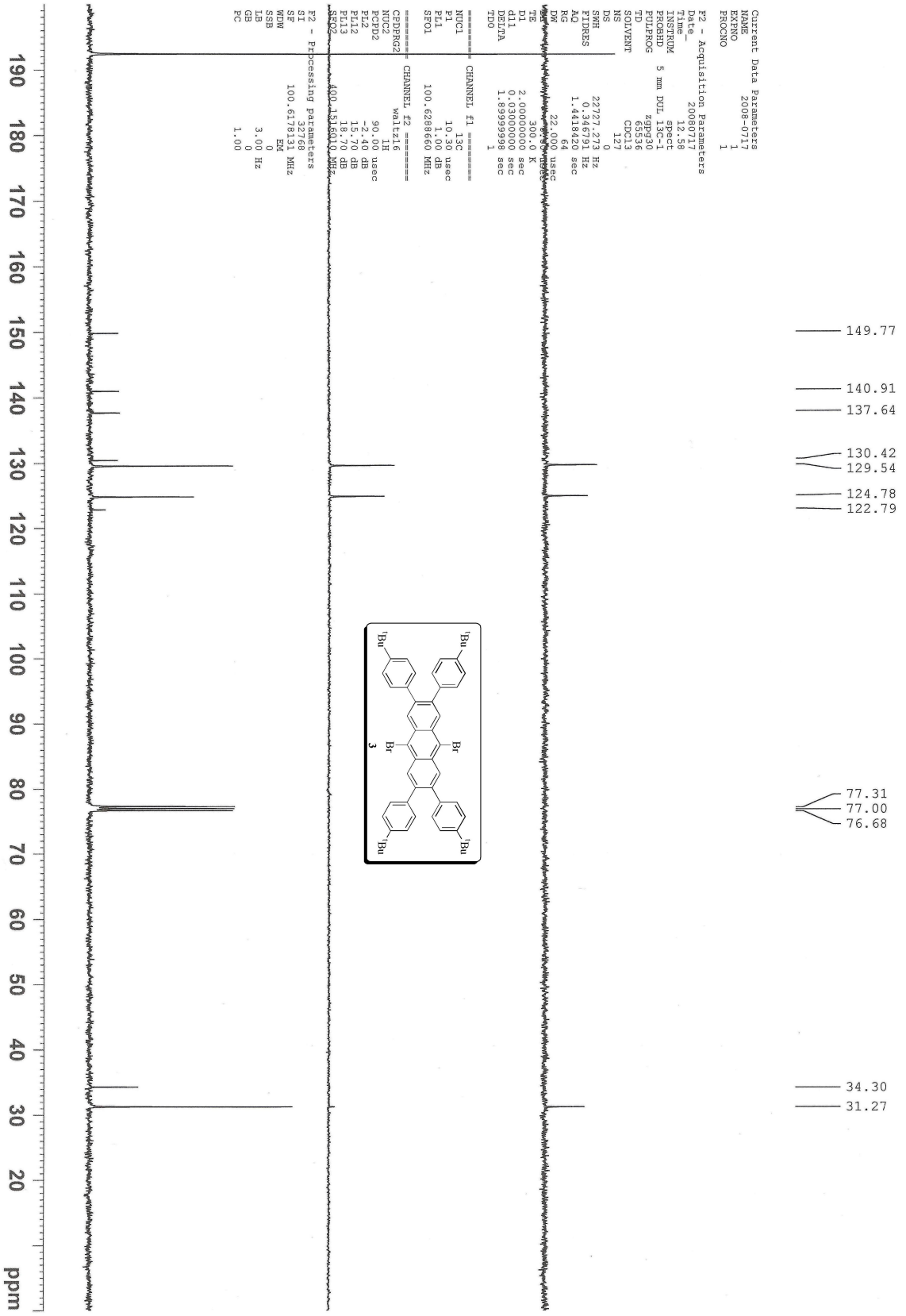
31.354
tBu
2c


Current Data Parameters
NAME
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD 5 mm DUL 13C-1
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
TD0
CHANNEL f1
NUC1
P1
PL1
SFO1
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC
8.575
7.301
7.279
7.241
7.233
7.212
1.543
1.315
0.98
2.24
2.10
9.82
ppm
tBu
Br
3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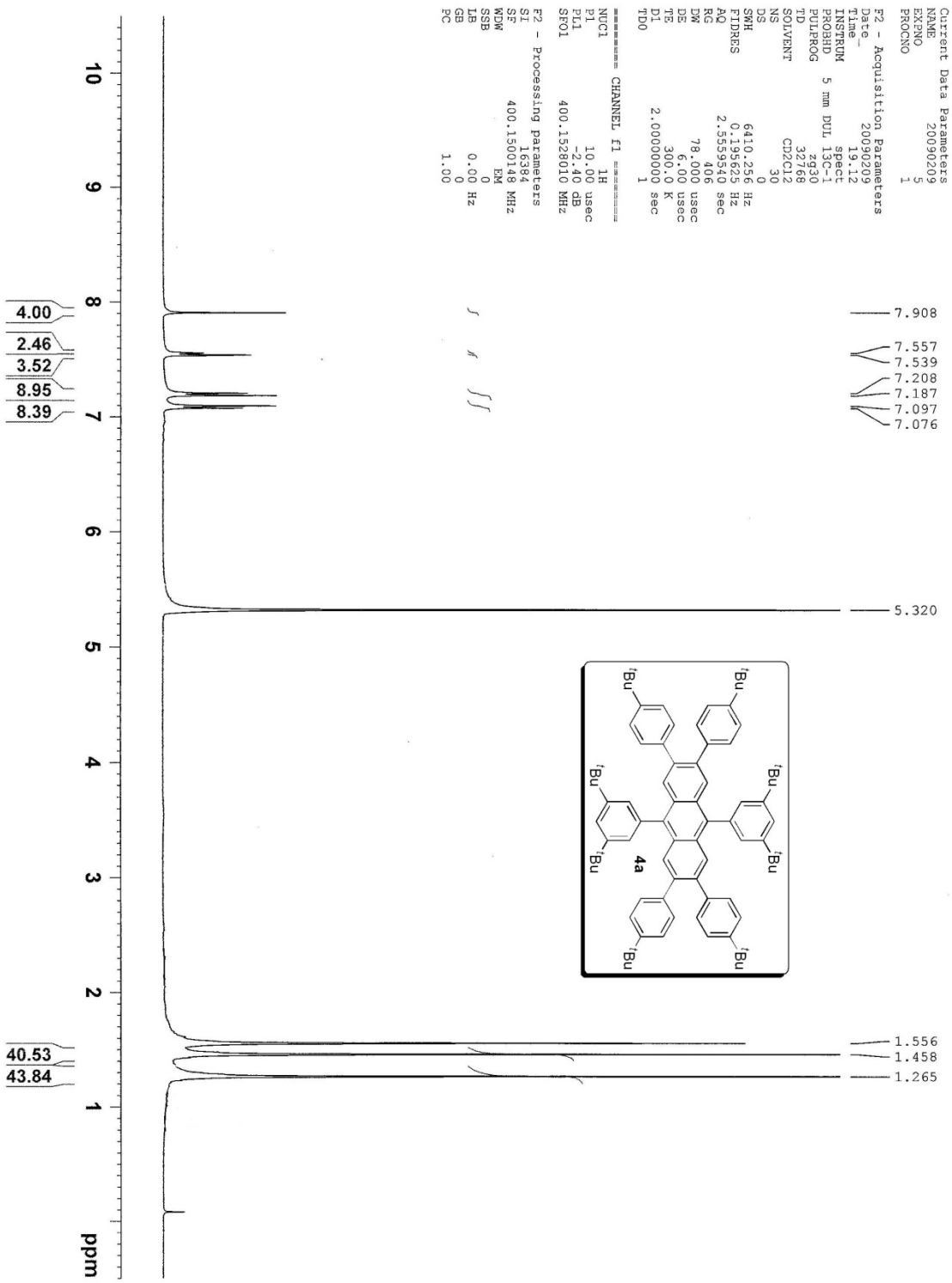
NAME 2008-0717
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080717
Time 12.58
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 127
