Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

New efficient fused-ring spiro[benzoanthracene-fluorene] dopant materials for blue fluorescent organic light-emitting diodes

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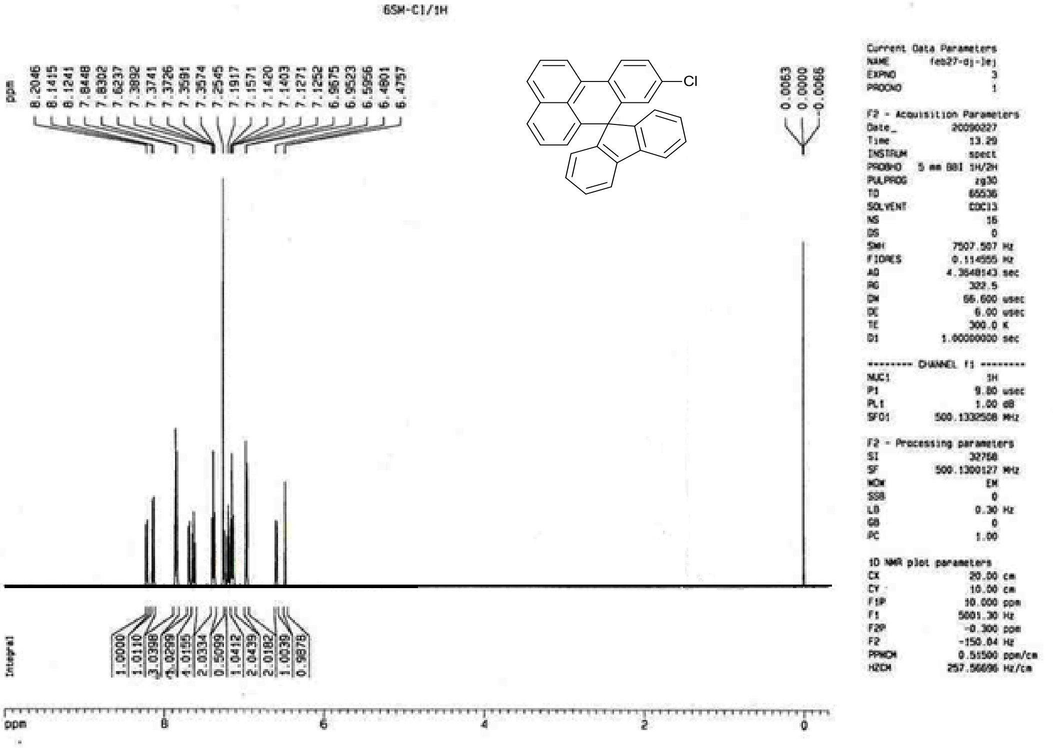
Following is the description of analytical instruments we used for structure characterization. It may be inserted somewhere in the main manuscript or supplementary. The ^1H and ^{13}C nuclear magnetic resonance (NMR) spectra were taken on a Bruker, Avance 600 nuclear magnetic resonance spectroscope (NMR, 600 MHz). Energy levels were measured with a low-energy photo-electron spectrometer (AC-2; Riken-Keiki, Union City, CA, USA). High resolution mass spectra were recorded using an HP 6890 (Brea, CA, USA) and Agilent Technologies 5975C MSD in FAB mode (Palo Alto, CA, USA).



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PROCNO                   1

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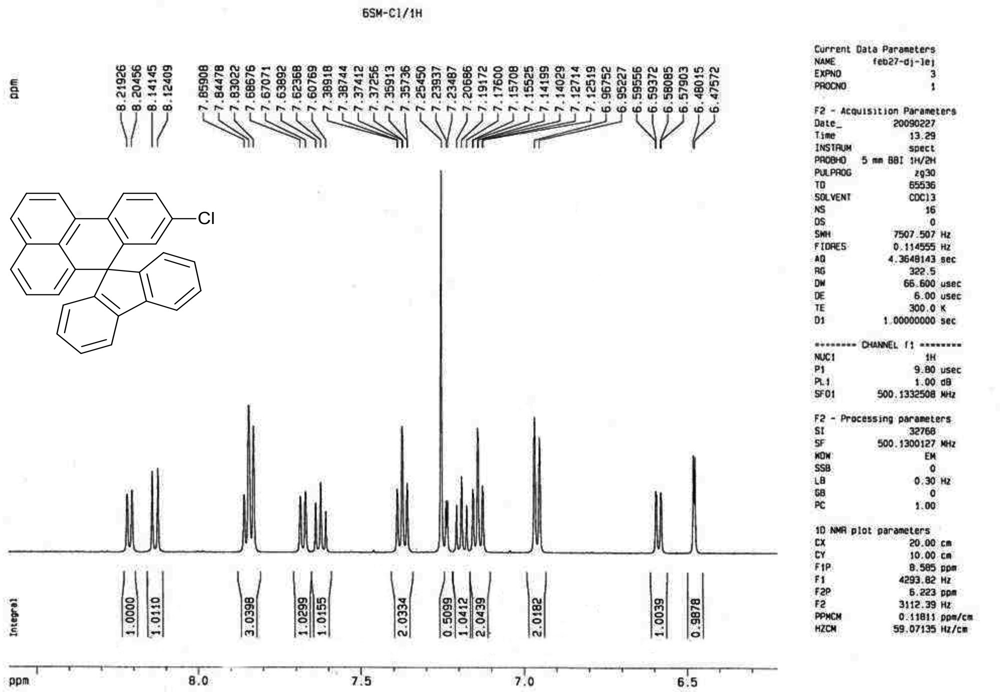
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       0
SWH               7507.507 Hz
FIDRES            0.114555 Hz
AQ               4.3648143 sec
RG                   322.5
DW                  66.600 usec
DE                    6.00 usec
TE                   300.0 K
D1              1.00000000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                    9.80 usec
PL1                   1.00 dB
SFO1           500.1332508 MHz

F2 - Processing parameters
SI                   32768
SF             500.1300127 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00

