Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information

Fluoranthene-based triarylamines as hole-transporting and emitting materials for efficient electroluminescent devices

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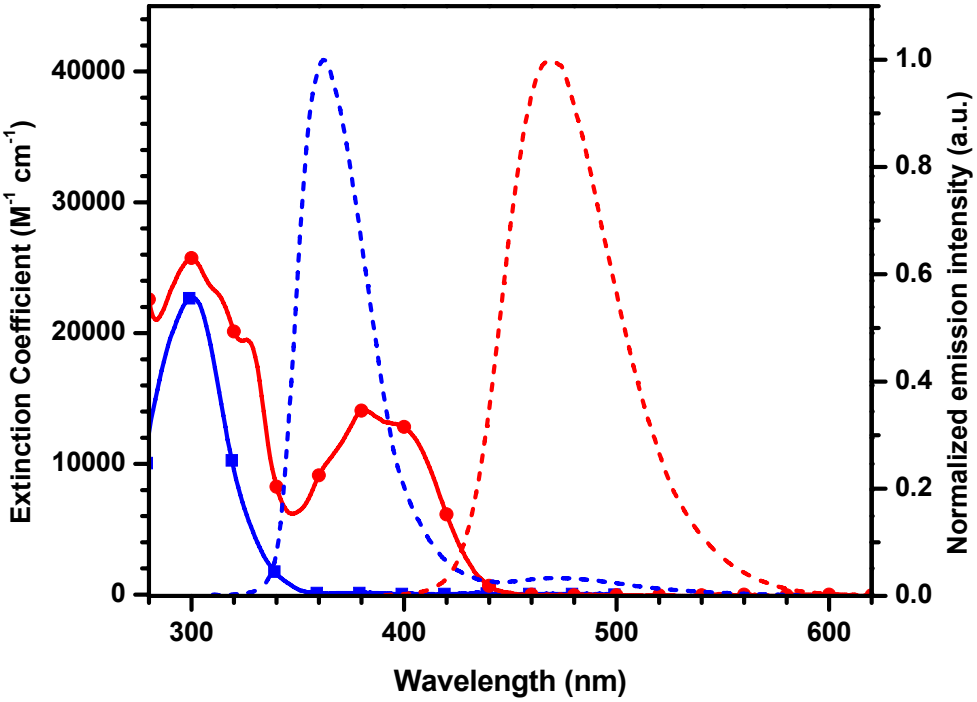


Figure S1. Absorption (solid line) and emission spectra (dashed line) recorded for dichloromethane solutions of triphenylamine (blue) and *N*,*N*-diphenylpyren-1-amine (red).

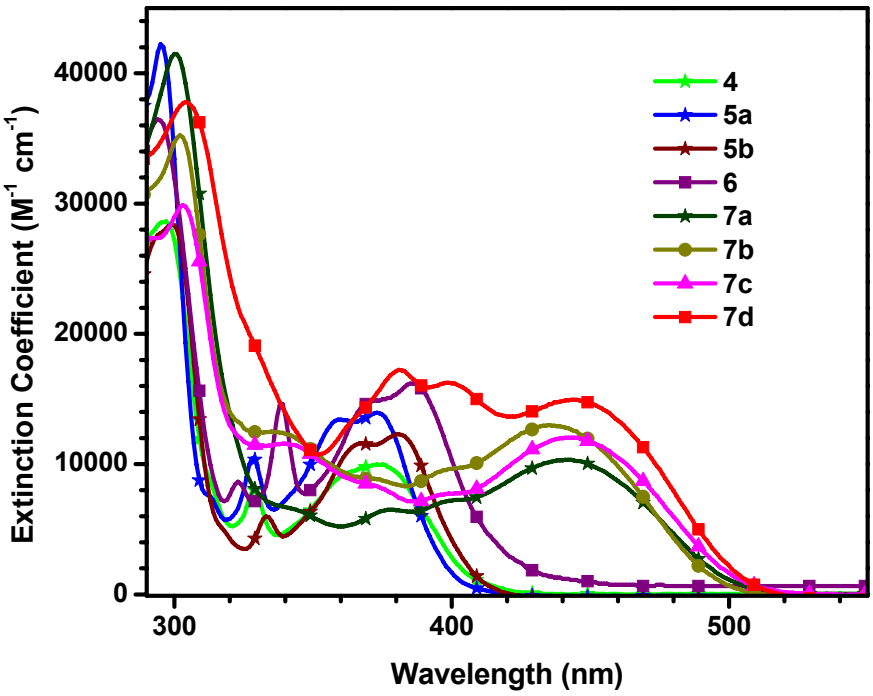


Figure S2. Absorption spectra of the (**4**, **5a, 5b, 6, 7a-7d**) measured for dichloromethane solutions.

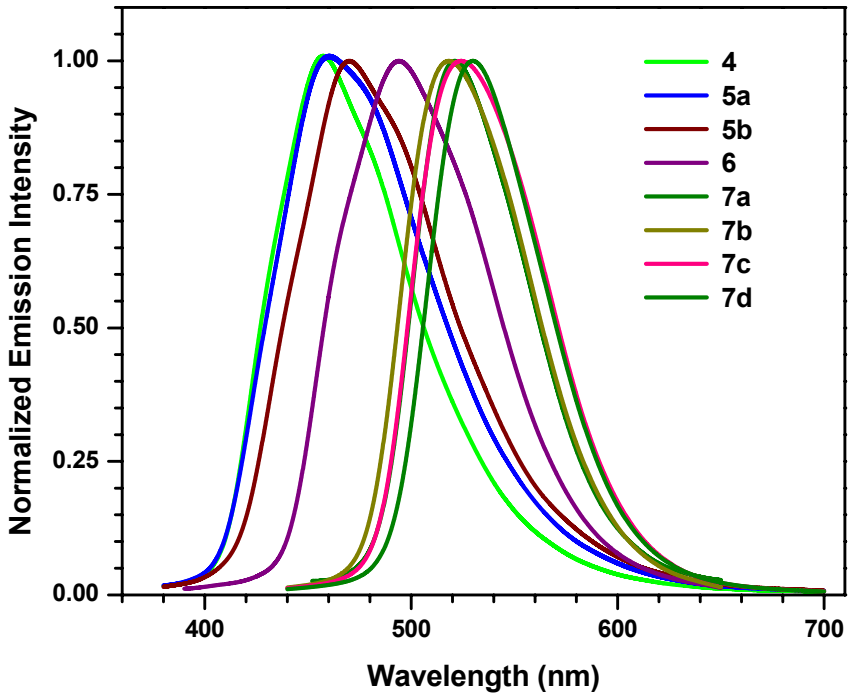
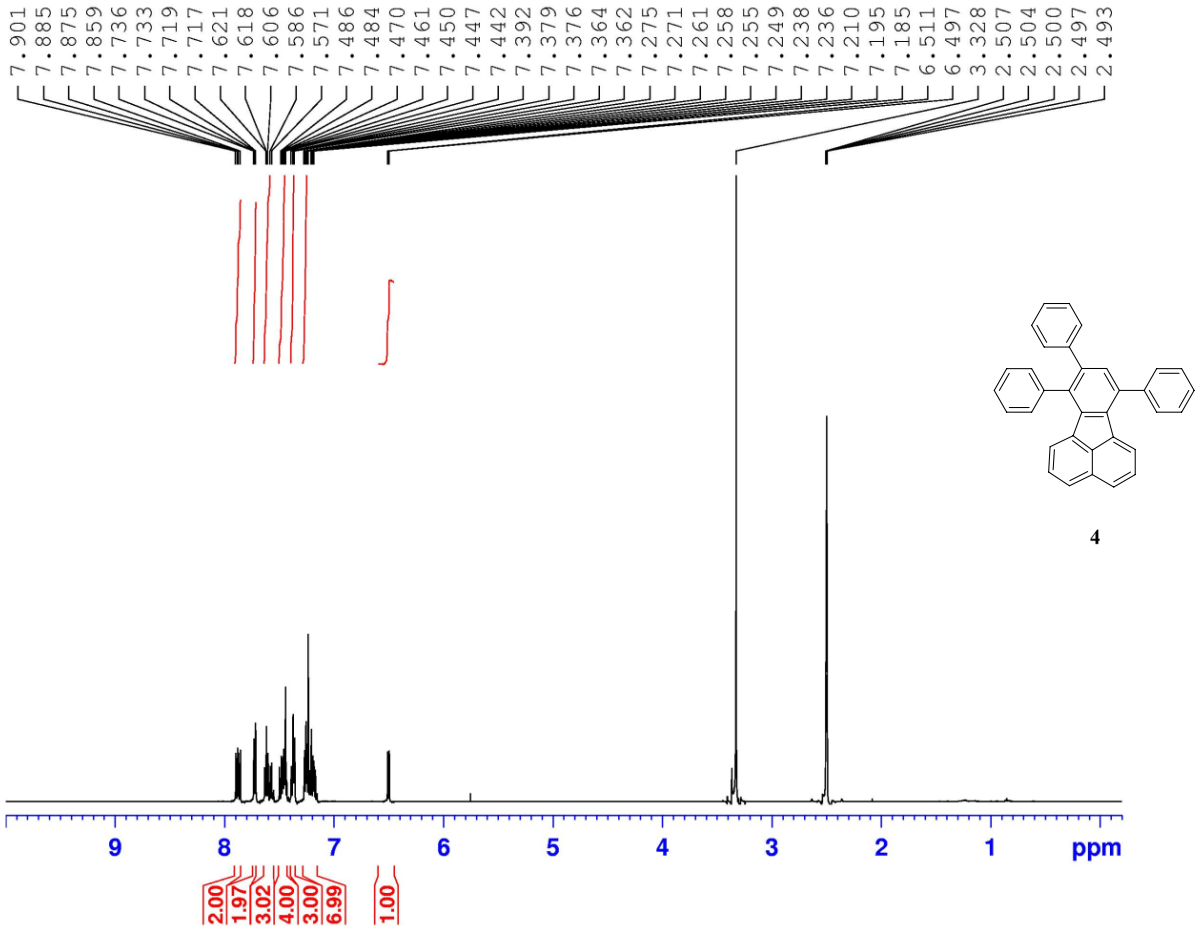