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 64
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.30 usec
PL1 1.00 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.70 dB
PL13 18.70 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178131 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
149.77
140.91
137.64
130.42
129.54
124.78
122.79
77.31
77.00
76.68
34.30
31.27
tBu
Br
3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
ppm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EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090209
Time 19.12
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PULPROG zg30
TD 32768
SOLVENT CD2Cl2
NS 30
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 406
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500148 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
4.00
2.46
3.52
8.95
8.39
40.53
43.84
7.908
7.557
7.539
7.208
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7.097
7.076
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1.556
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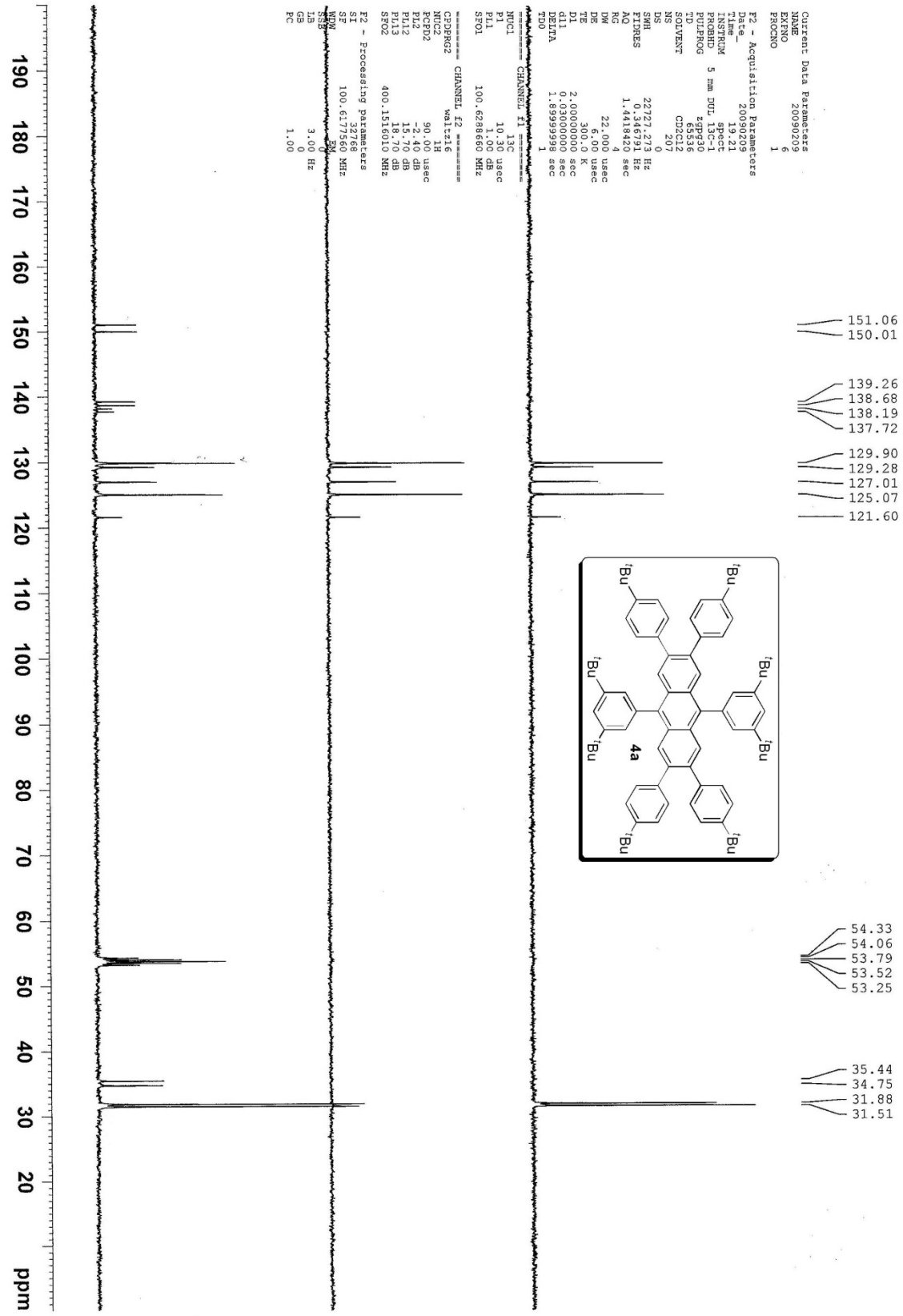
1.265
tBu
4a
10
9
8
7
6
5
4
3
2
1
ppm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137.72