1D NMR plot parameters
CX                   20.00 cm
CY                   10.00 cm
F1P                 10.000 ppm
F1                 5001.30 Hz
F2P                 -0.300 ppm
F2                 -150.04 Hz
PPMCM              0.51500 ppm/cm
HZCM             257.56696 Hz/cm
```

Figure S1. ^{1}H NMR spectrum of CSBAF.



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Current Data Parameters
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EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
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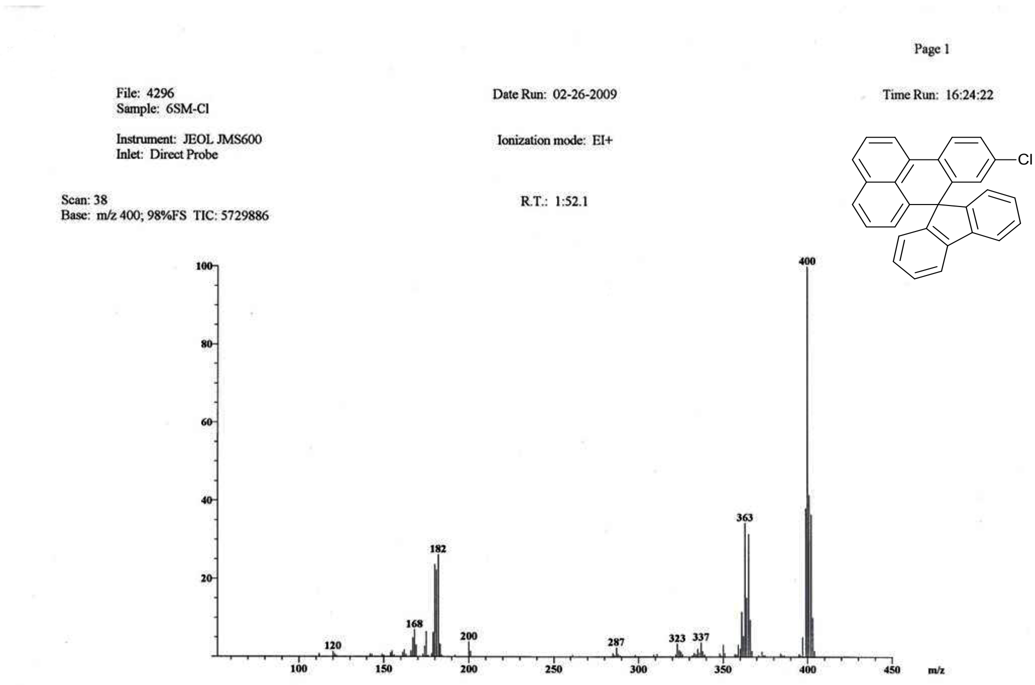
Time                 13.29
INSTRUM              spect
PROBHD    5 mm BBI 1H/2H
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       0
SWH               7507.507 Hz
FIDRES            0.114555 Hz
AQ               4.3648143 sec
RG                   322.5
DW                  66.600 usec
DE                    6.00 usec
TE                   300.0 K
D1              1.00000000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                    9.80 usec
PL1                   1.00 dB
SFO1           500.1332508 MHz

F2 - Processing parameters
SI                   32768
SF             500.1300127 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00

1D NMR plot parameters
CX                   20.00 cm
CY                   10.00 cm
F1P                  8.585 ppm
F1                 4293.82 Hz
F2P                  6.223 ppm
F2                 3112.39 Hz
PPMCM              0.11811 ppm/cm
HZCM              59.07135 Hz/cm
```

Figure S1-1. Enlarged ^{1}H NMR spectrum of CSBAF in the 6.0-8.5 ppm range.



Page 1

File: 4296
Sample: 6SM-Cl

Date Run: 02-26-2009

Time Run: 16:24:22

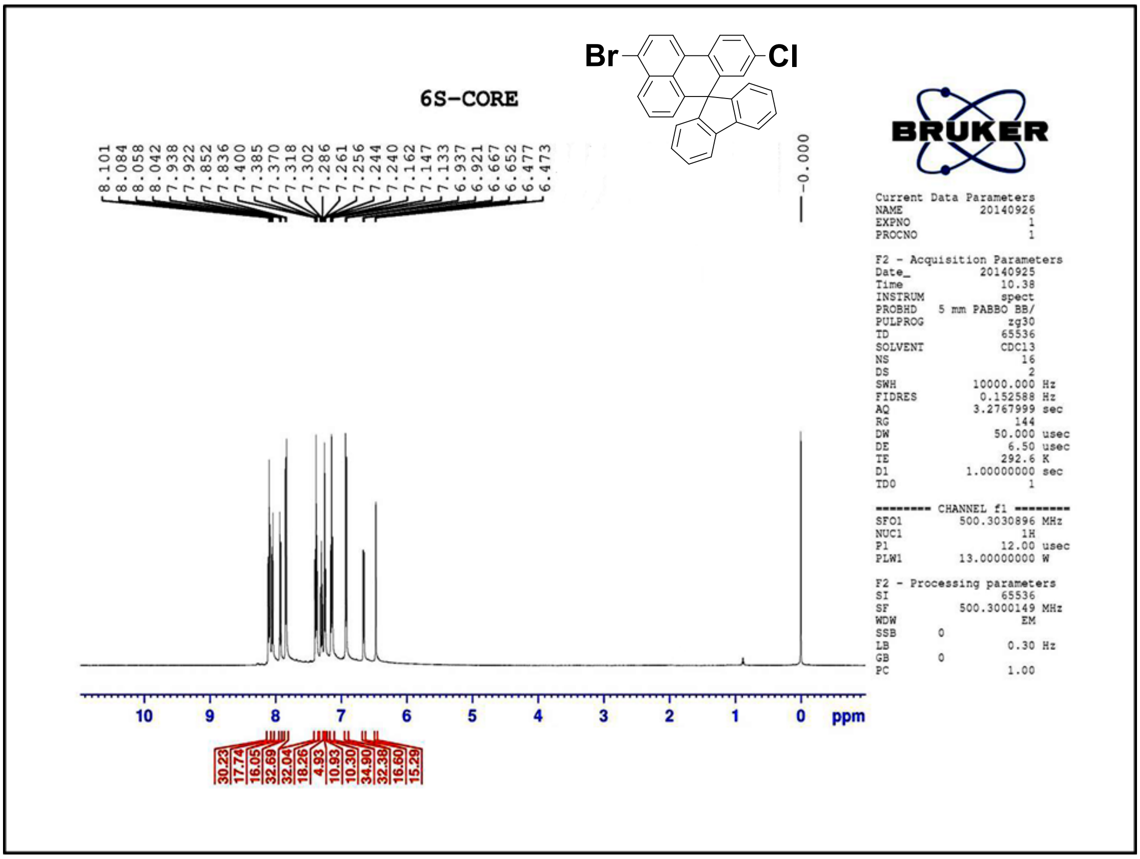
Instrument: JEOL JMS600
Inlet: Direct Probe