Figure S3. Emission spectra of the compounds (**4**, **5a-b**, **6**, **7a-7d**) measured for toluene solutions.



4

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TD                      65536
SOLVENT                  DMSO
NS                         16
DS                          2
SWH                 10330.578 Hz
FIDRES                0.157632 Hz
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RG                        287
DW                       48.400 usec
DE                        6.00 usec
TE                       298.0 K
D1                    1.00000000 sec
TD0                          1

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F2 - Processing parameters
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SSB                          0
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GB                           0
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Figure S4. ^{1}H NMR of **4**.

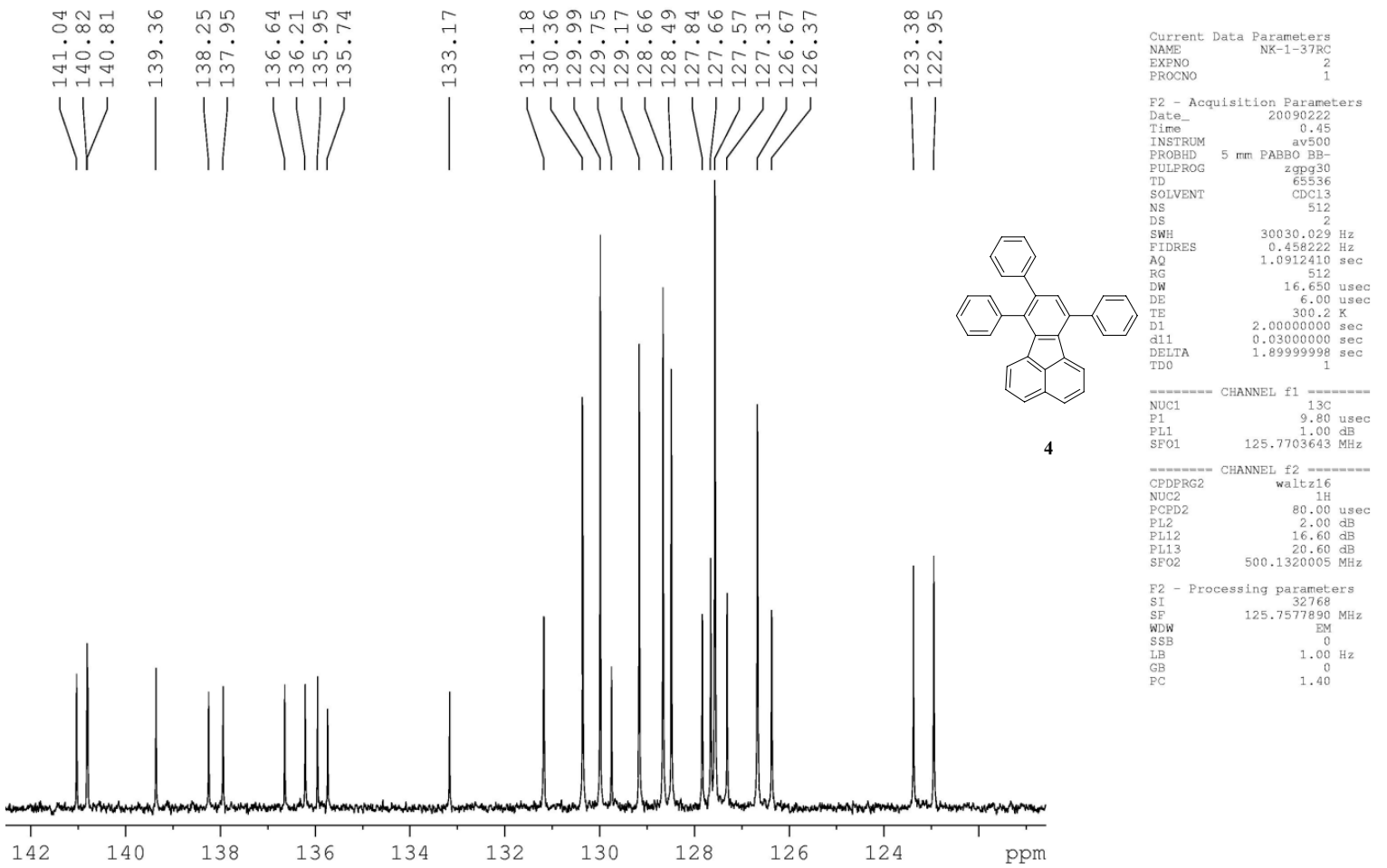
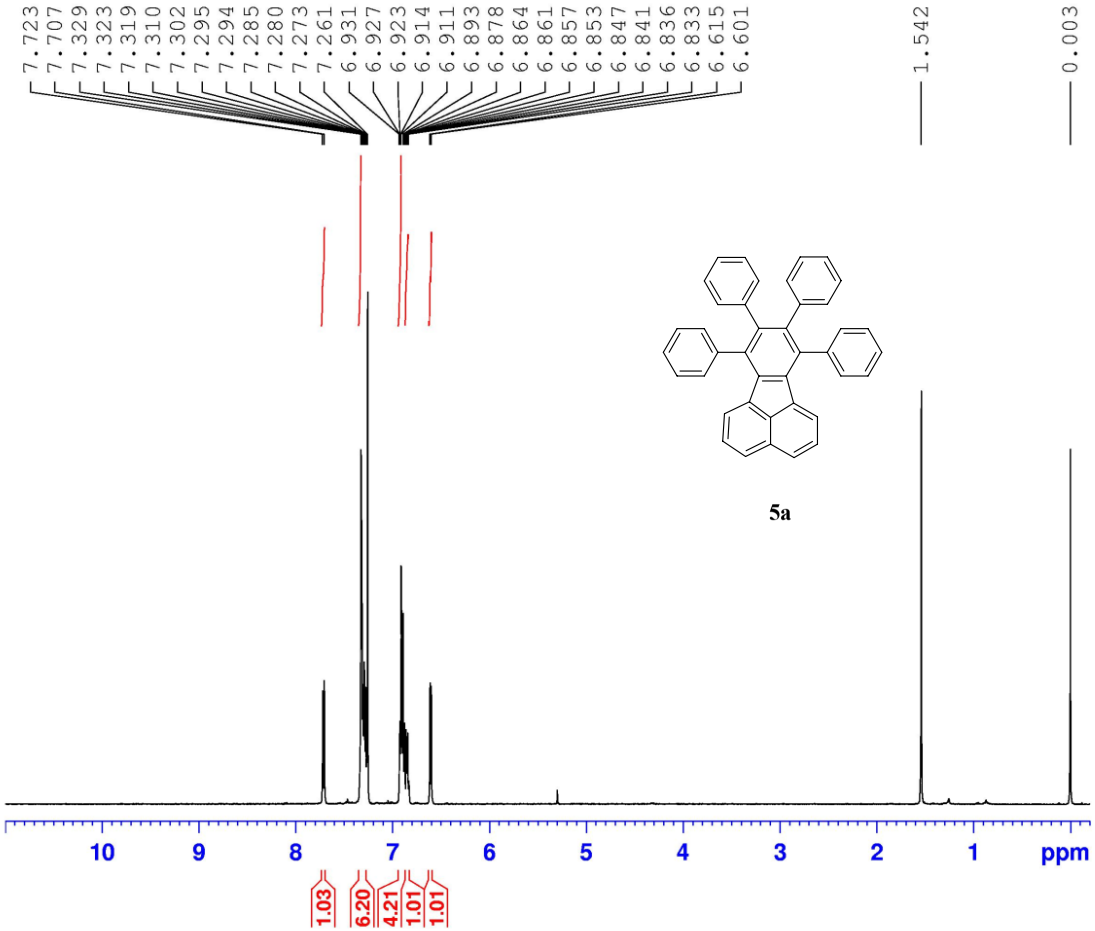


Figure S5. ^{13}C NMR of **4**.