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125.07
121.60
54.33
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31.51
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150
140
130
120
110
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80
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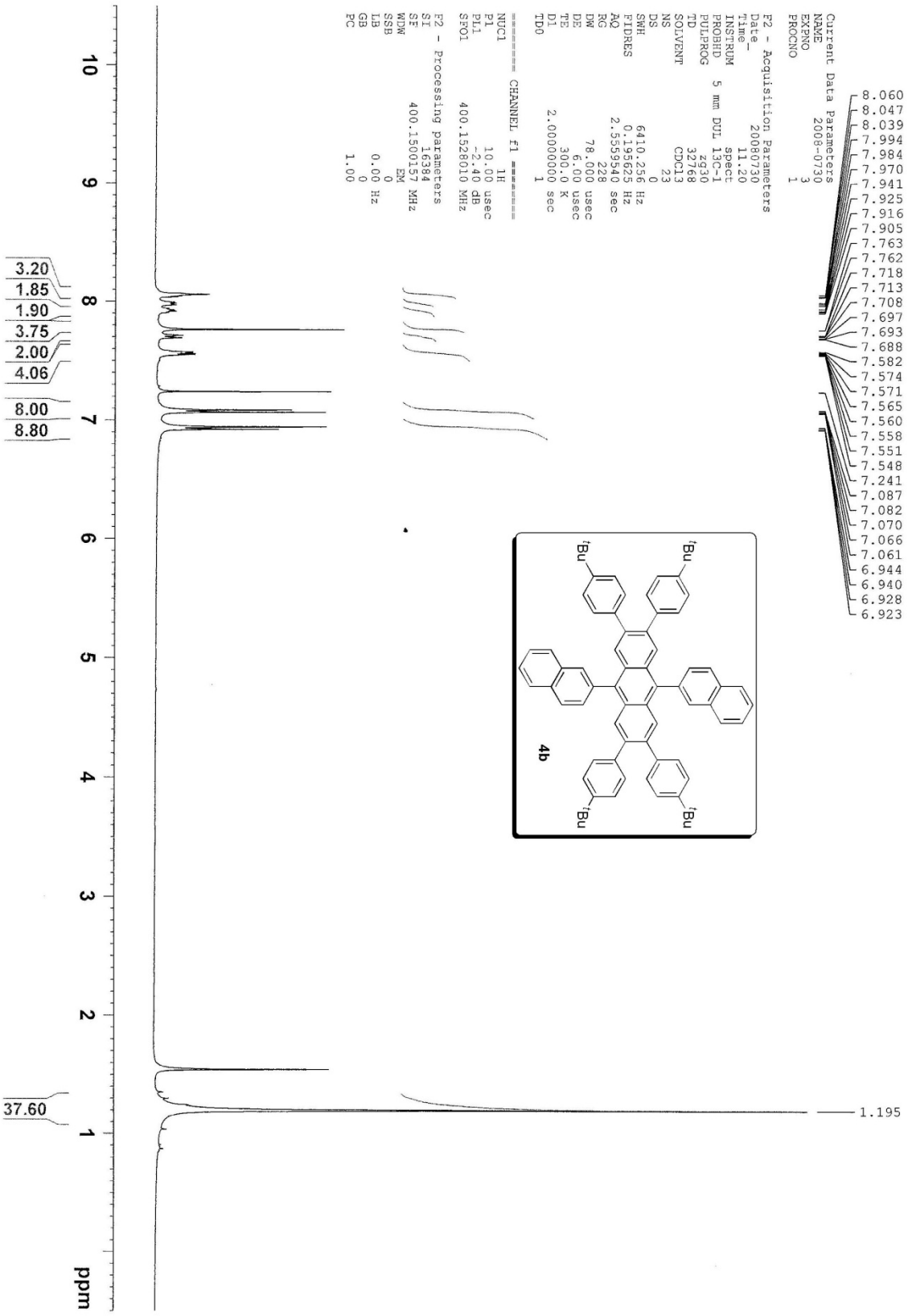
50
40
30
20
ppm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NAME
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080730
Time_ 11.20
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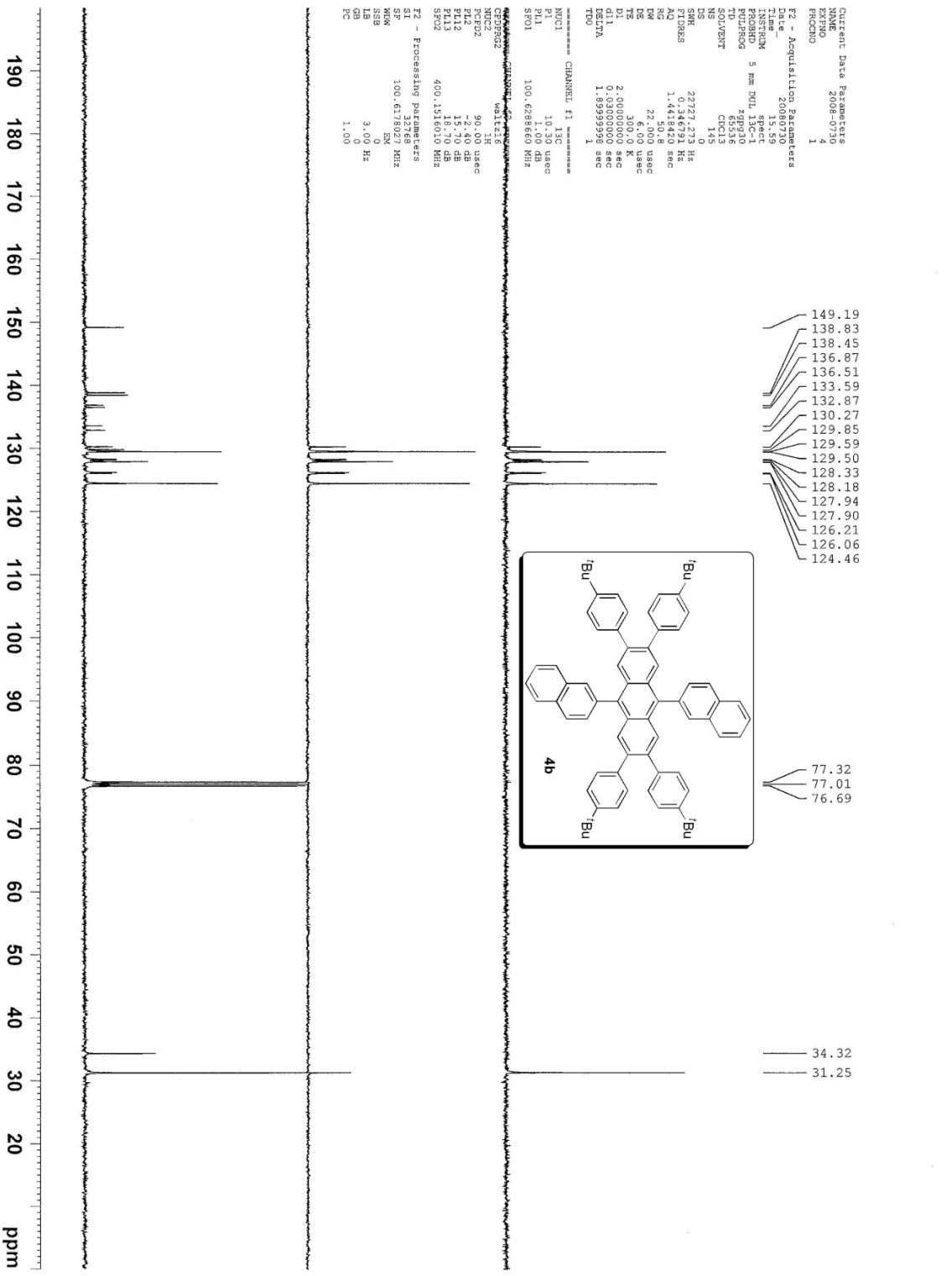
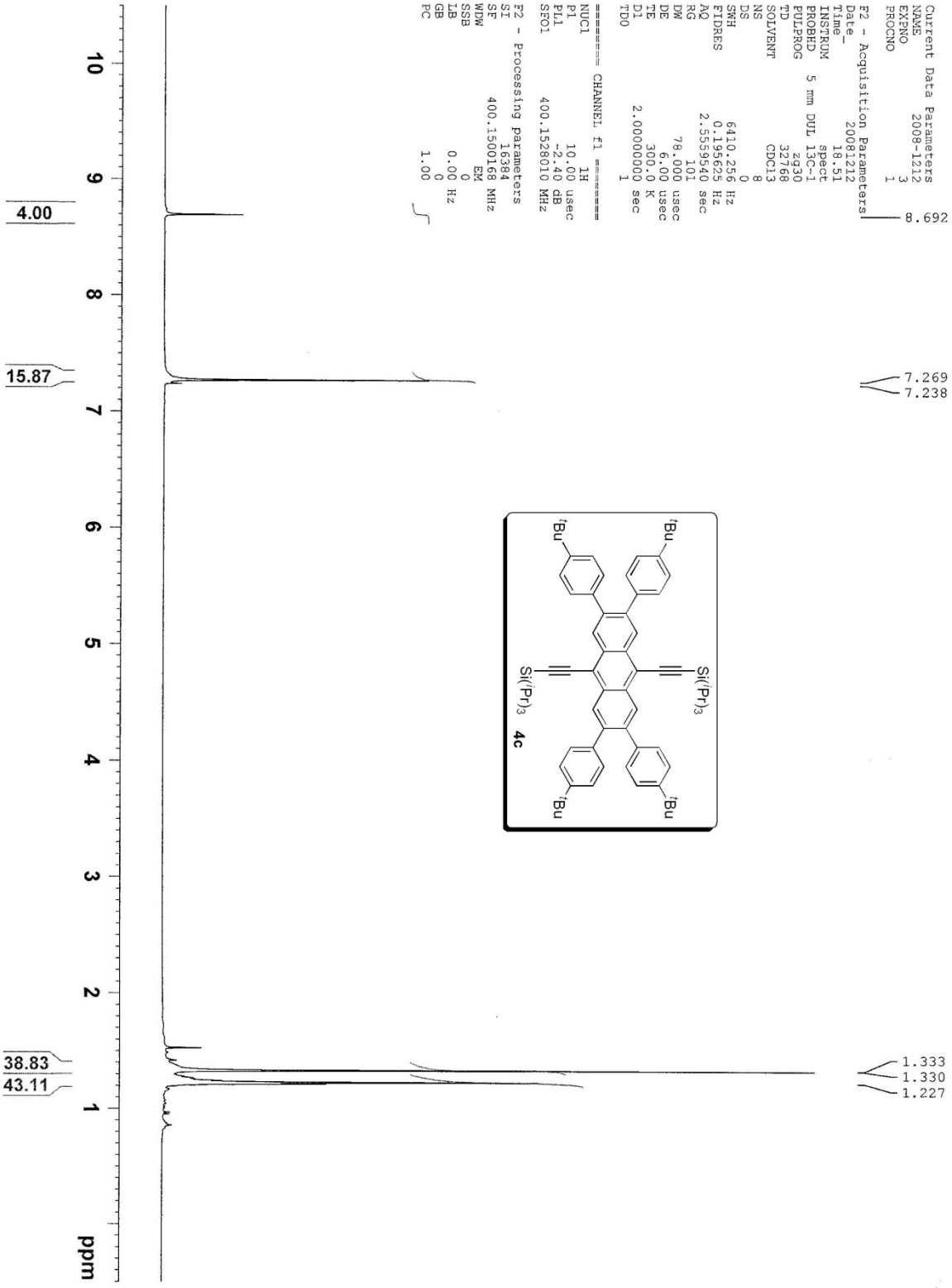