Ionization mode: EI+

Scan: 38
Base: m/z 400; 98%FS TIC: 5729886

R.T.: 1:52.1

Figure S2. Mass spectrum of CSBAF.



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NAME            20140926
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140925
Time               10.38
INSTRUM            spect
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PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES          0.152588 Hz
AQ             3.2767999 sec
RG                   144
DW                50.000 usec
DE                  6.50 usec
TE                 292.6 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.3030896 MHz
NUC1                  1H
P1                 12.00 usec
PLW1         13.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.3000149 MHz
WDW                   EM
SSB      0
LB                  0.30 Hz
GB       0
PC                  1.00
```

Figure S3. ^{1}H NMR spectrum of CBSBAF.

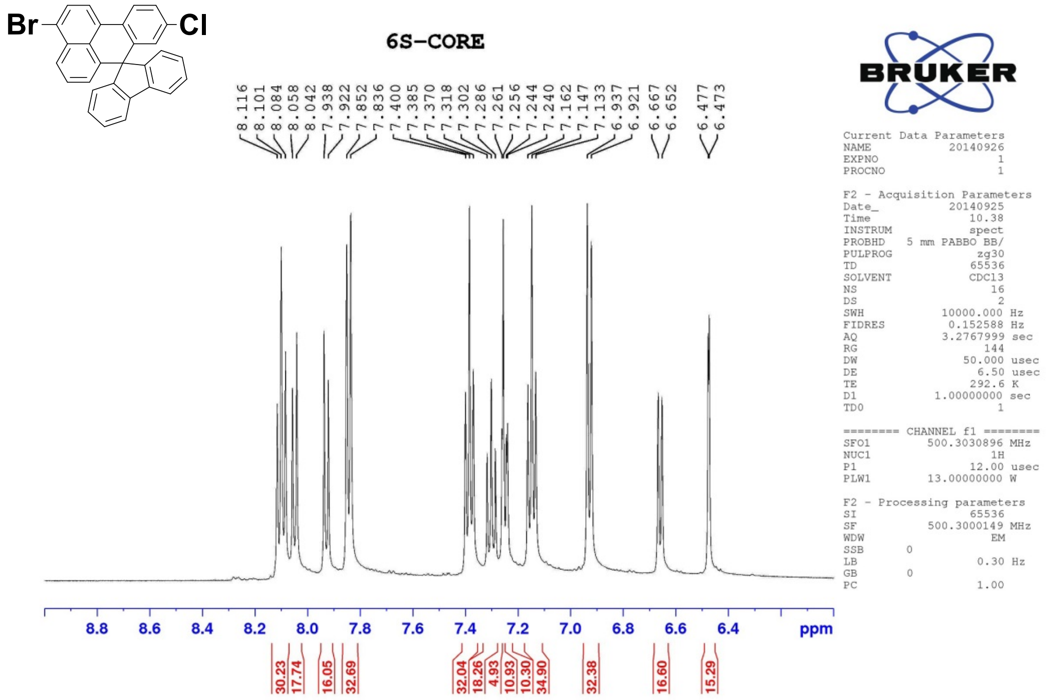
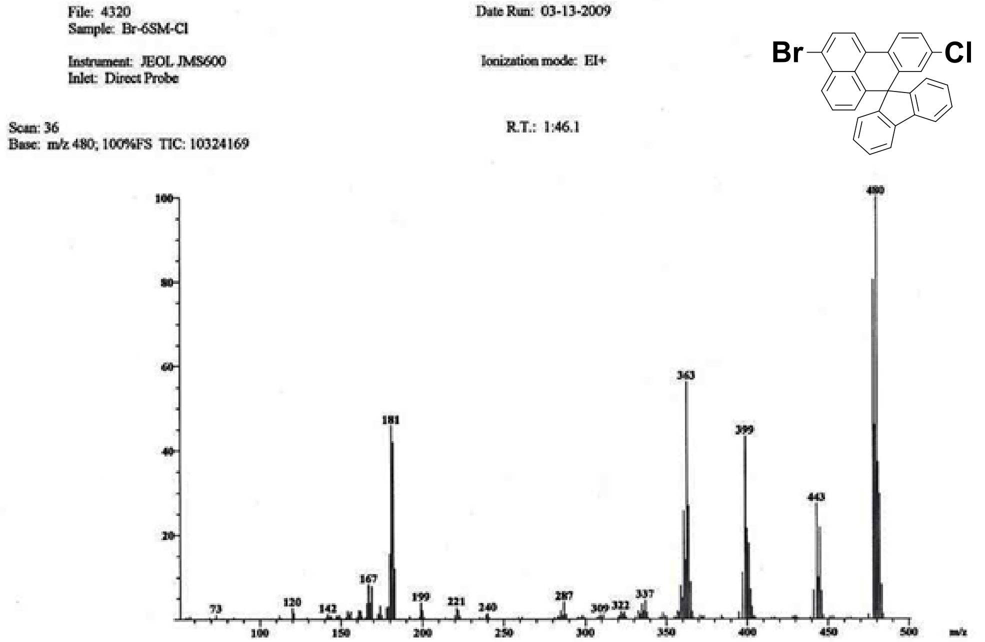


Figure S3-1. Enlarged ^{1}H NMR spectrum of CBSBAF in the 6.0-8.5 ppm range.



File: 4320
Sample: Br-6SM-Cl

Instrument: JEOL JMS600