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TD                      65536
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AQ                    3.1720407 sec
RG                         406
DW                      48.400 usec
DE                       6.00 usec
TE                      296.2 K
D1                    1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
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P1                       14.90 usec
PL1                       2.00 dB
SFO1               500.1330885 MHz

F2 - Processing parameters
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SF                 500.1299256 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
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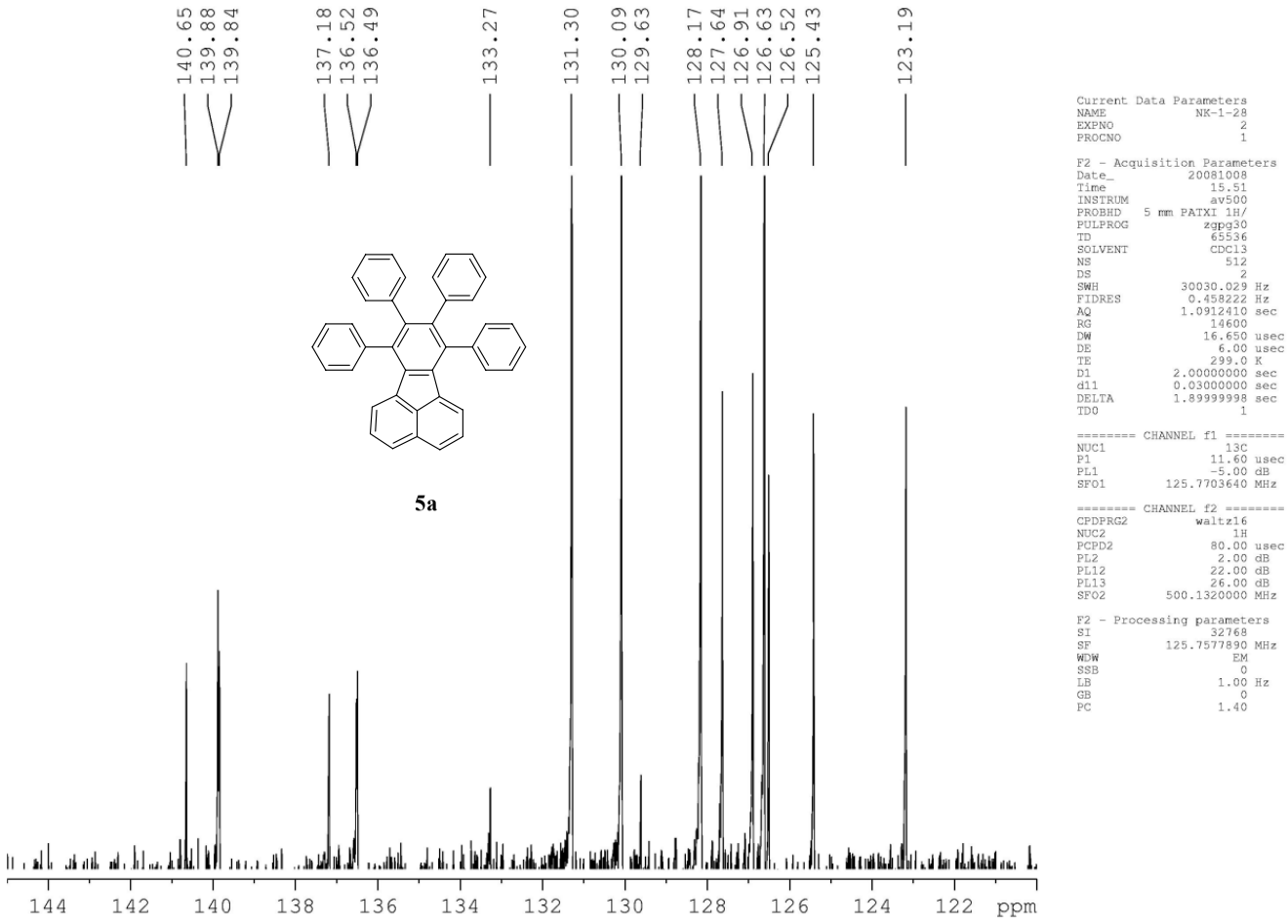
Figure S6. ^{1}H NMR of **5a**.

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TD                      65536
SOLVENT                CDCl3
NS                        512
DS                          2
SWH                30030.029 Hz
FIDRES                0.458222 Hz
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RG                        14600
DW                       16.650 usec
DE                        6.00 usec
TE                       299.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                         1

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P1                      11.60 usec
PL1                     -5.00 dB
SFO1               125.7703640 MHz

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CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                      2.00 dB
PL12                    22.00 dB
PL13                    26.00 dB
SFO2               500.1320000 MHz

F2 - Processing parameters
SI                        32768
SF                 125.7577890 MHz
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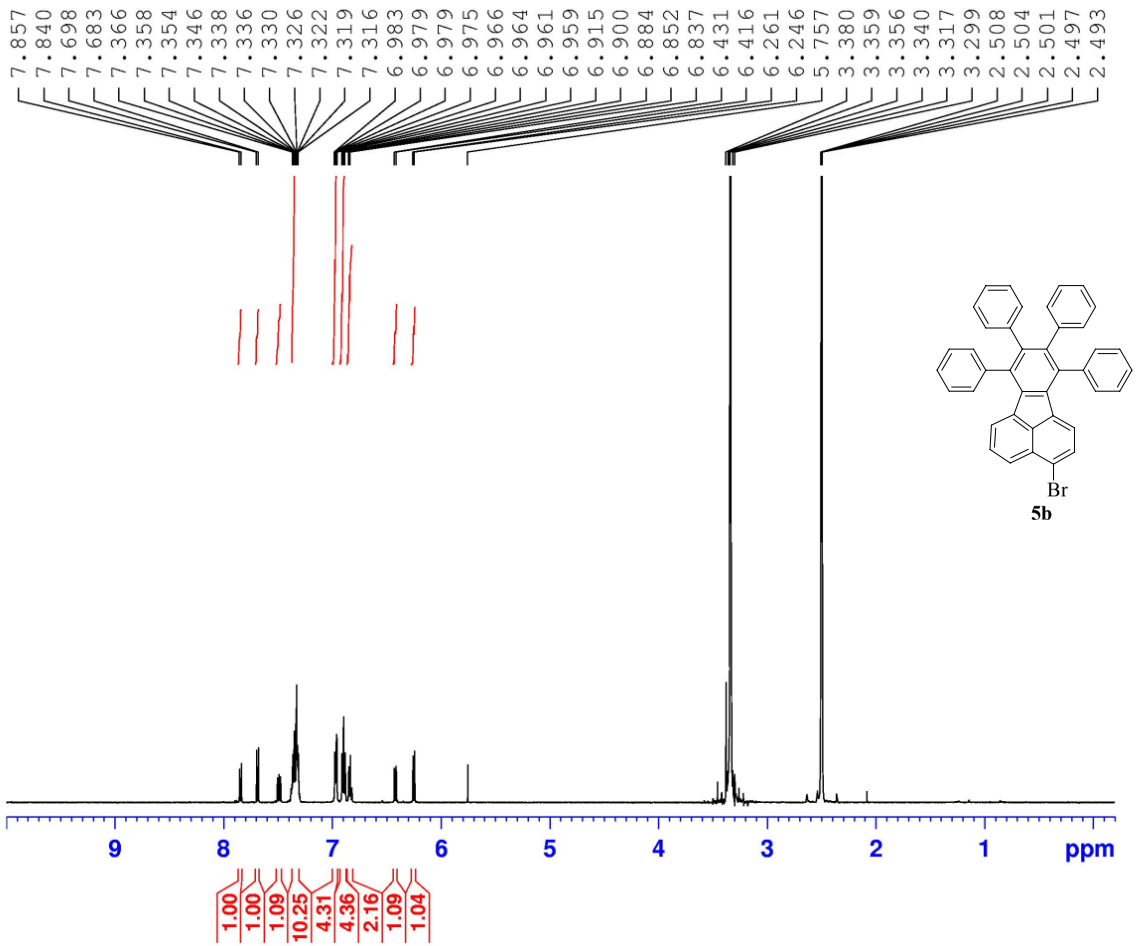
Figure S7. ^{13}C NMR of **5a**.