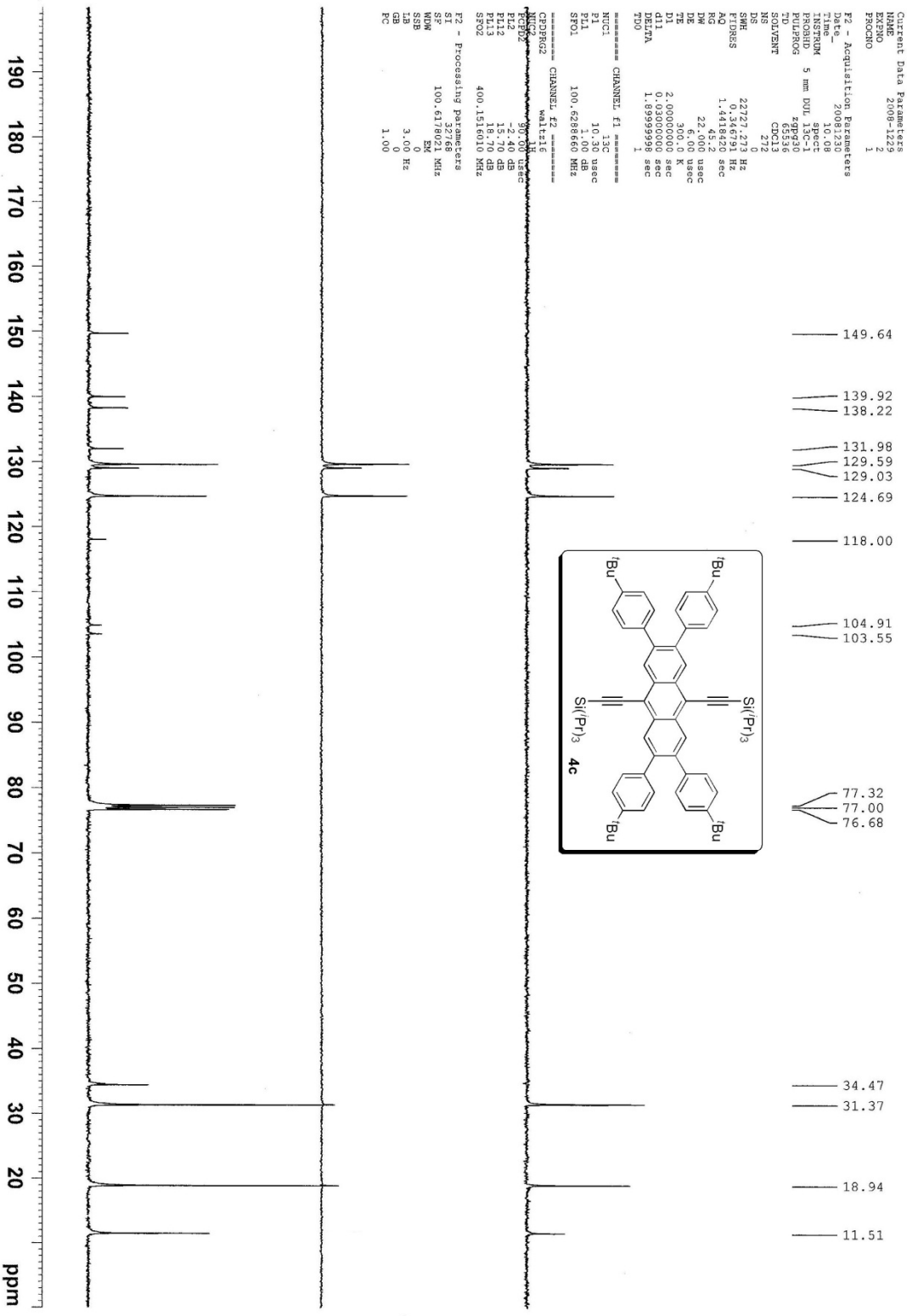
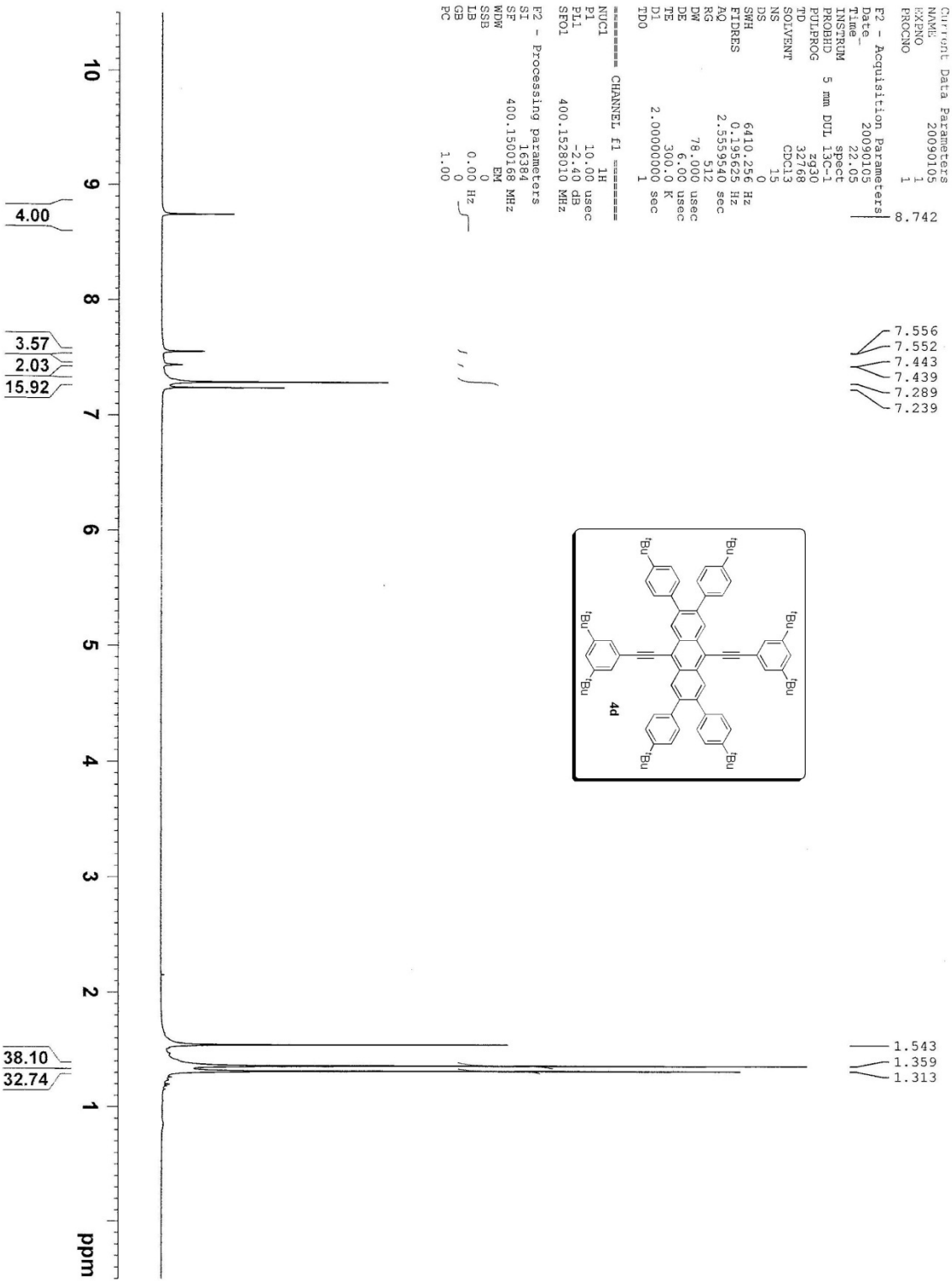
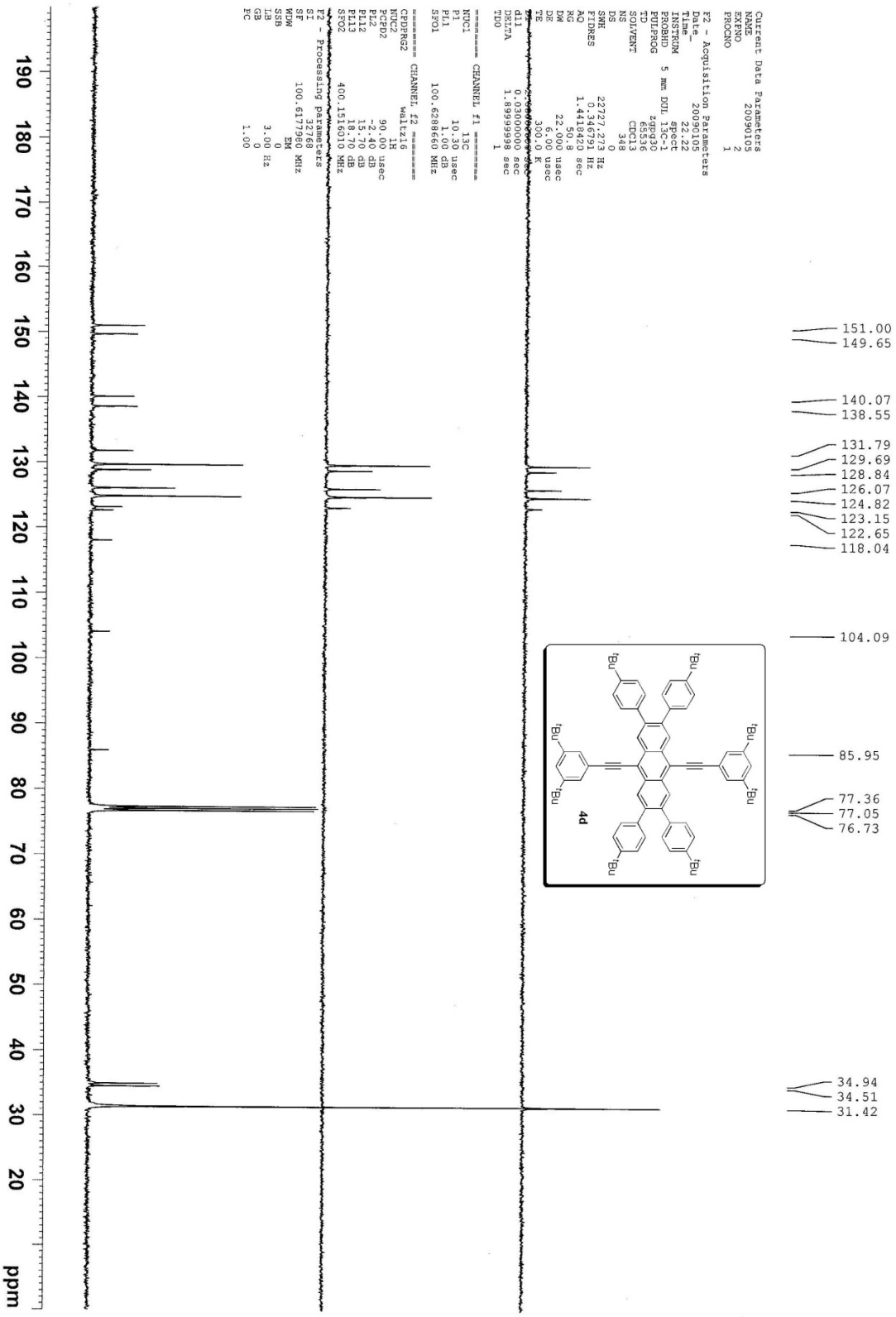
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 23
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 228
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500157 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.060
8.047
8.039
7.994
7.984
7.970
7.941
7.925
7.916
7.905
7.763
7.762
7.718
7.713
7.708
7.697
7.693
7.688
7.582
7.574
7.571
7.565
7.560
7.558
7.551
7.548
7.241
7.087
7.082
7.070
7.066
7.061
6.944
6.940
6.928
6.923
3.20
1.85
1.90
3.75
2.00
4.06
8.00
8.80
37.60
1.195
tBu
4b
ppm