Inlet: Direct Probe

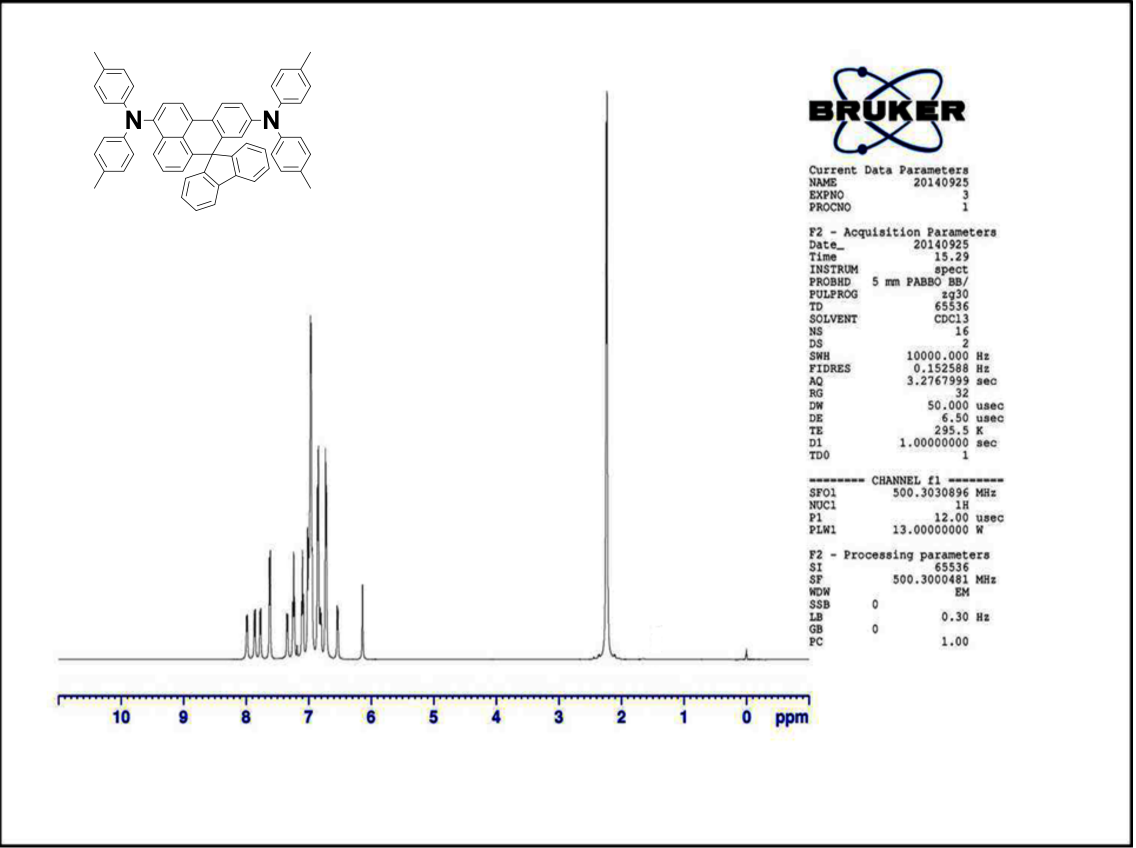
Scan: 36
Base: m/z 480; 100%FS TIC: 10324169

Date Run: 03-13-2009

Ionization mode: EI+

R.T.: 1:46.1

Figure S4. Mass spectrum of CBSBAF .



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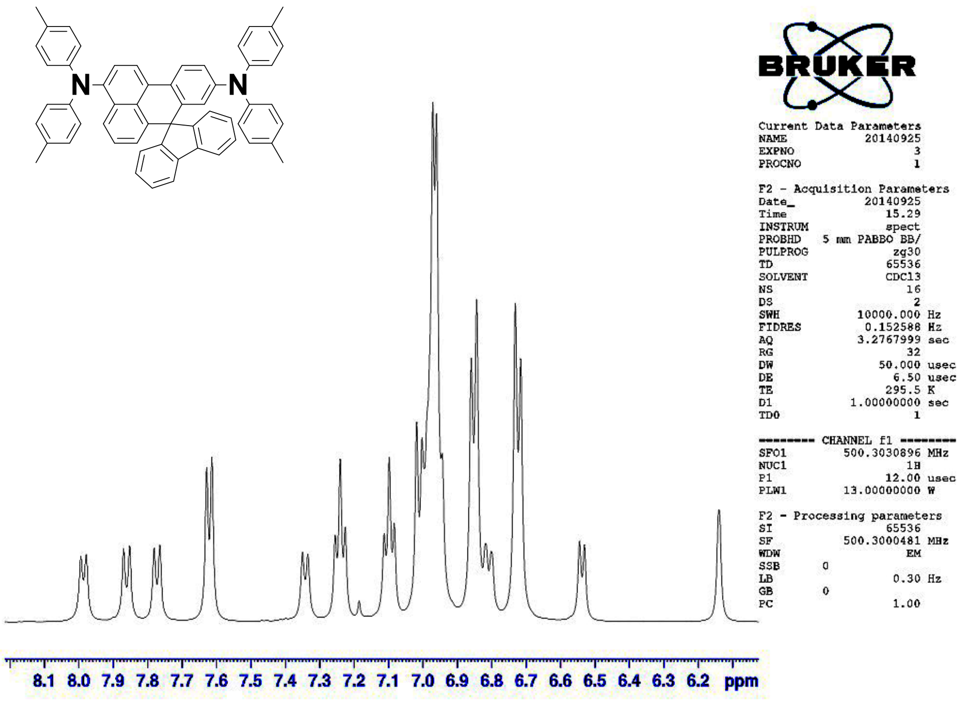
Current Data Parameters
NAME              20140925
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_             20140925
Time                 15.29
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH              10000.000 Hz
FIDRES            0.152588 Hz
AQ               3.2767999 sec
RG                      32
DW                  50.000 usec
DE                    6.50 usec
TE                   295.5 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           500.3030896 MHz
NUC1                    1H
P1                   12.00 usec
PLW1           13.00000000 W

F2 - Processing parameters
SI                   65536
SF             500.3000481 MHz
WDW                     EM
SSB      0
LB                    0.30 Hz
GB       0
PC                    1.00
```

Figure S5. ^{1}H NMR spectrum of DTSBAF.