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PULPROG                   zg30
TD                       65536
SOLVENT                   DMSO
NS                          16
DS                           2
SWH                  10330.578 Hz
FIDRES                0.157632 Hz
AQ                    3.1720407 sec
RG                          456
DW                       48.400 usec
DE                        6.00 usec
TE                       296.4 K
D1                  1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                        7.70 usec
PL1                       2.00 dB
SFO1                500.1330885 MHz

F2 - Processing parameters
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SF                  500.1300051 MHz
WDW                          EM
SSB                           0
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GB                            0
PC                        1.00
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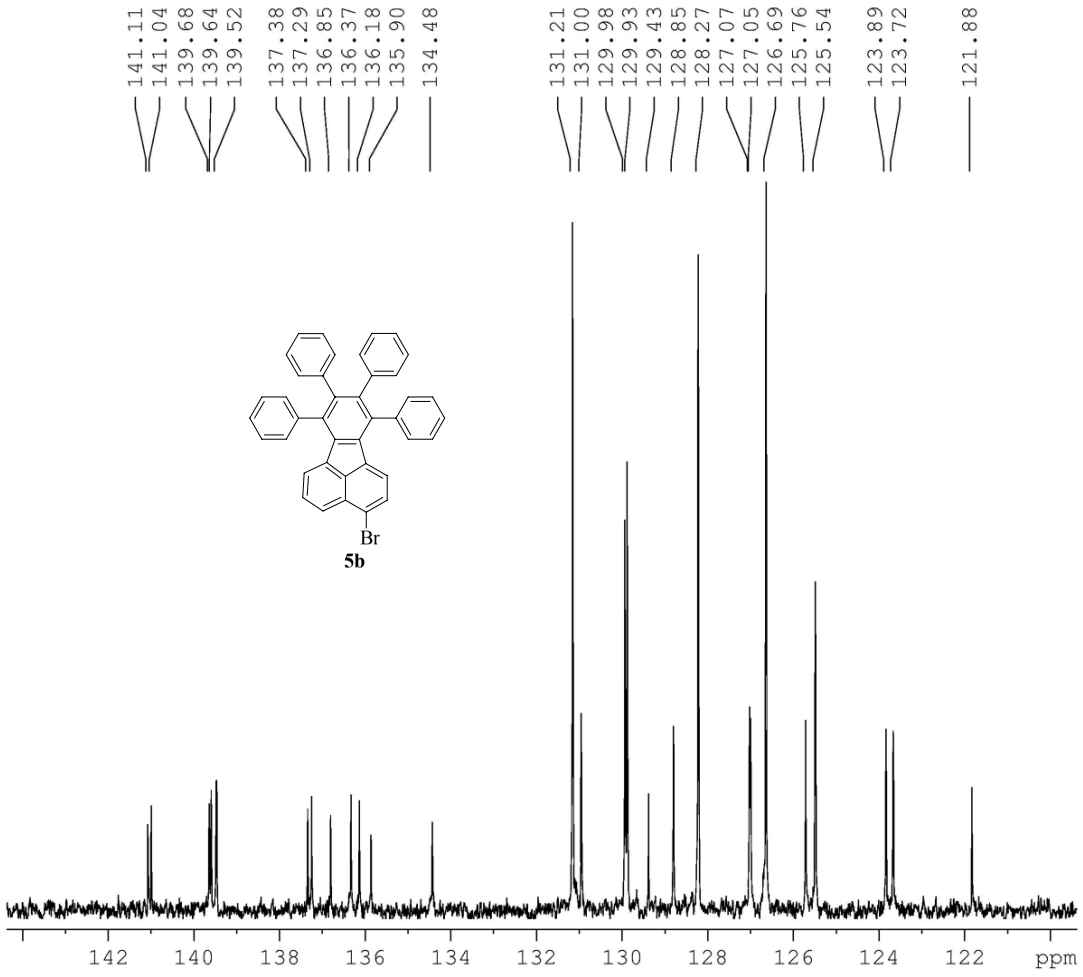
Figure S8. ^{1}H NMR of **5b**.

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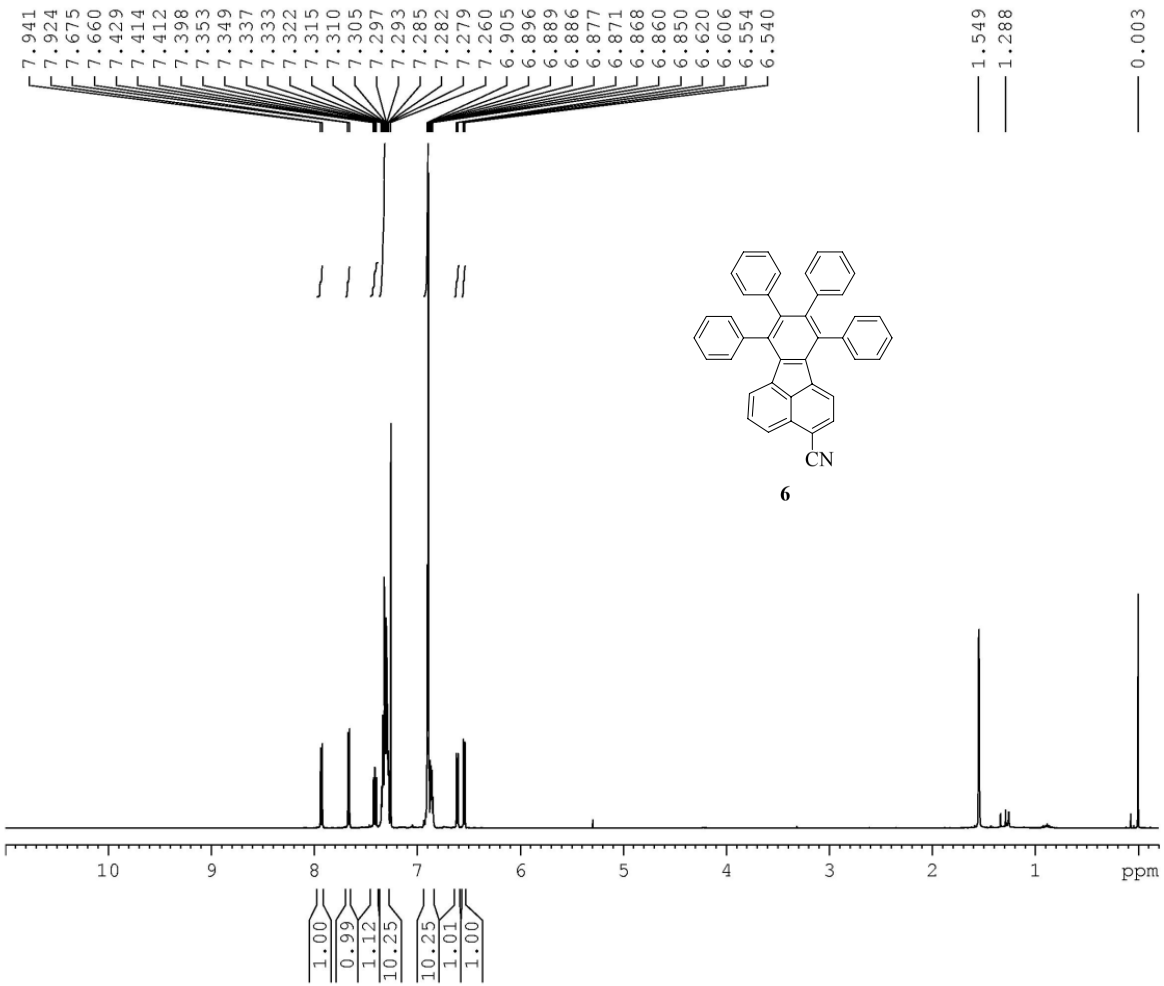
TD                    65536
SOLVENT                CDCl3
NS                       256
DS                         2
SWH               30030.029 Hz
FIDRES             0.458222 Hz
AQ                1.0912410 sec
RG                       456
DW                  16.650 usec
DE                   6.00 usec
TE                   299.4 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                    9.80 usec
PL1                   1.00 dB
SFO1            125.7703640 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                80.00 usec
PL2                   2.00 dB
PL12                 16.60 dB
PL13                 20.60 dB
SFO2            500.1320000 MHz