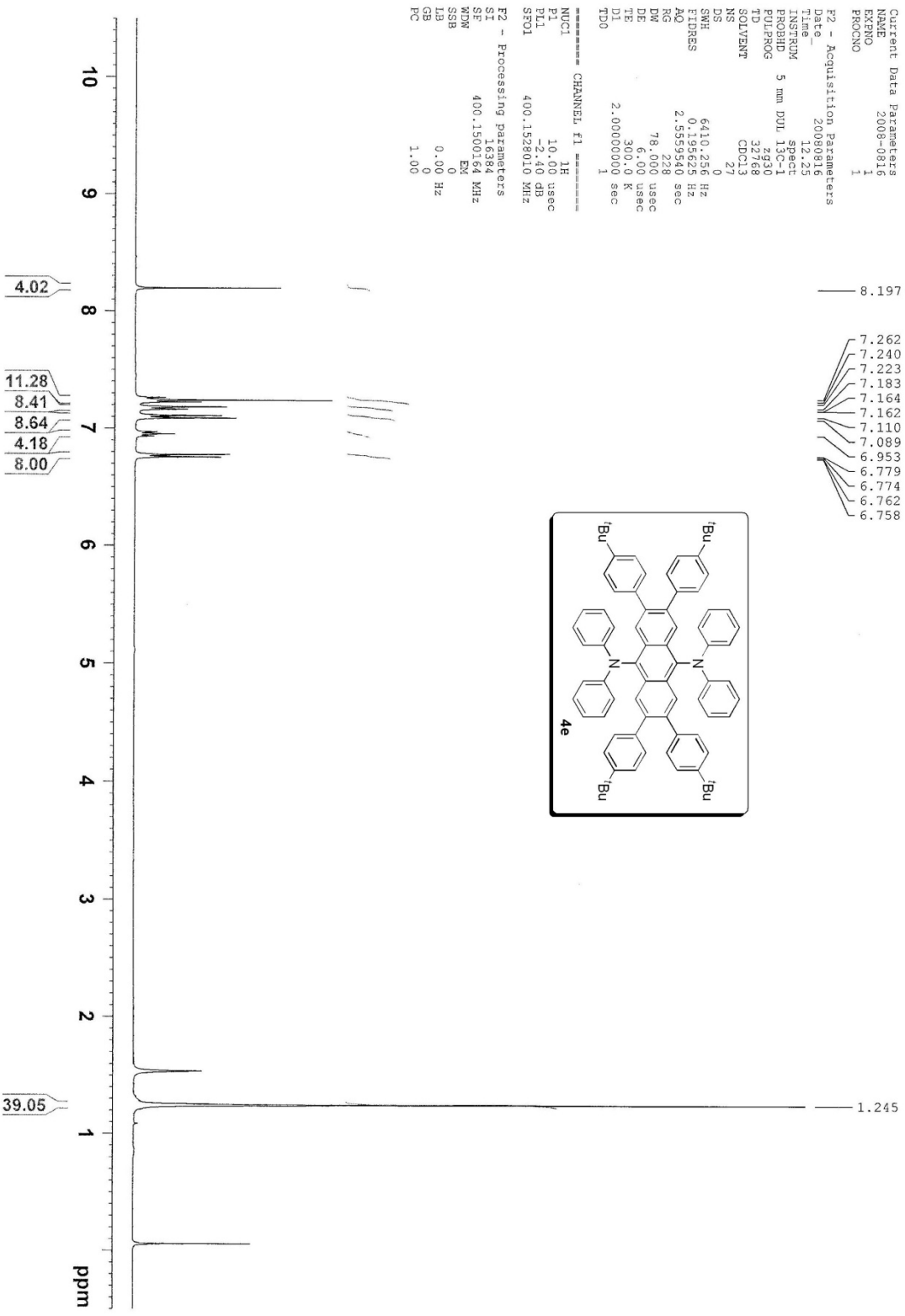

149.19
138.83
138.45
136.87
136.51
133.59
132.87
130.27
129.85
129.59
129.50
128.33
128.18
127.94
127.90
126.21
126.06
124.46
77.32
77.01
76.69
34.32
31.25
4b
tBu
ppm

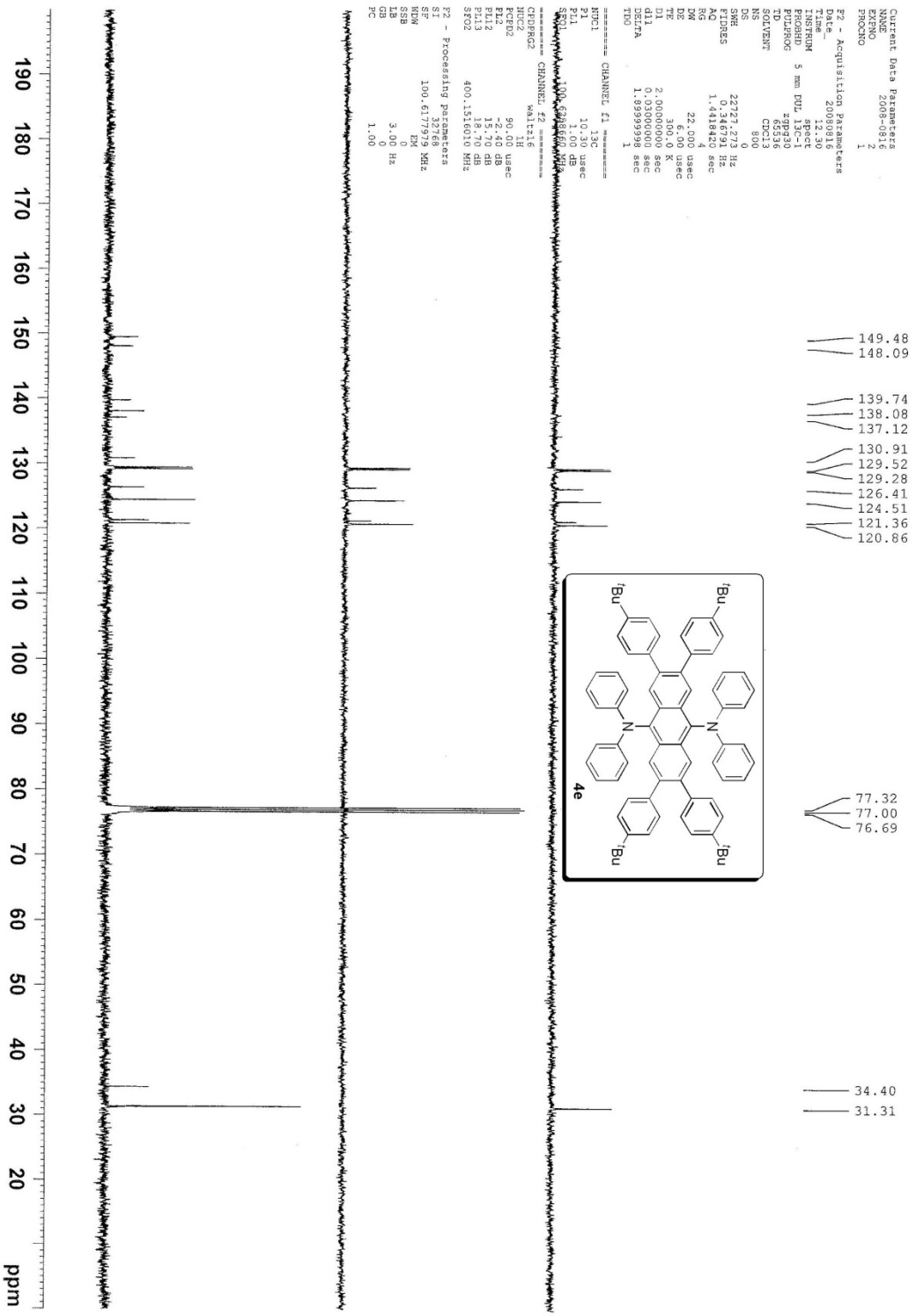

Current Data Parameters
NAME 2008-1212
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081212
Time_ 18.51
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 101
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.692
7.269
7.238
1.333
1.330
1.227
4.00
15.87
38.83
43.11
10
9
8
7
6
5
4
3
2
1
ppm
tBu
Si(iPr)3
4c