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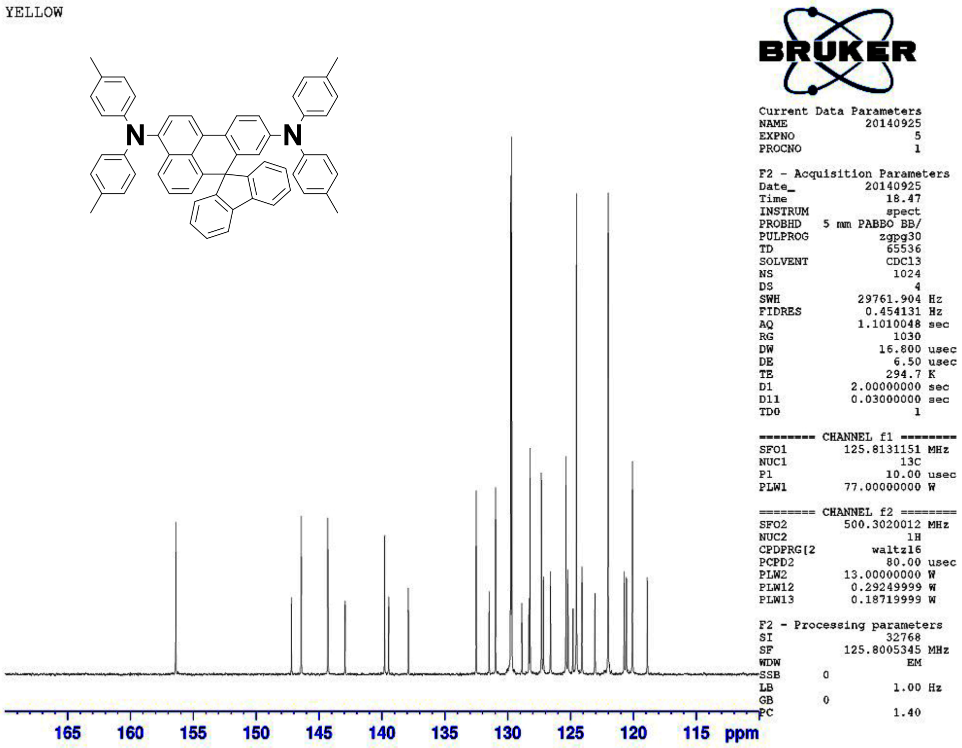
Current Data Parameters
NAME             20140925
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140925
Time                15.29
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             10000.000 Hz
FIDRES           0.152588 Hz
AQ              3.2767999 sec
RG                     32
DW                 50.000 usec
DE                   6.50 usec
TE                  295.5 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          500.3030896 MHz
NUC1                   1H
P1                  12.00 usec
PLW1          13.00000000 W

F2 - Processing parameters
SI                  65536
SF            500.3000481 MHz
WDW                    EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

Figure S5-1. Enlarged ^{1}H NMR spectrum of DTSBAF in the 6.0-8.5 ppm range.



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Current Data Parameters
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EXPNO                      5
PROCNO                     1

F2 - Acquisition Parameters
Date_               20140925
Time                   18.47
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH               29761.904 Hz
FIDRES             0.454131 Hz
AQ                1.1010048 sec
RG                      1030
DW                    16.800 usec
DE                      6.50 usec
TE                     294.7 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             125.8131151 MHz
NUC1                     13C
P1                     10.00 usec
PLW1             77.00000000 W

======== CHANNEL f2 ========
SFO2             500.3020012 MHz
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                  80.00 usec
PLW2             13.00000000 W
PLW12             0.29249999 W
PLW13             0.18719999 W