F2 - Processing parameters
SI                       32768
SF              125.7577943 MHz
WDW                         EM
SSB                          0
LB                    1.00 Hz
GB                           0
PC                    1.40
```

Figure S9. ^{13}C NMR of **5b**.

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PROCNO                      1

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PROBHD    5 mm PATXI 1H/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               10330.578 Hz
FIDRES             0.157632 Hz
AQ                3.1720407 sec
RG                      256
DW                   48.400 usec
DE                    6.00 usec
TE                   297.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    7.70 usec
PL1                   2.00 dB
SFO1           500.1330885 MHz

F2 - Processing parameters
SI                    32768
SF             500.1300132 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```

Figure S10. ^{1}H NMR of **6**.

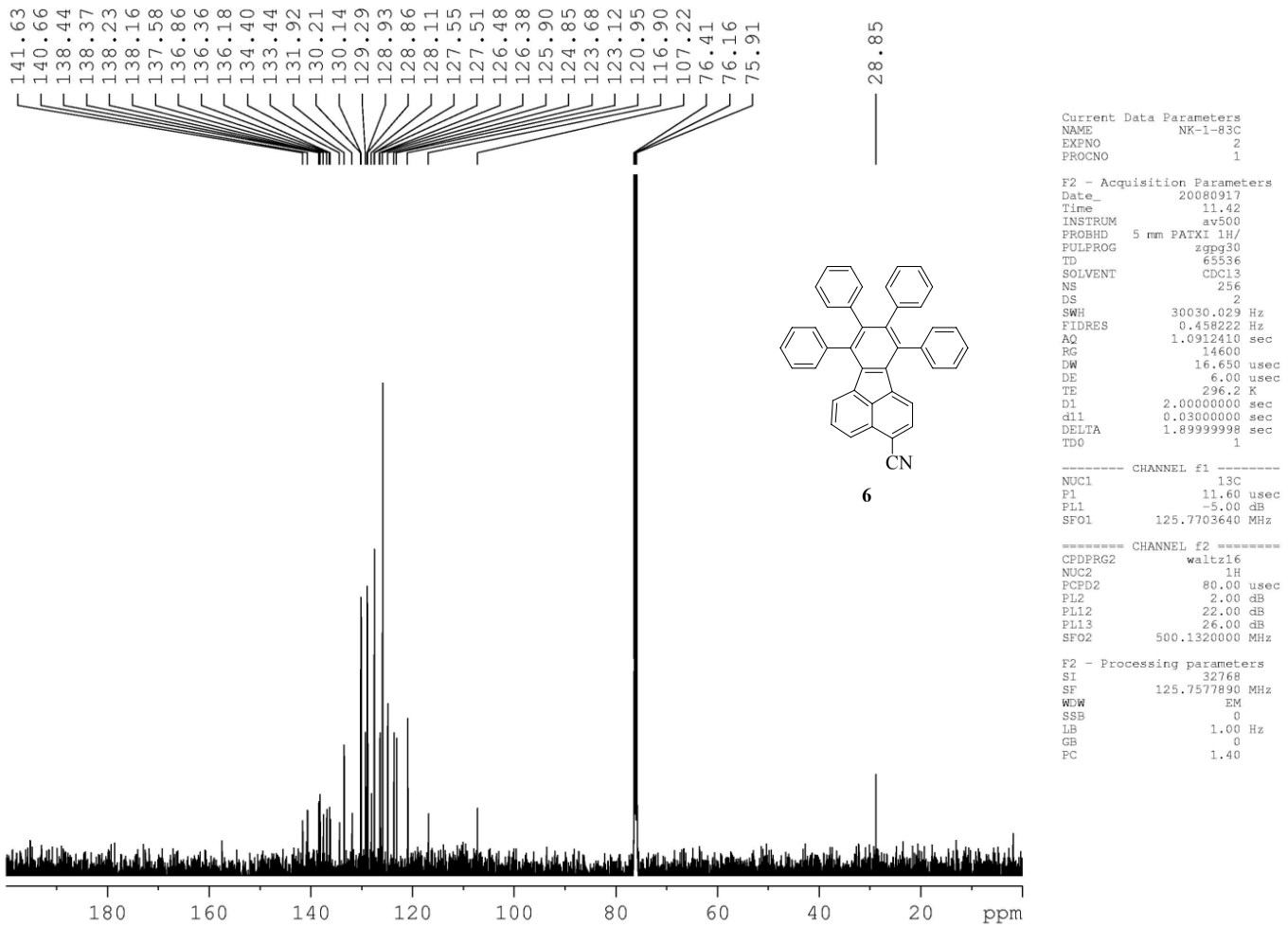


Figure S11. ^{13}C NMR of **6**.

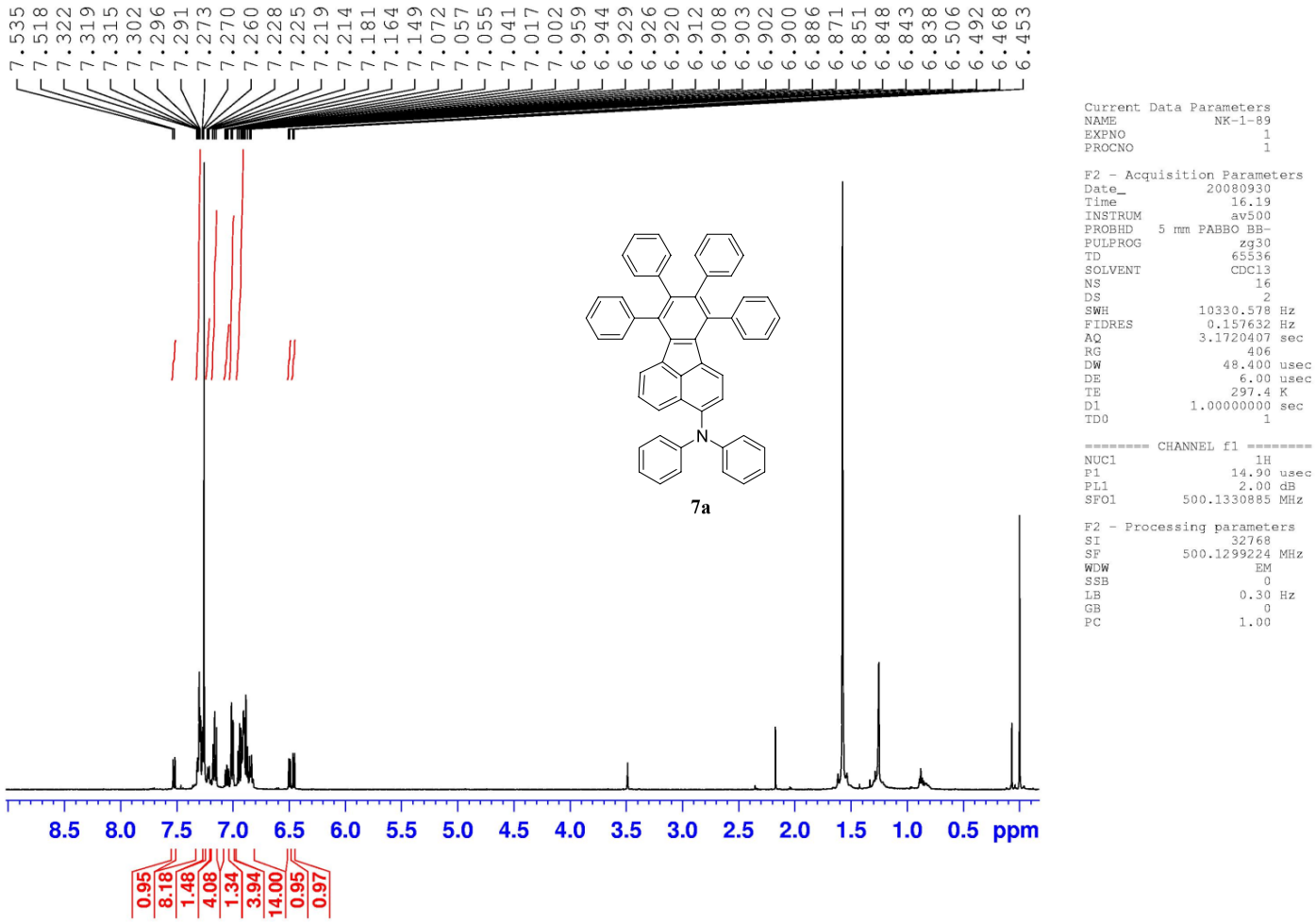
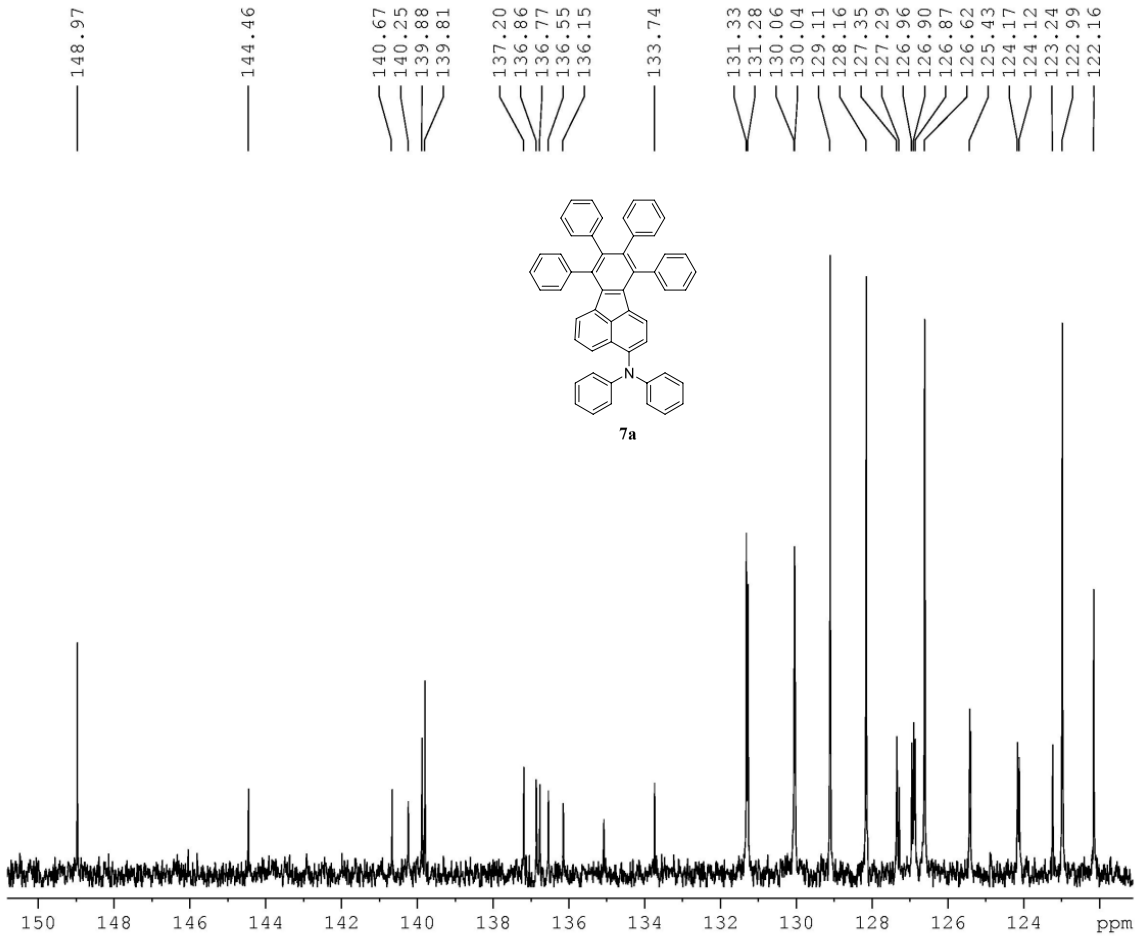


Figure S12. ^{1}H NMR of **7a**.

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PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       512
DS                         2
SWH               30030.029 Hz
FIDRES             0.458222 Hz
AQ                 1.0912410 sec
RG                       575
DW                    16.650 usec
DE                     6.00 usec
TE                    298.7 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.80 usec
PL1                      1.00 dB
SFO1             125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                      2.00 dB
PL12                    16.60 dB
PL13                    20.60 dB
SFO2             500.1320005 MHz

F2 - Processing parameters
SI                       32768
SF               125.7577890 MHz
WDW                         EM
SSB                          0
LB                       1.00 Hz
GB                           0
PC                       1.40
```

Figure S13. ^{13}C NMR of **7a**.

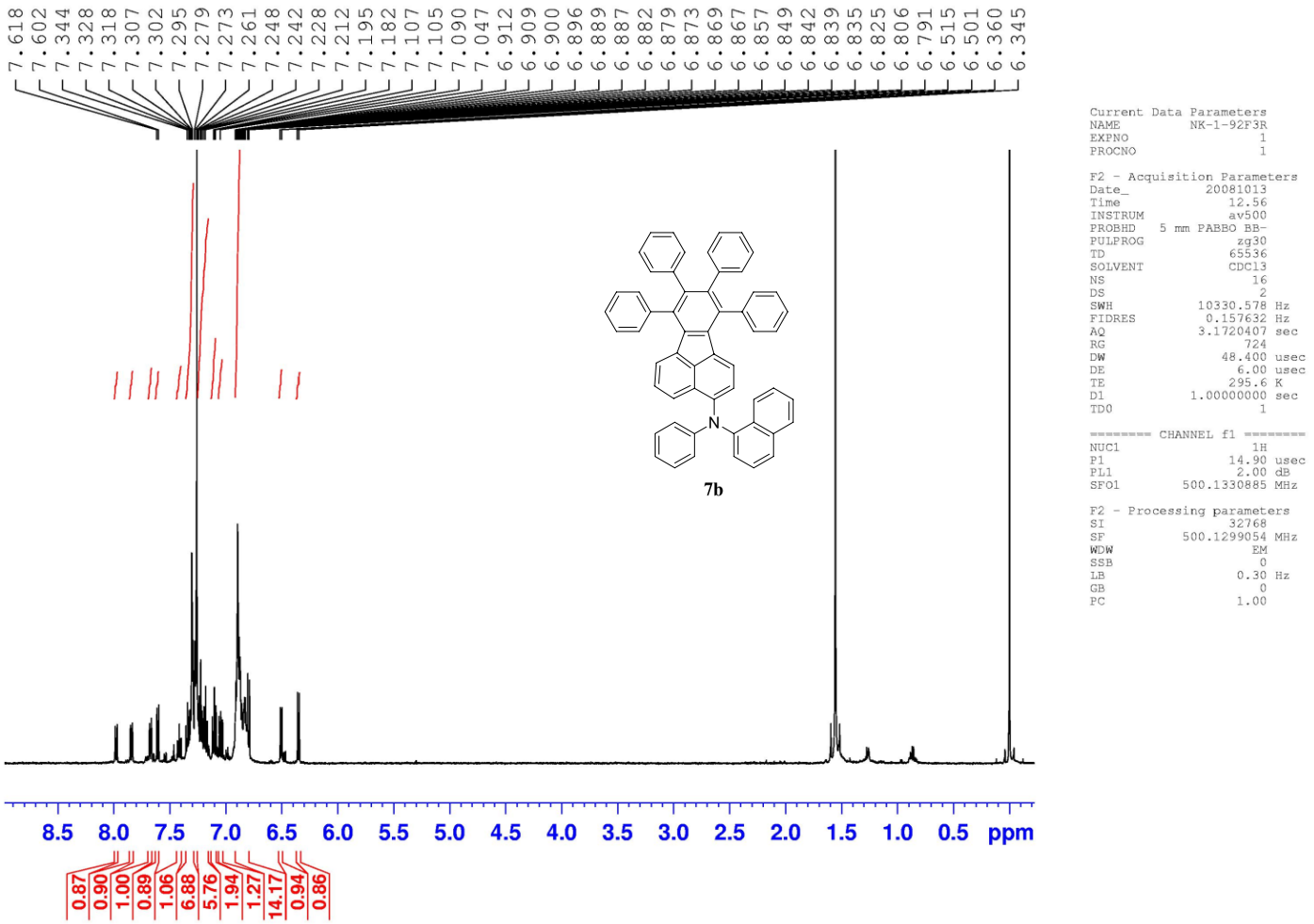
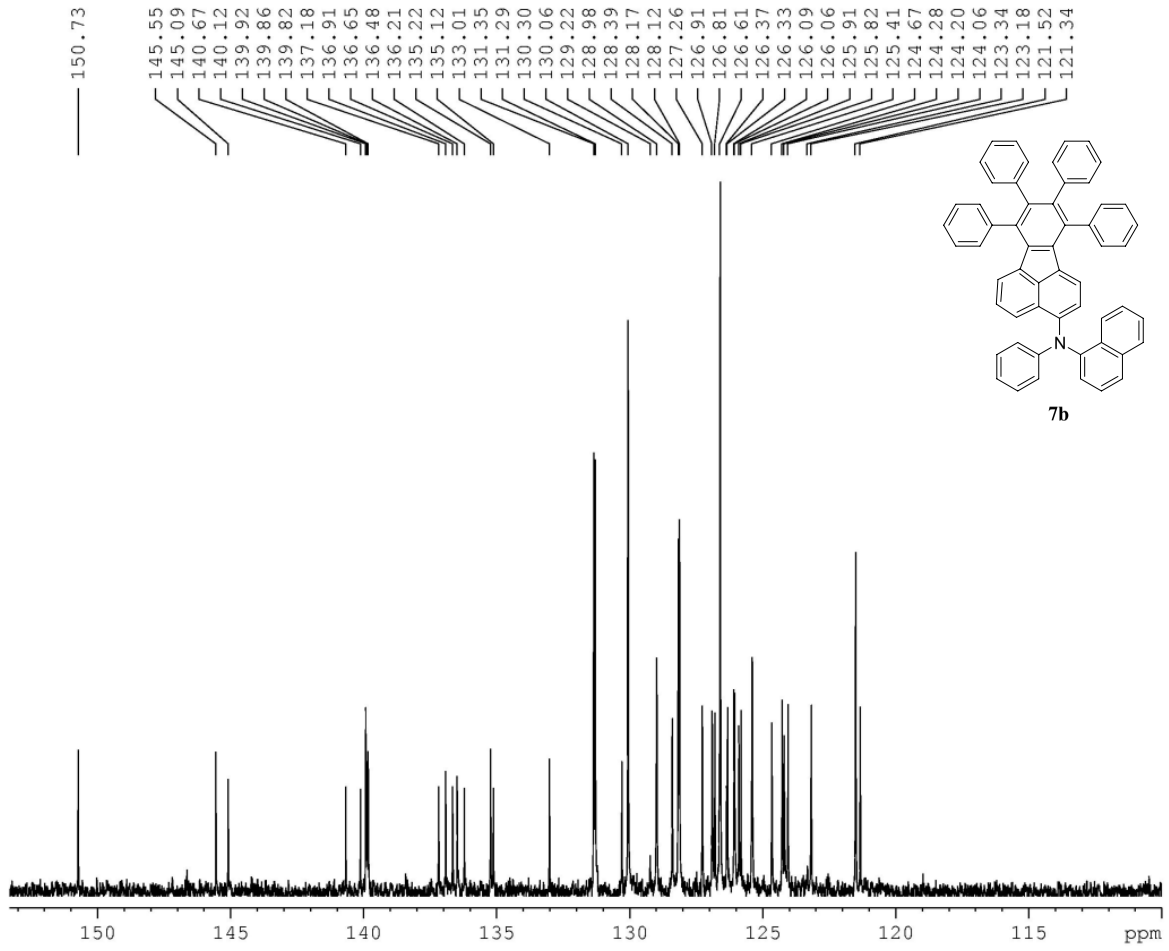


Figure S14. ^{1}H NMR of **7b**.

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PROCNO                        1

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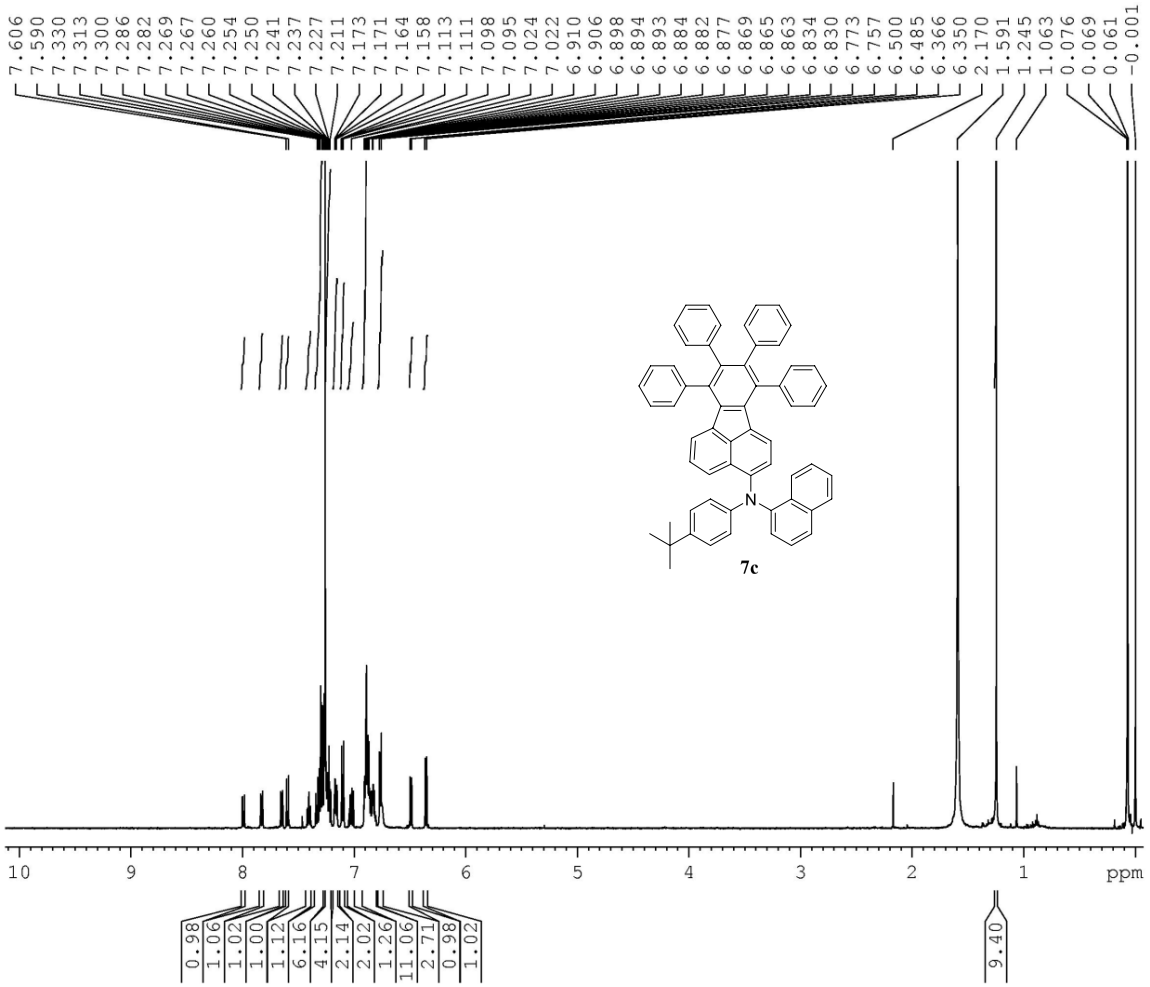
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         512
DS                           2
SWH                  30030.029 Hz
FIDRES                0.458222 Hz
AQ                    1.0912410 sec
RG                         1030
DW                       16.650 usec
DE                        6.00 usec
TE                       300.4 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        13C
P1                        9.80 usec
PL1                       1.00 dB
SFO1                125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                    80.00 usec
PL2                       2.00 dB
PL12                     16.60 dB
PL13                     20.60 dB
SFO2                500.1320005 MHz

F2 - Processing parameters
SI                        32768
SF                  125.7577890 MHz
WDW                          EM
SSB                           0
LB                        1.00 Hz
GB                            0
PC                        1.40
```

Figure S15. ^{13}C NMR of **7b**.

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PROCNO                     1

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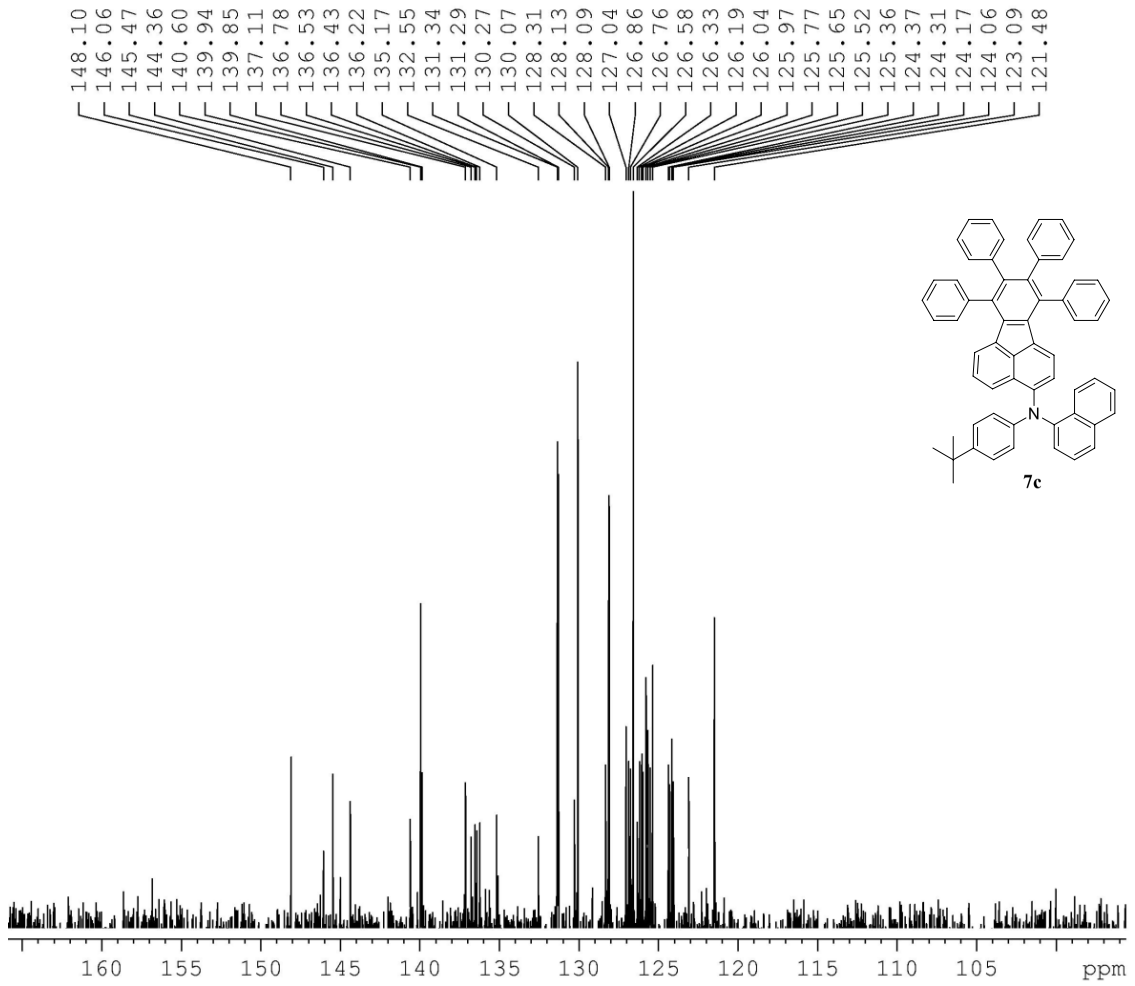
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               10330.578 Hz
FIDRES            0.157632 Hz
AQ                3.1720407 sec
RG                      456
DW                   48.400 usec
DE                    6.00 usec
TE                   298.5 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.90 usec
PL1                     2.00 dB
SFO1           500.1330885 MHz

F2 - Processing parameters
SI                        32768
SF             500.1299413 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00
```

Figure S16. ^{1}H NMR of **7c**.

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PROCNO                     1

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PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT                CDC13
NS                       256
DS                         2
SWH               30030.029 Hz
FIDRES             0.458222 Hz
AQ                1.0912410 sec
RG                       456
DW                  16.650 usec
DE                   6.00 usec
TE                   299.5 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                    9.80 usec
PL1                   1.00 dB
SF01            125.7703640 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                80.00 usec
PL2                   2.00 dB
PL12                 16.60 dB
PL13                 20.60 dB
SF02            500.1320000 MHz

F2 - Processing parameters
SI                       32768
SF              125.7577890 MHz
WDW                         EM
SSB                          0
LB                    1.00 Hz
GB                           0
PC                    1.40
```

Figure S17. ^{13}C NMR of **7c**.

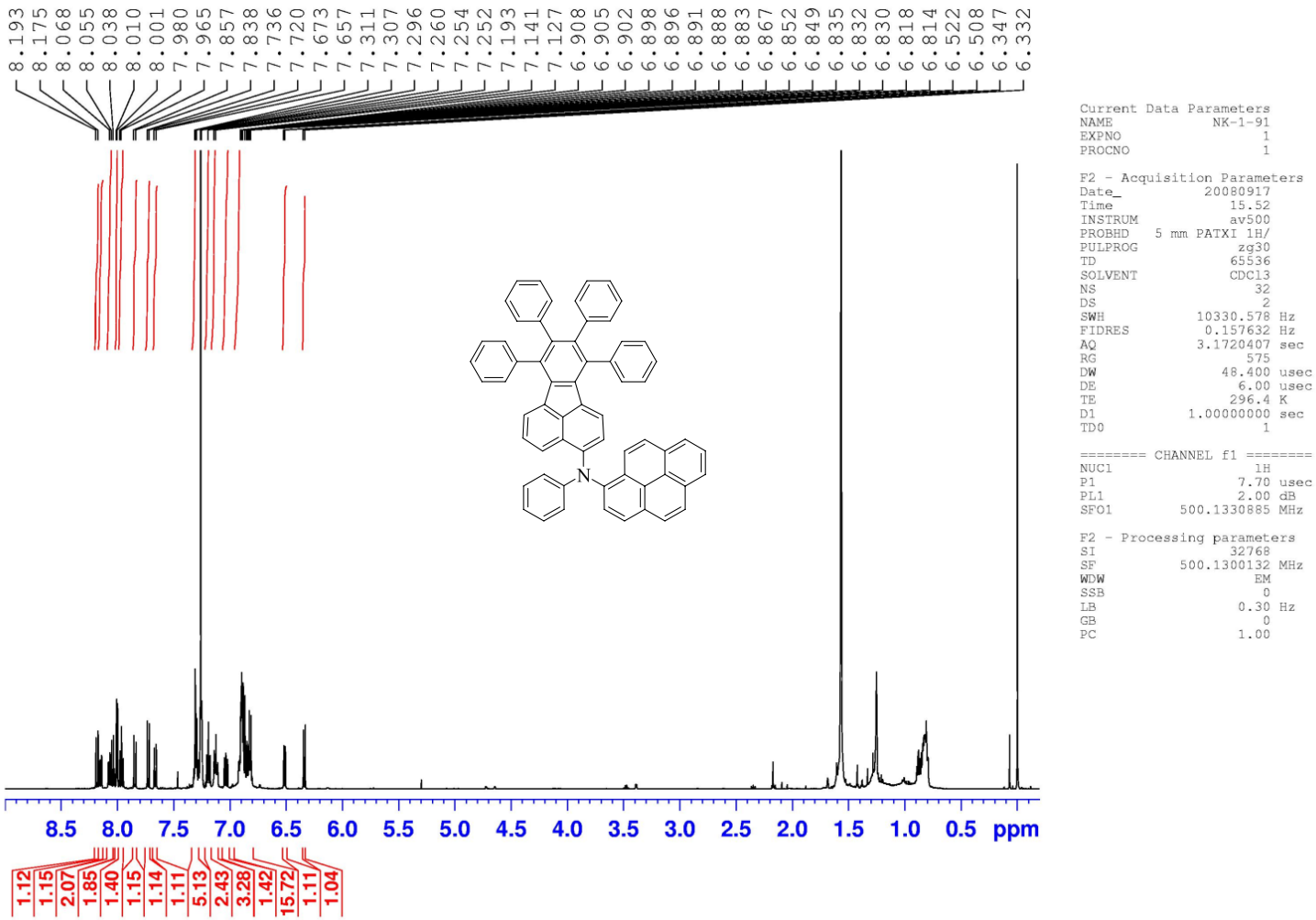
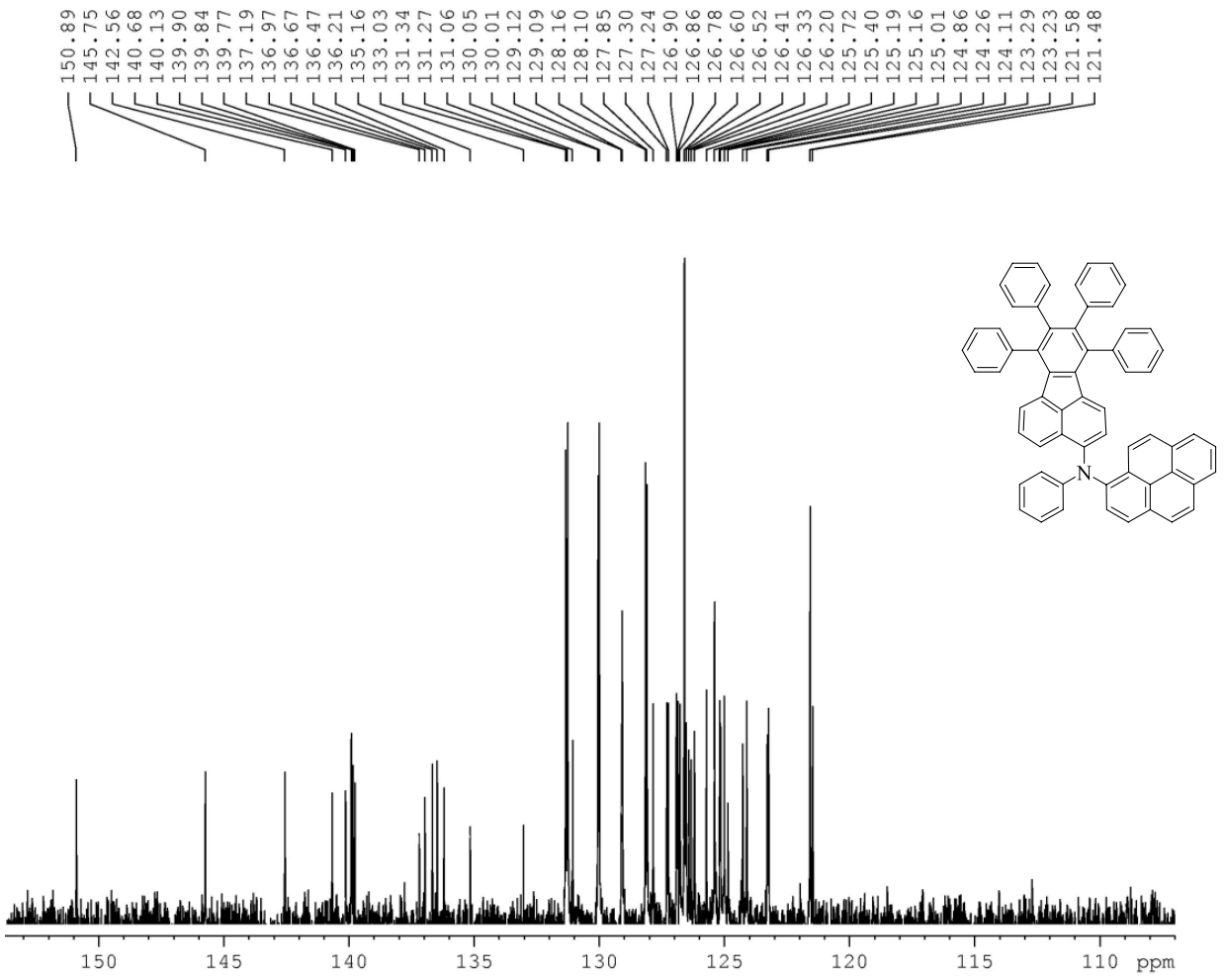


Figure S18. ^{1}H NMR of **7d**.

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PROCNO                1

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PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 512
DS                   2
SWH          30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0912410 sec
RG                 575
DW              16.650 usec
DE               6.00 usec
TE              300.3 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                9.80 usec
PL1               1.00 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               2.00 dB
PL12             16.60 dB
PL13             20.60 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF          125.7577890 MHz
WDW                   EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```

Figure S19. ^{13}C NMR of **7**.