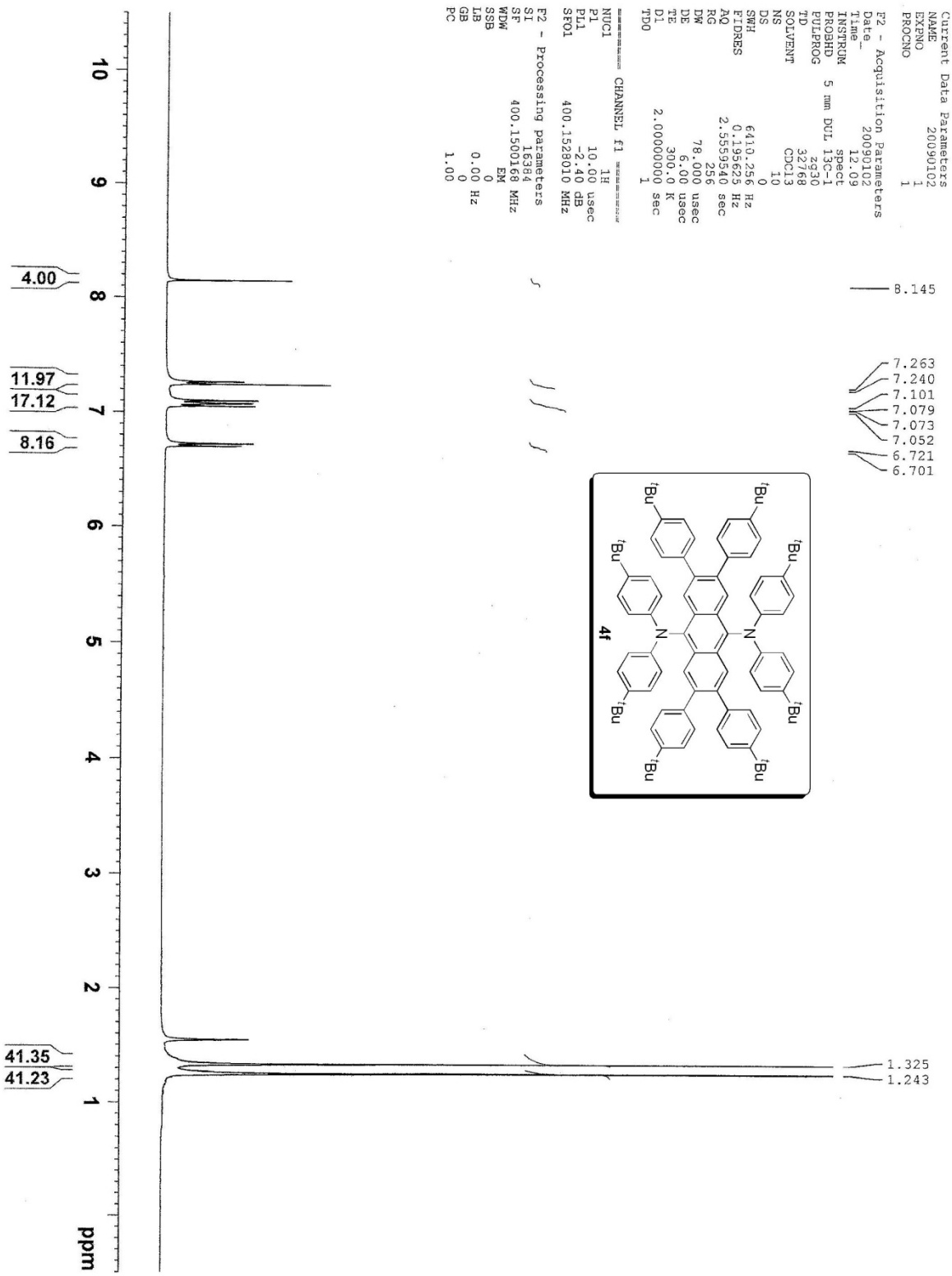

149.64
139.92
138.22
131.98
129.59
129.03
124.69
118.00
104.91
103.55
77.32
77.00
76.68
34.47
31.37
18.94
11.51
ppm
Si(iPr)3
Si(iPr)3
tBu
4c

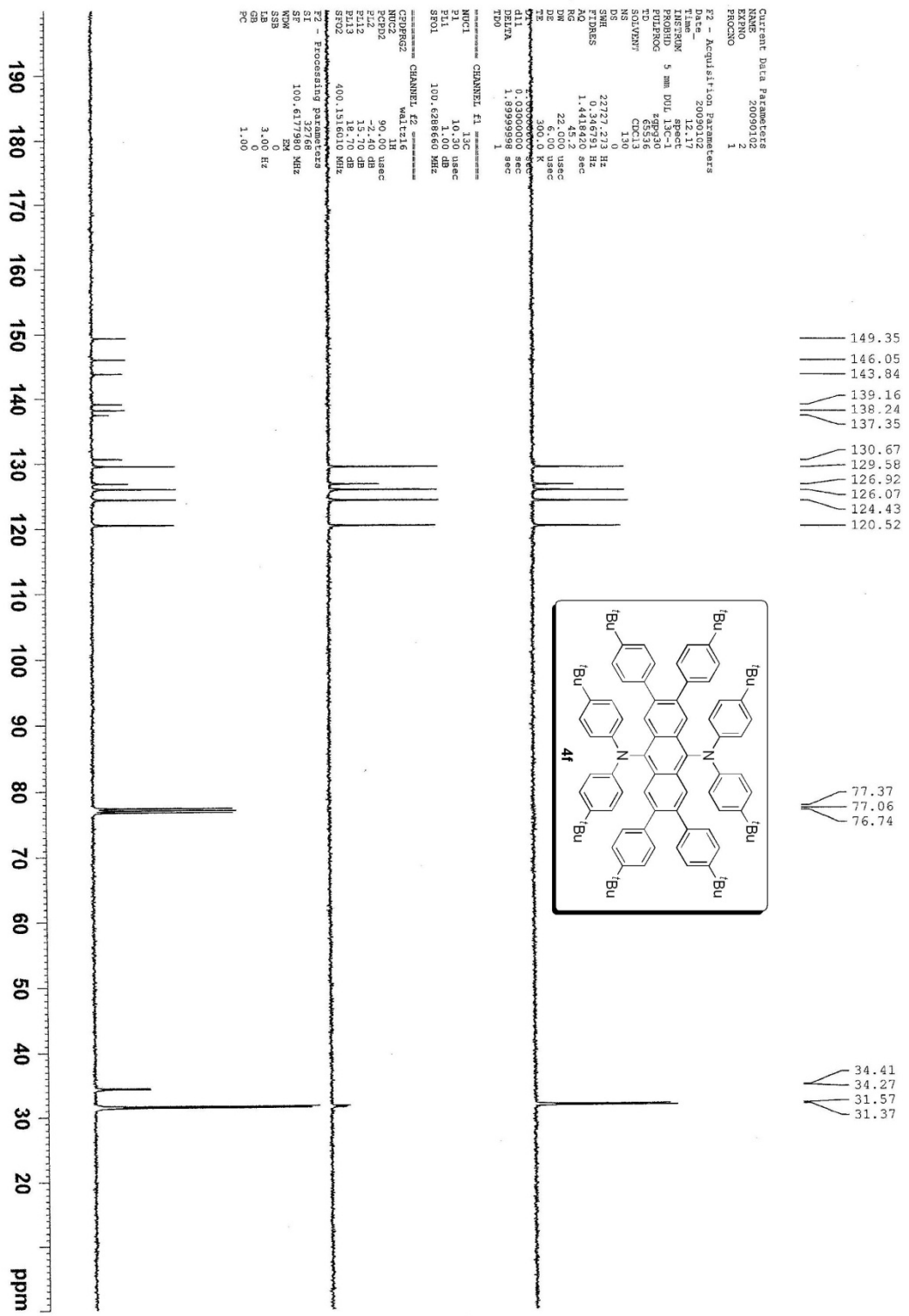

Current Data Parameters
NAME 20090105
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090105
Time_ 22.05
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 15
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 512
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.742
7.556
7.552
7.443
7.439
7.289
7.239
1.543
1.359
1.313
4.00
3.57
2.03
15.92
38.10
32.74
ppm
4d