F2 - Processing parameters
SI                     32768
SF               125.8005345 MHz
WDW                       EM
SSB        0
LB                      1.00 Hz
GB         0
PC                      1.40
```

Figure S6. ^{13}C NMR spectrum of DTSBAF.

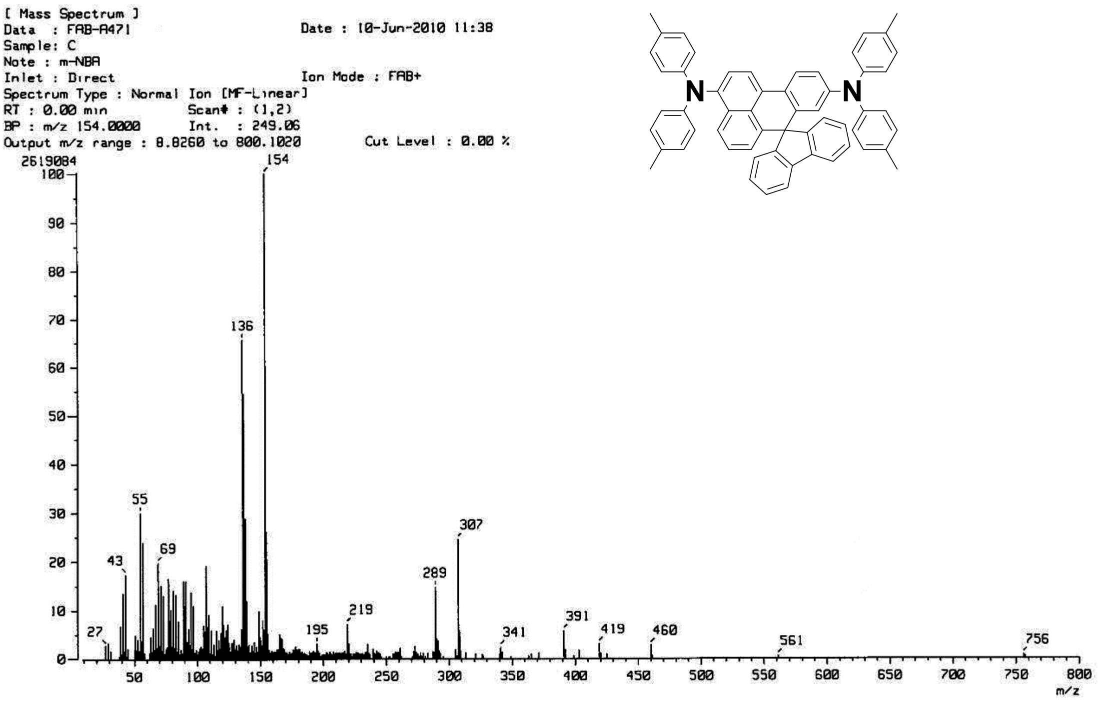
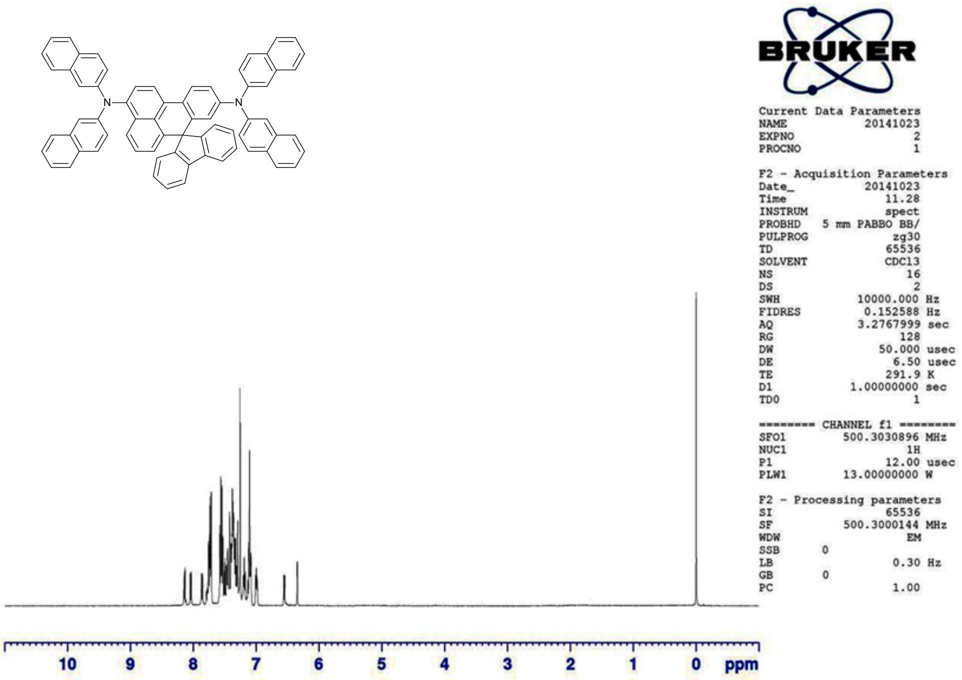

[Mass Spectrum]
Data : FAB-A471
Date : 10-Jun-2010 11:38
Sample: C
Note : m-NBA
Inlet : Direct
Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.00 min
Scan# : (1,2)
BP : m/z 154.0000
Int. : 249.06
Output m/z range : 8.8260 to 800.1020
Cut Level : 0.00 %

Figure S7. Mass spectrum of DTSBAF .



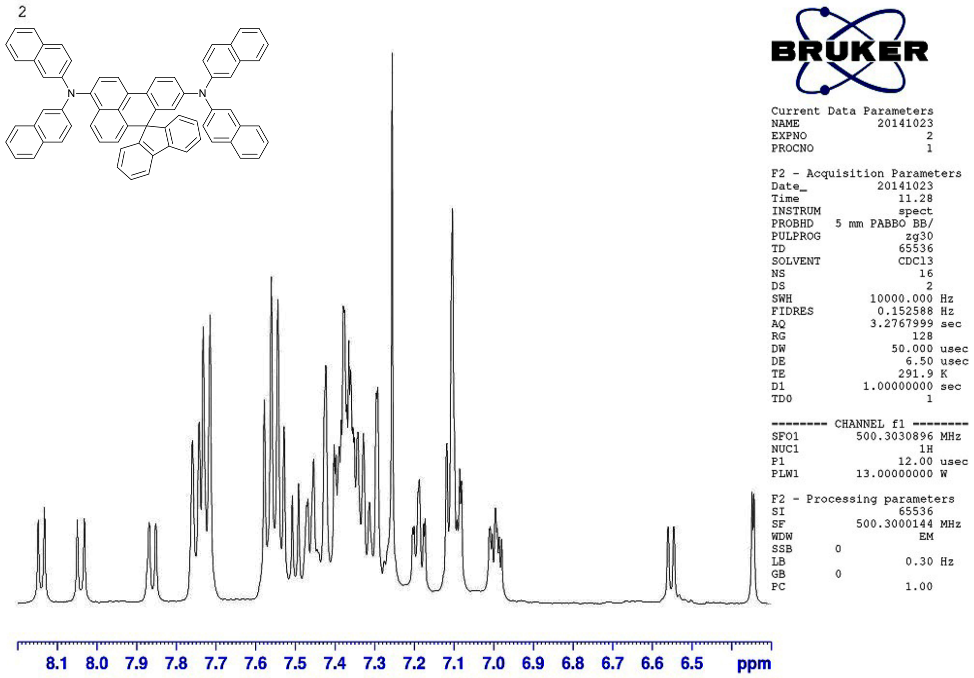
```
Current Data Parameters
NAME             20141023
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20141023
Time                11.28
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             10000.000 Hz
FIDRES           0.152588 Hz
AQ              3.2767999 sec
RG                    128
DW                 50.000 usec
DE                   6.50 usec
TE                  291.9 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          500.3030896 MHz
NUC1                   1H
P1                  12.00 usec
PLW1          13.00000000 W

F2 - Processing parameters
SI                  65536
SF            500.3000144 MHz
WDW                    EM
SSB      0
LB                   0.30 Hz
GB       0
PC                   1.00
```

Figure S8. ^{1}H NMR spectrum of DBSBAF.



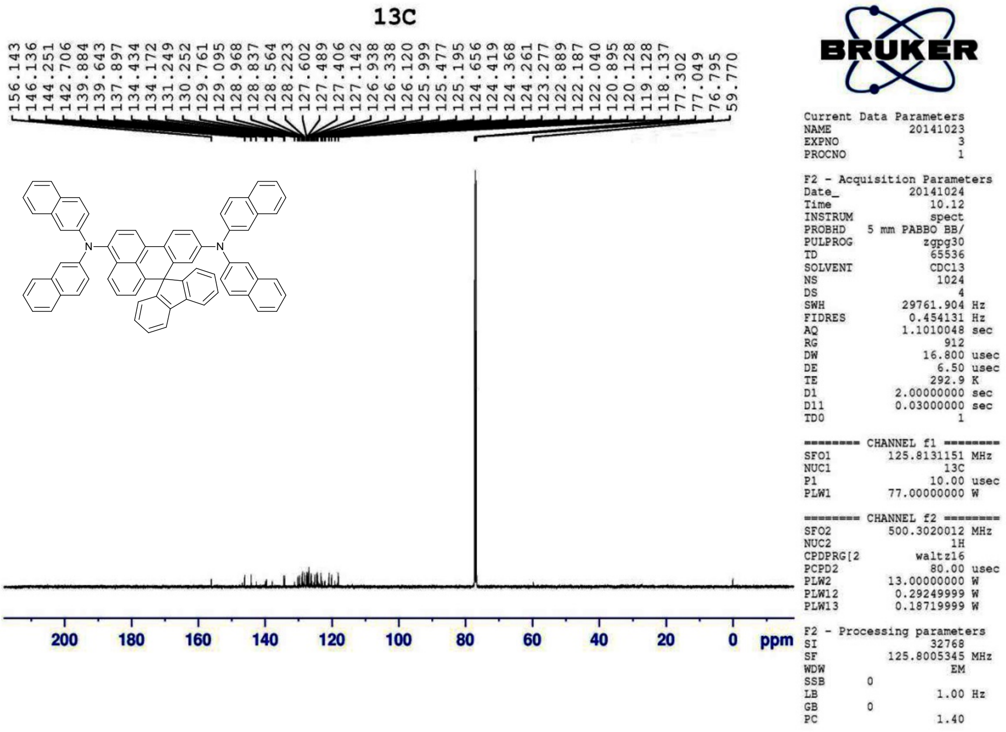
```
Current Data Parameters
NAME             20141023
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20141023
Time                11.28
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ            3.2767999 sec
RG                    128
DW               50.000 usec
DE                 6.50 usec
TE                291.9 K
D1           1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1        500.3030896 MHz
NUC1                   1H
P1                  12.00 usec
PLW1        13.00000000 W

F2 - Processing parameters
SI                  65536
SF          500.3000144 MHz
WDW                    EM
SSB      0
LB                   0.30 Hz
GB       0
PC                   1.00
```

Figure S8-1. Enlarged ^1H NMR spectrum of DBSBAF in the 6.0-8.5 ppm range.



```
Current Data Parameters
NAME               20141023
EXPNO                     3
PROCNO                    1

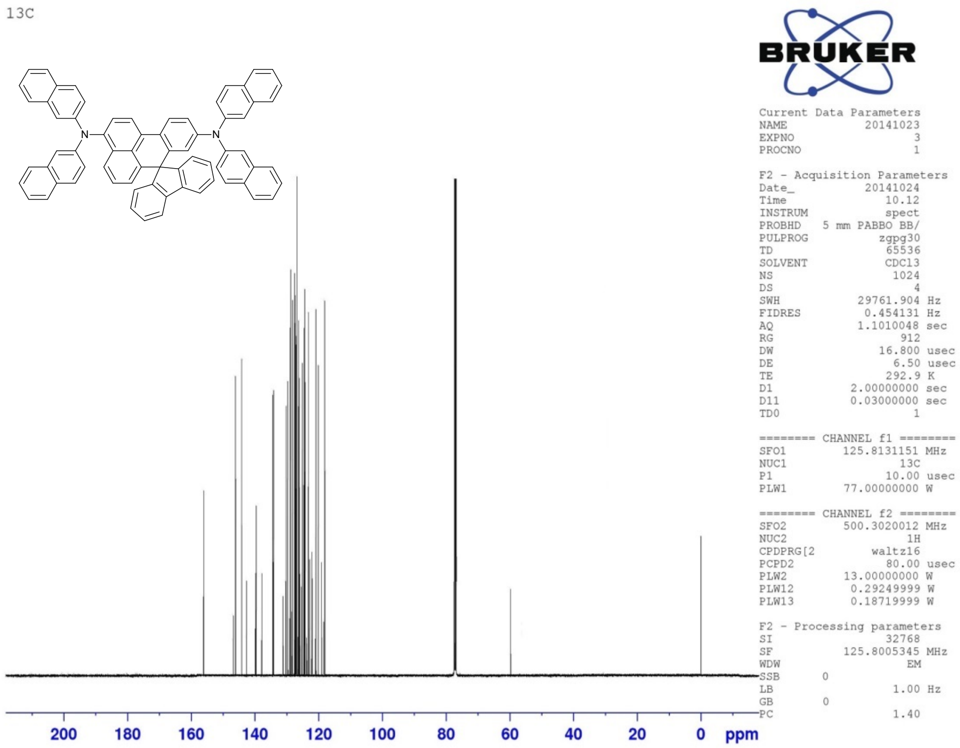
F2 - Acquisition Parameters
Date_              20141024
Time                  10.12
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDC13
NS                     1024
DS                        4
SWH               29761.904 Hz
FIDRES             0.454131 Hz
AQ                1.1010048 sec
RG                      912
DW                   16.800 usec
DE                     6.50 usec
TE                    292.9 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            125.8131151 MHz
NUC1                    13C
P1                    10.00 usec
PLW1            77.00000000 W

======== CHANNEL f2 ========
SFO2            500.3020012 MHz
NUC2                     1H
CPDPRG[2            waltz16
PCPD2                 80.00 usec
PLW2            13.00000000 W
PLW12            0.29249999 W
PLW13            0.18719999 W

F2 - Processing parameters
SI                    32768
SF              125.8005345 MHz
WDW                      EM
SSB      0
LB                     1.00 Hz
GB       0
PC                     1.40
```

Figure S9. ^{13}C NMR spectrum of DBSBAF.



```
Current Data Parameters
NAME             20141023
EXPNO                   3
PROCNO                  1

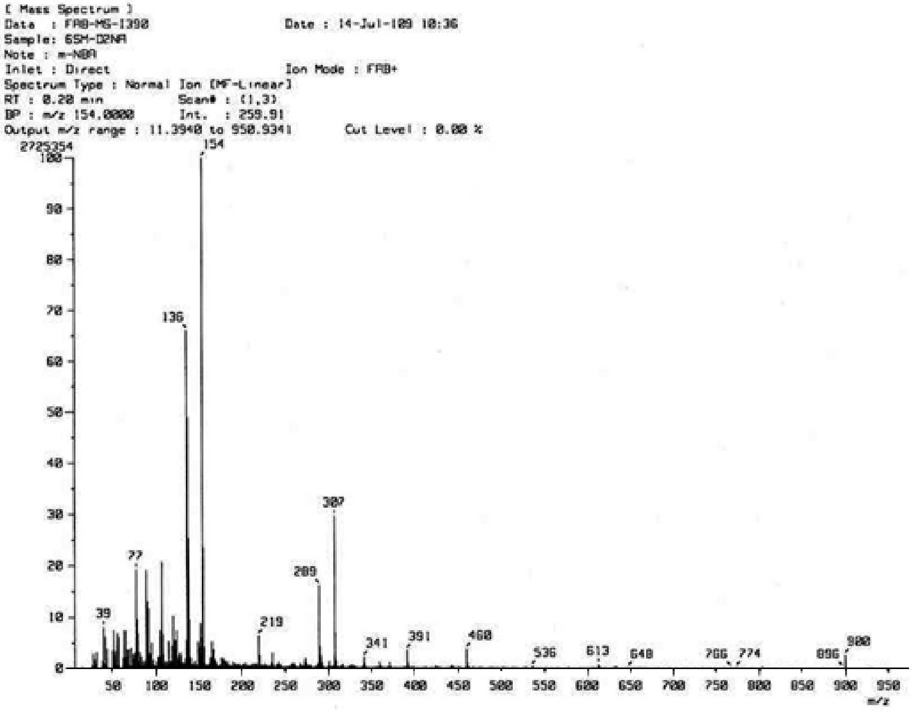
F2 - Acquisition Parameters
Date_            20141024
Time                10.12
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ             1.1010048 sec
RG                   912
DW                16.800 usec
DE                  6.50 usec
TE                 292.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.8131151 MHz
NUC1                 13C
P1                 10.00 usec
PLW1         77.00000000 W

======== CHANNEL f2 ========
SFO2         500.3020012 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         13.00000000 W
PLW12         0.29249999 W
PLW13         0.18719999 W

F2 - Processing parameters
SI                 32768
SF           125.8005345 MHz
WDW                   EM
SSB      0
LB                  1.00 Hz
GB       0
PC                  1.40
```

Figure S9-1. Enlarged ^{13}C NMR spectrum of DBSBAF.



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[ Mass Spectrum ]
Data  : FAB-MS-1390                    Date : 14-Jul-109 10:36
Sample: 6SM-D2NA
Note : m-NBA
Inlet : Direct                         Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.20 min          Scan# : (1,3)
BP : m/z 154.0000      Int.   : 259.91
Output m/z range : 11.3940 to 950.9341        Cut Level : 0.00 %
```

Figure S10. Mass spectrum of DBSBAF .

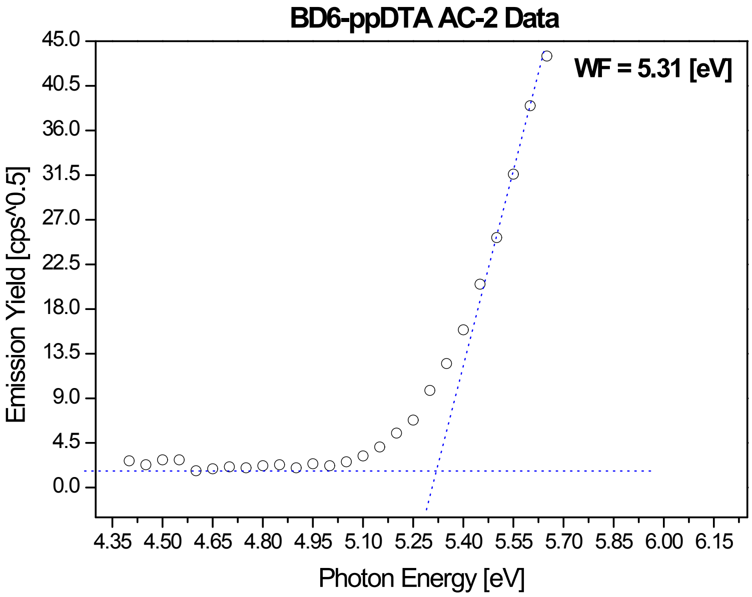

Figure S11. Photoelectron spectrum of DTSBAF by AC2.