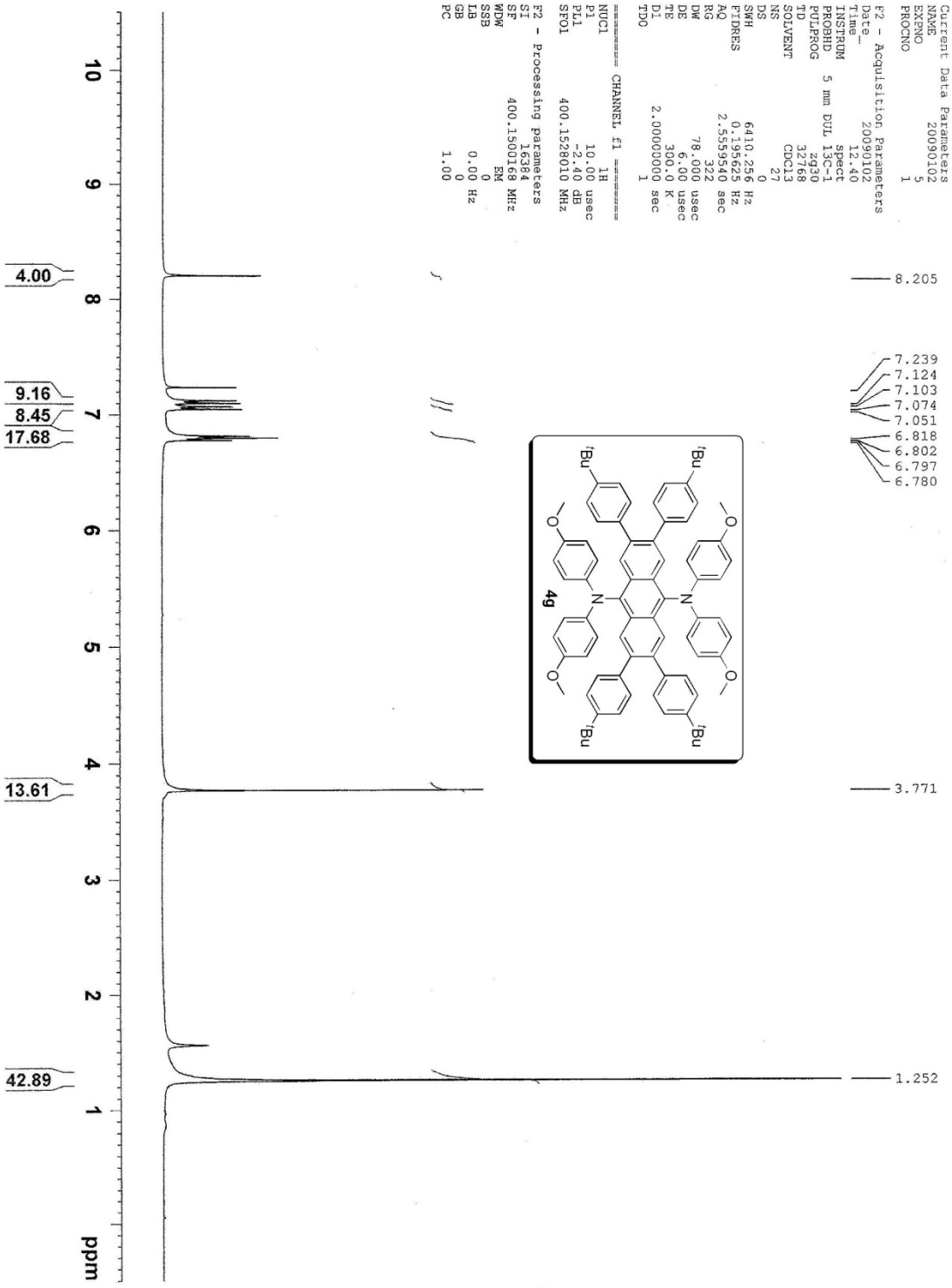

151.00
149.65
140.07
138.55
131.79
129.69
128.84
126.07
124.82
123.15
122.65
118.04
104.09
85.95
77.36
77.05
76.73
34.94
34.51
31.42
4d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

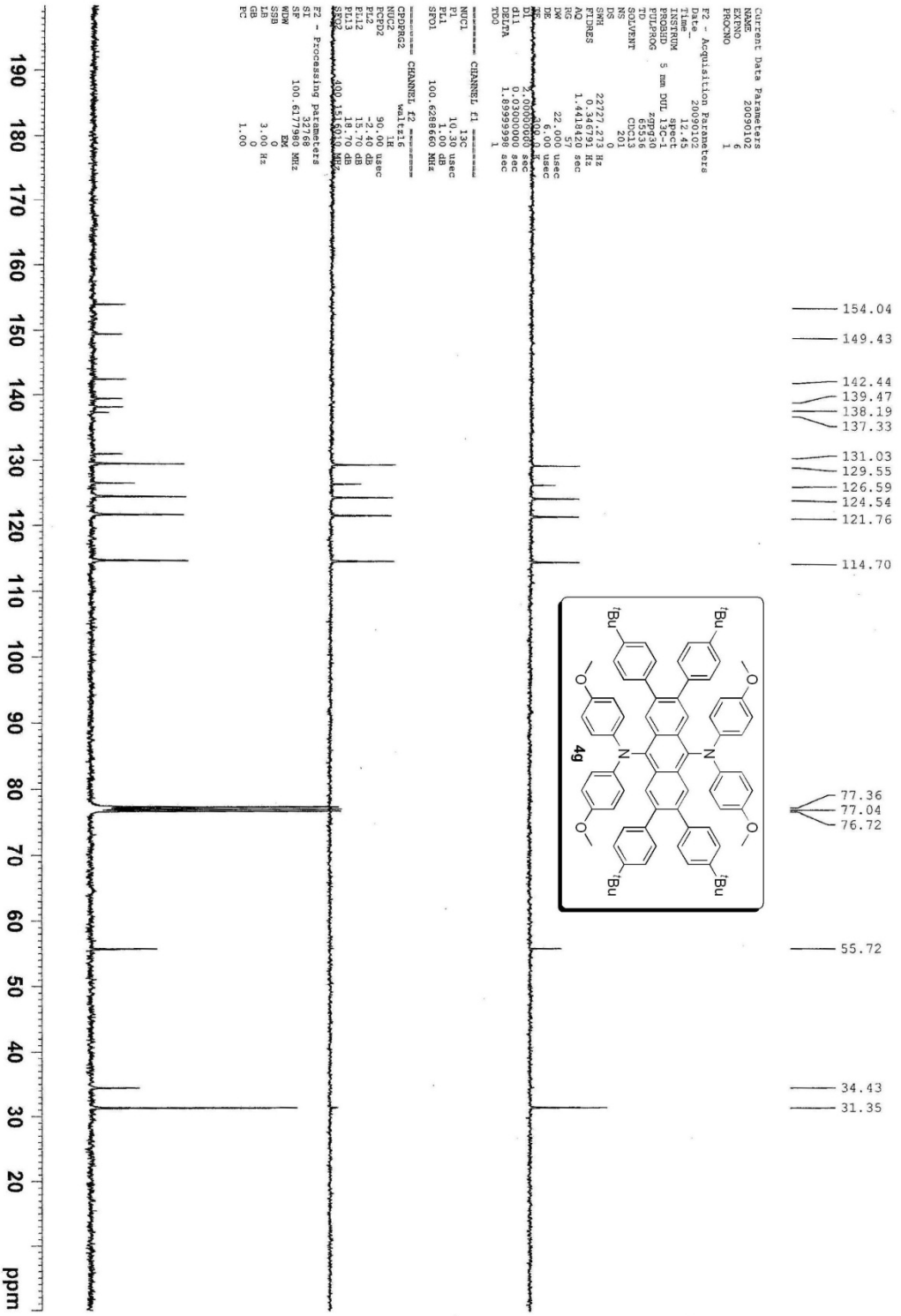

Current Data Parameters
NAME
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080816
Time_ 12.25
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 27
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 228
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500164 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
4.02
11.28
8.41
8.64
4.18
8.00
39.05
8.197
7.262
7.240
7.223
7.183
7.164
7.162
7.110
7.089
6.953
6.779
6.774
6.762
6.758
1.245
tBu
N
4e
ppm


149.48
148.09
139.74
138.08
137.12
130.91
129.52
129.28
126.41
124.51
121.36
120.86
77.32
77.00
76.69
34.40
31.31
4e
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


Current Data Parameters
NAME 20090102
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090102
Time 12.09
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 256
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.145
7.263
7.240
7.101
7.079
7.073
7.052
6.721
6.701
1.325
1.243
4.00
11.97
17.12
8.16
41.35
41.23
4f
tBu
N
ppm


149.35
146.05
143.84
139.16
138.24
137.35
130.67
129.58
126.92
126.07
124.43
120.52
77.37
77.06
76.74
34.41
34.27
31.57
31.37
4f
ppm


Current Data Parameters
NAME 20090102
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090102
Time 12.40
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 27
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 322
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528610 MHz
F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.205
7.239
7.124
7.103
7.074
7.051
6.818
6.802
6.797
6.780
3.771
1.252
4.00
9.16
8.45
17.68
13.61
42.89
4g
ppm


154.04
149.43
142.44
139.47
138.19
137.33
131.03
129.55
126.59
124.54
121.76
114.70
77.36
77.04
76.72
55.72
34.43
31.35
4g
tBu
O
N
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm