# EFFECT OF END GROUPS ON THE BAND GAP OF DONOR-ACCEPTOR BASED SMALL MOLECULES CONTAINING DIKETOPYRROLOPYRROLE

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**Figure S1.** $^{1}$H-NMR spectrum of **DPPTCN**.

**Figure S2.** $^{13}$C-NMR spectrum of **DPPTCN**.

**Figure S3.** HRMS (FAB) spectrum of **DPPTCN**.

**Figure S4.** $^{1}$H-NMR spectrum of **DPPPhCN**.

**Figure S5.** $^{13}$C-NMR spectrum of **DPPPhCN**

**Figure S6.** HRMS (FAB) spectrum of **DPPPhCN**.

**Figure S7.** $^{1}$H-NMR spectrum of compound **9**.

**Figure S8.** $^{13}$C-NMR spectrum of compound **9**.

**Figure S9.** HRMS (FAB) spectrum of compound **9**.

**Figure S10.** $^{1}$H-NMR spectrum of compound **11**.

**Figure S11.** $^{13}$C-NMR spectrum of compound **11**.

**Figure S12.** HRMS (FAB) spectrum of compound **11**.

**Figure S13.** $^{1}$H-NMR spectrum of **DPPT2CN**.

**Figure S14.** $^{13}$C-NMR spectrum of **DPPT2CN**.

**Figure S15.** HRMS (FAB) spectrum of **DPPT2CN**.

**Figure S16.** $^{1}$H-NMR spectrum of **DPPPh2CN**.

**Figure S17.** $^{13}$C-NMR spectrum of **DPPPh2CN**.

**Figure S18.** HRMS (FAB) spectrum of **DPPPh2CN**.

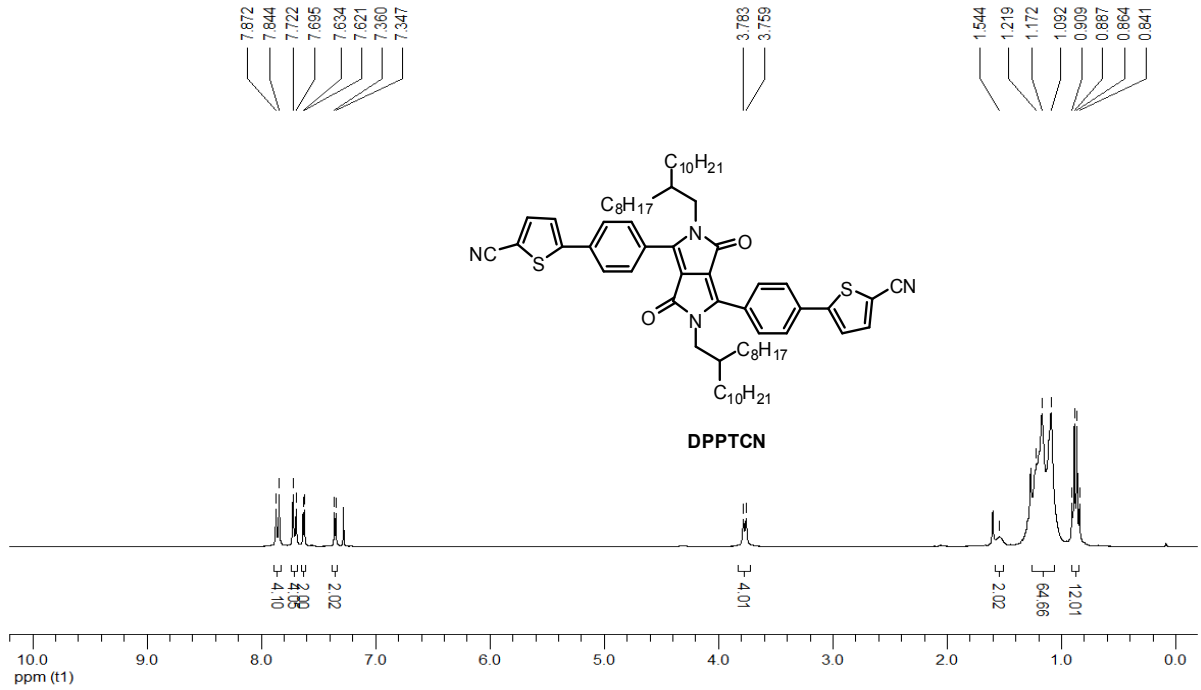



**Figure S1.** $^{1}$H-NMR spectrum of **DPPTCN**.

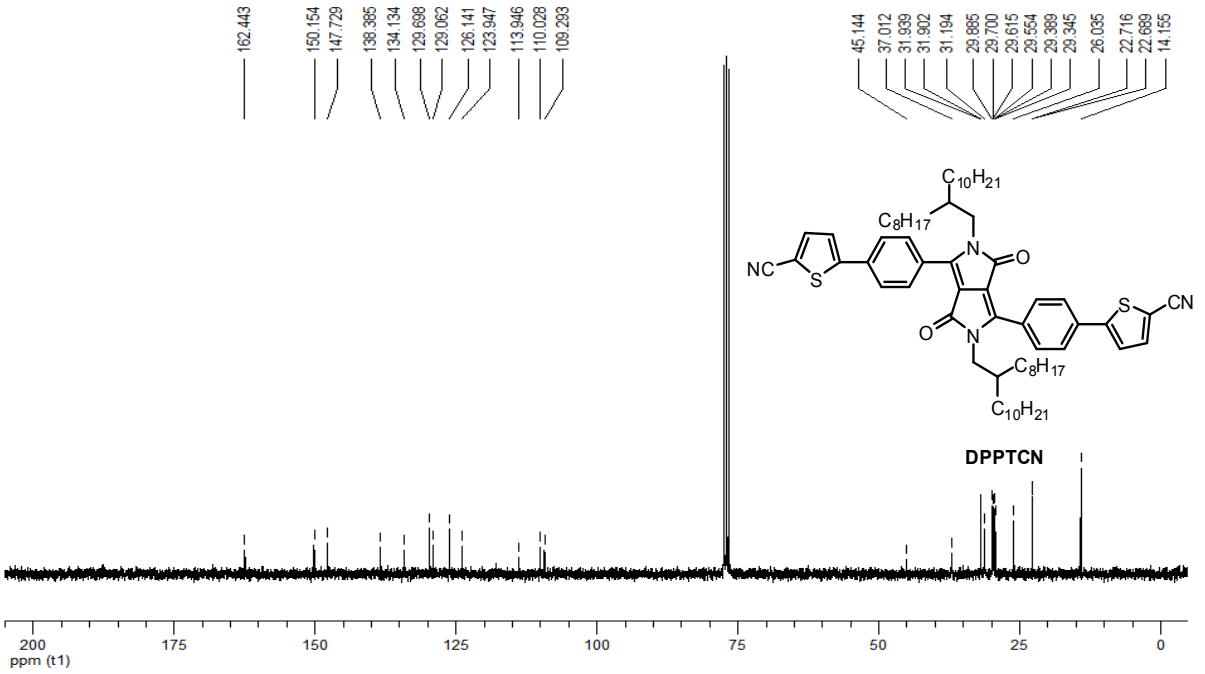
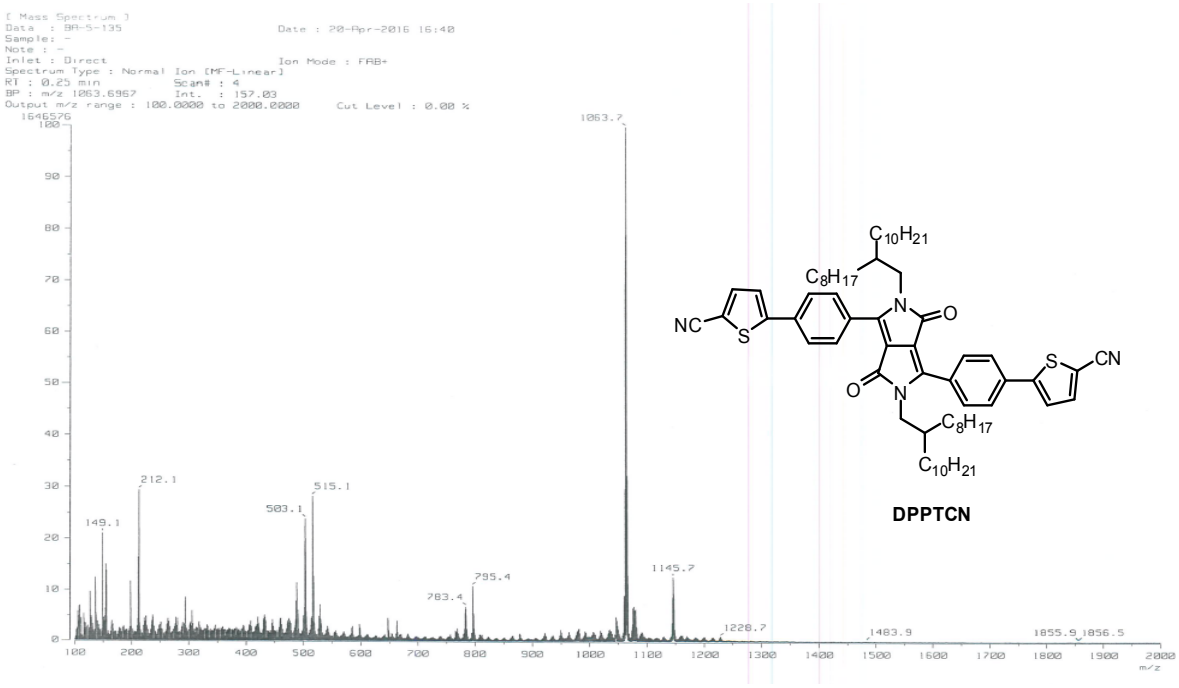



**Figure S2.** $^{13}$C-NMR spectrum of **DPPTCN**.

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[ Elemental Composition ]
Data  : BA-5-135-HR                    Date : 21-Apr-2016 16:22
Sample: -
Note : -
Inlet : Direct                         Ion Mode : FAB+
RT : 1.92 min                          Scan#: 24
Elements : C 100/1, H 150/1, N 10/1, O 4/1, S 4/1
Mass Tolerance       : 100ppm, 3mmu if m/z > 30
Unsaturation (U.S.) : 0.0 - 30.0

Observed m/z Int%   Err[ppm / mmu]     U.S.  Composition
 1063.6899     1.2     +2.2 /  +2.3    29.0  C 73 H 93 N O 3 S
                       +1.5 /  +1.6    26.0  C 66 H 93 N 7 O S 2
                       +0.3 /  +0.3    25.5  C 68 H 95 N 4 O 2 S 2
                       -1.0 /  -1.0    25.0  C 70 H 97 N O 3 S 2
                       -1.6 /  -1.7    22.0  C 63 H 97 N 7 O S 3
                       +2.2 /  +2.3    18.0  C 58 H 97 N 9 O 3 S 3
                       +0.9 /  +0.9    17.5  C 60 H 99 N 6 O 4 S 3
                       -1.0 /  -1.1    14.0  C 55 H 101 N 9 O 3 S 4
                       -2.3 /  -2.4    13.5  C 57 H 103 N 6 O 4 S 4
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**Figure S3.** HRMS (FAB) spectrum of **DPPTCN**.

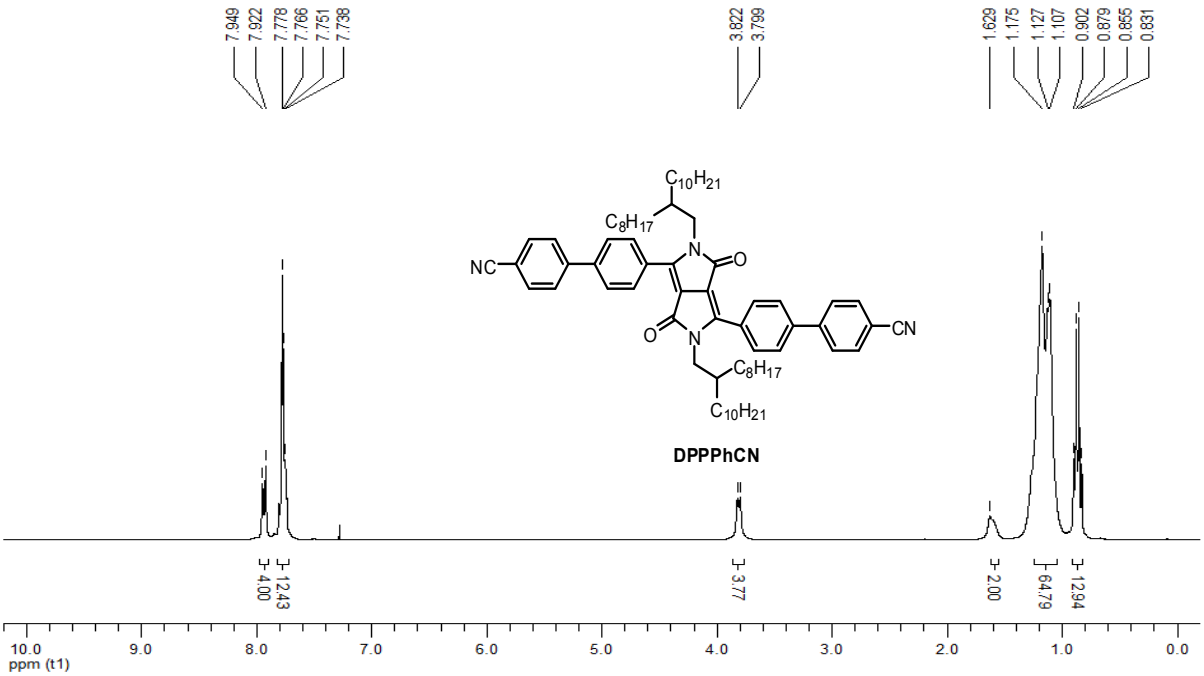



**Figure S4.** [1]H-NMR spectrum of **DPPPhCN**.

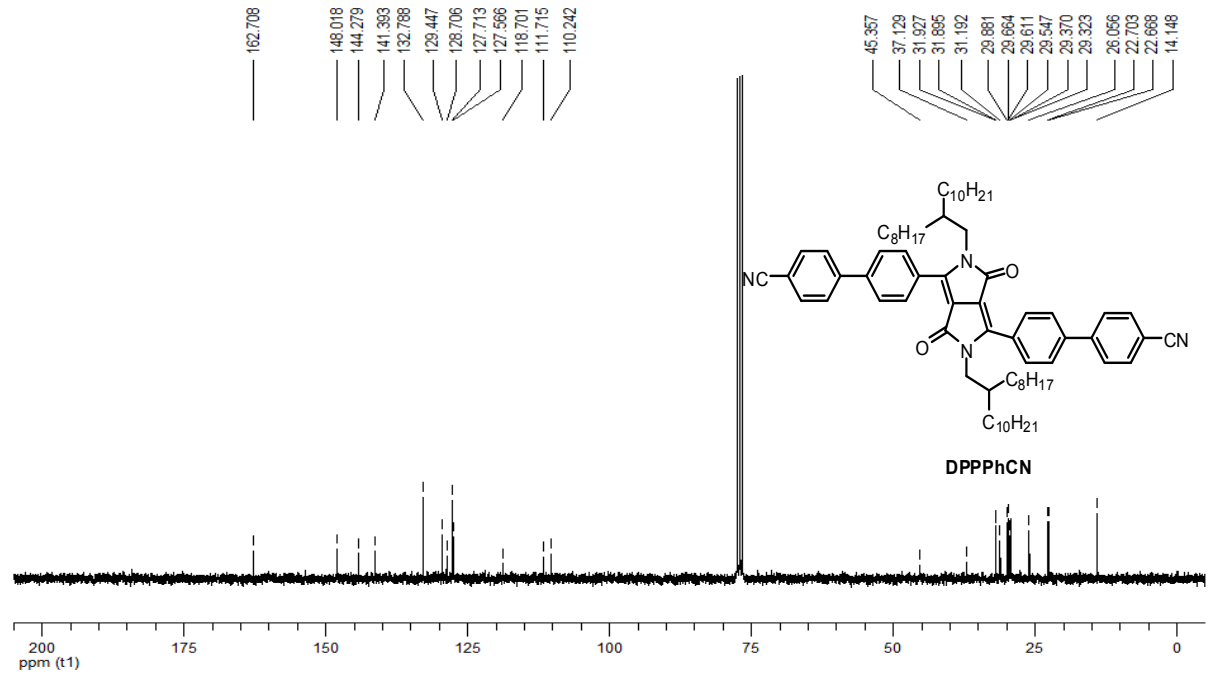
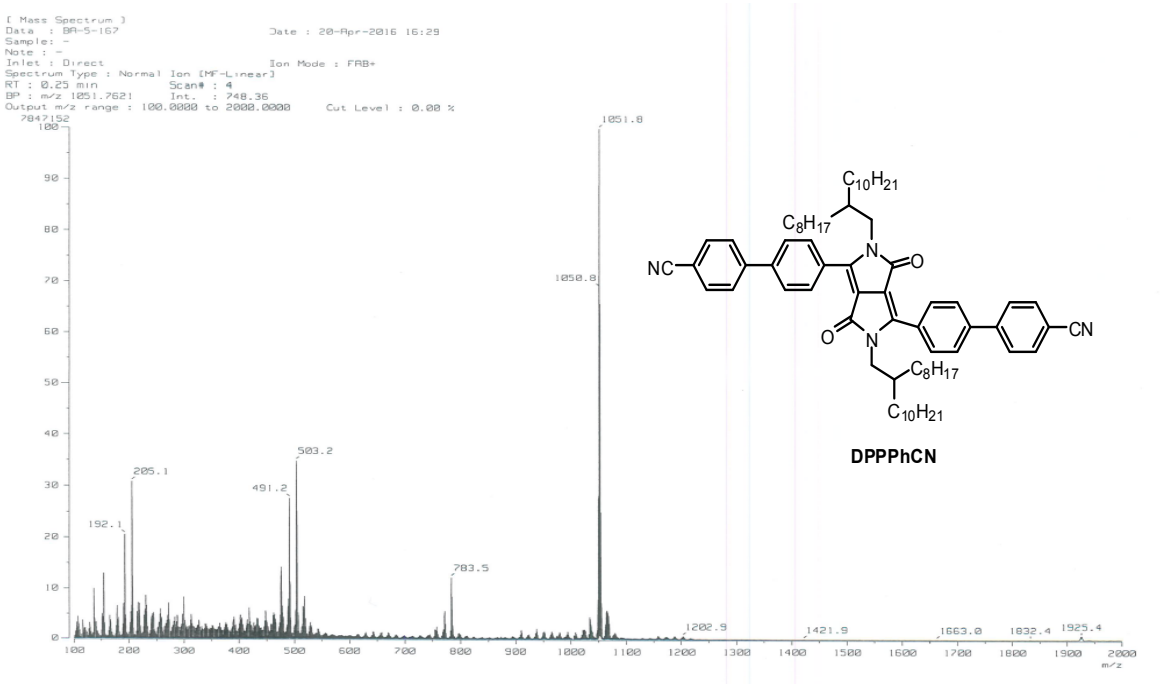



**Figure S5.** [13]C-NMR spectrum of **DPPPhCN**




[ Elemental Composition ]
Data : BA-5-167-HR Date : 21-Apr-2016 14:40
Sample: -
Note : -
Inlet : Direct Ion Mode : FAB+
RT : 0.92 min Scan#: 12
Elements : C 100/1, H 150/1, N 10/1, O 10/1
Mass Tolerance : 100ppm, 3mmu if m/z > 30
Unsaturation (U.S.) : 0.0 - 30.0

| Observed m/z | Int% | Err[ppm / mmu] | U.S. | Composition |
|---|---|---|---|---|
| 1051.7762 | 5.8 | +0.7 / +0.8 | 26.0 | C 70 H 97 N 7 O |
| | | -0.5 / -0.6 | 25.5 | C 72 H 99 N 4 O 2 |
| | | -1.8 / -1.9 | 25.0 | C 74 H 101 N O 3 |
| | | +2.0 / +2.1 | 21.0 | C 69 H 101 N 3 O 5 |
| | | -1.0 / -1.1 | 13.0 | C 58 H 101 N 9 O 8 |
| | | -2.3 / -2.4 | 12.5 | C 60 H 103 N 6 O 9 |

**Figure S6.** HRMS (FAB) spectrum of **DPPPhCN**.

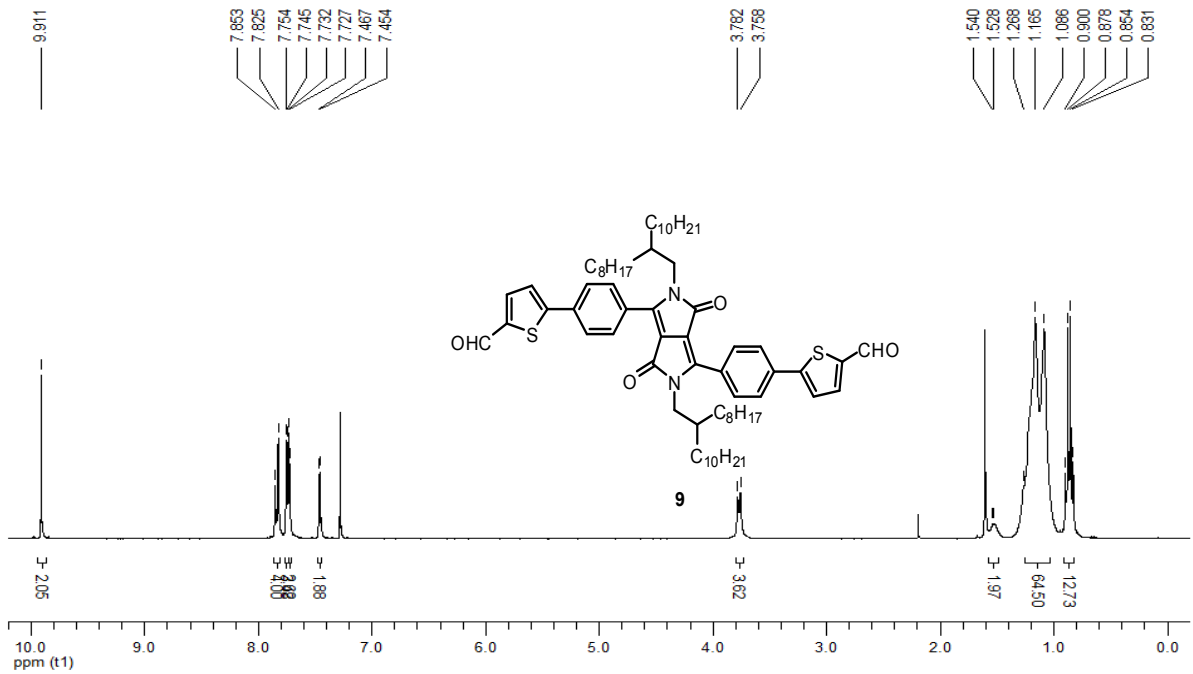



**Figure S7.** $^{1}$H-NMR spectrum of compound **9**.

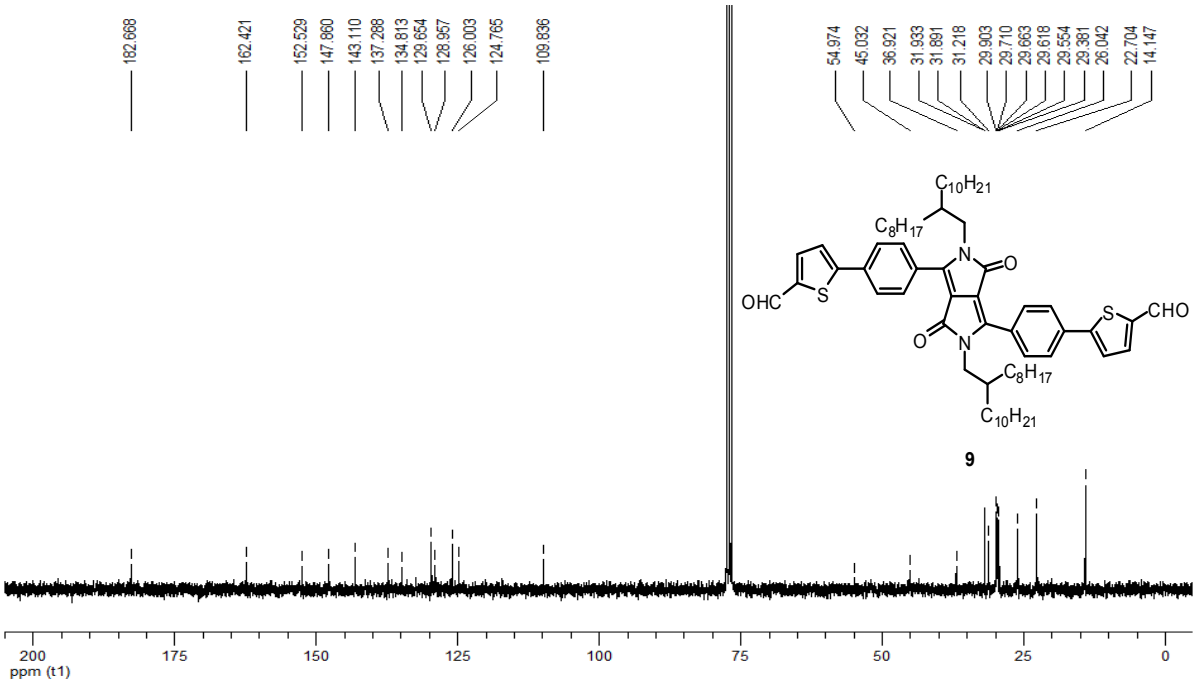
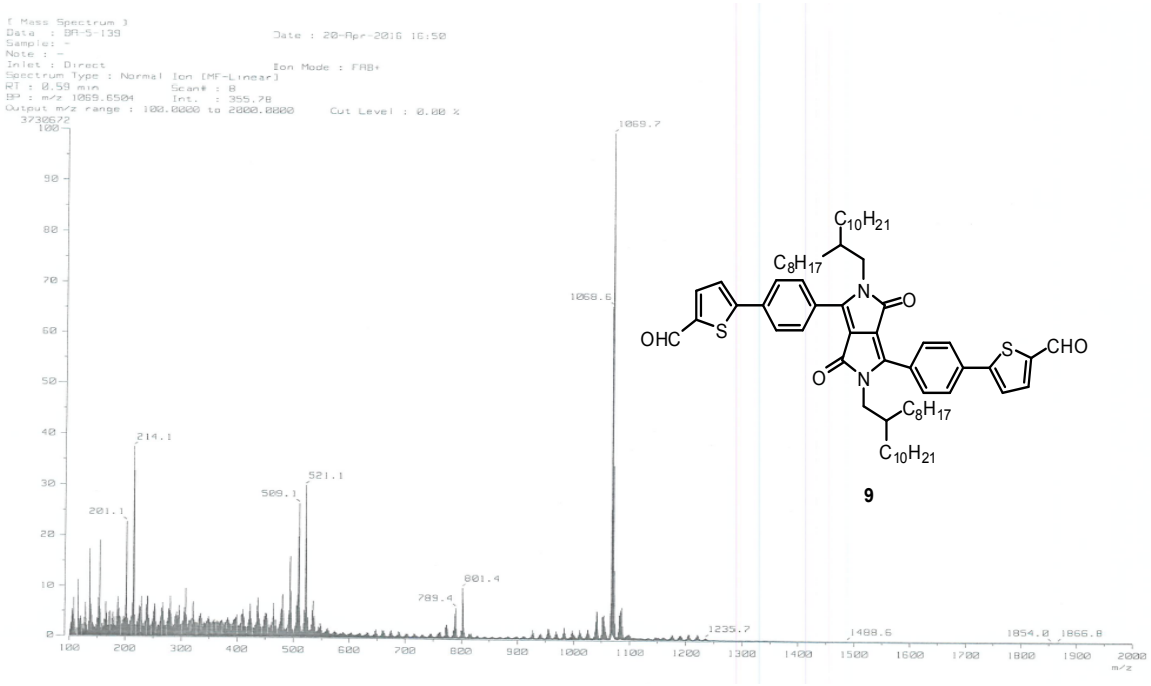



**Figure S8.** $^{13}$C-NMR spectrum of compound **9**.

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[ Elemental Composition ]
Data  : BA-5-139-HR                        Date : 21-Apr-2016 16:38
Sample: -
Note : -
Inlet : Direct                             Ion Mode : FAB+
RT : 1.84 min                              Scan#: 23
Elements : C 100/1, H 150/1, N 5/1, O 4/1, S 4/1
Mass Tolerance       : 100ppm, 5mmu if m/z > 50
Unsaturation (U.S.) : 0.0 - 30.0

Observed m/z Int%   Err[ppm / mmu]     U.S.  Composition
 1069.6930     6.3      -3.6 /  -3.8   27.5  C 70 H 93 N 4 O 3 S
                        +1.2 /  +1.3   28.0  C 71 H 95 N 3 O S 2
                        +3.8 /  +4.0   23.5  C 68 H 97 N 2 O 4 S 2
                        -1.9 /  -2.0   24.0  C 68 H 99 N 3 O S 3
                        +1.9 /  +2.0   20.0  C 63 H 99 N 5 O 3 S 3
                        +0.6 /  +0.6   19.5  C 65 H 101 N 2 O 4 S 3
                        -1.3 /  -1.4   16.0  C 60 H 103 N 5 O 3 S 4
                        -2.6 /  -2.7   15.5  C 62 H 105 N 2 O 4 S 4
```

**Figure S9.** HRMS (FAB) spectrum of compound **9**.

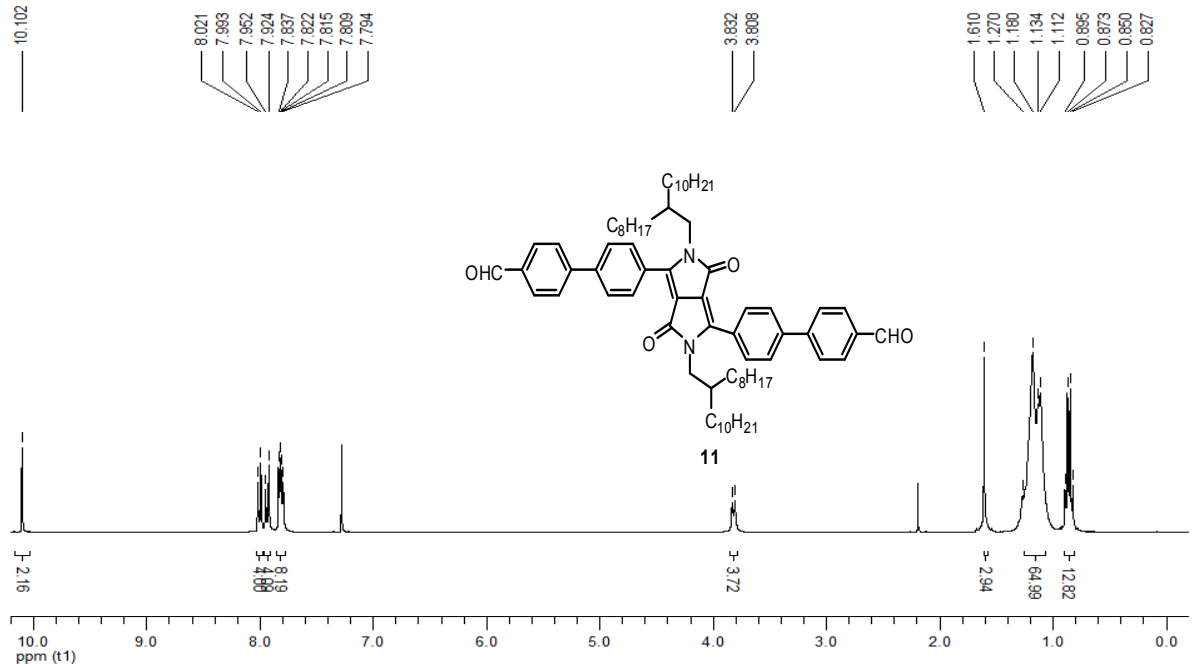



**Figure S10.** $^{1}$H-NMR spectrum of compound **11**.

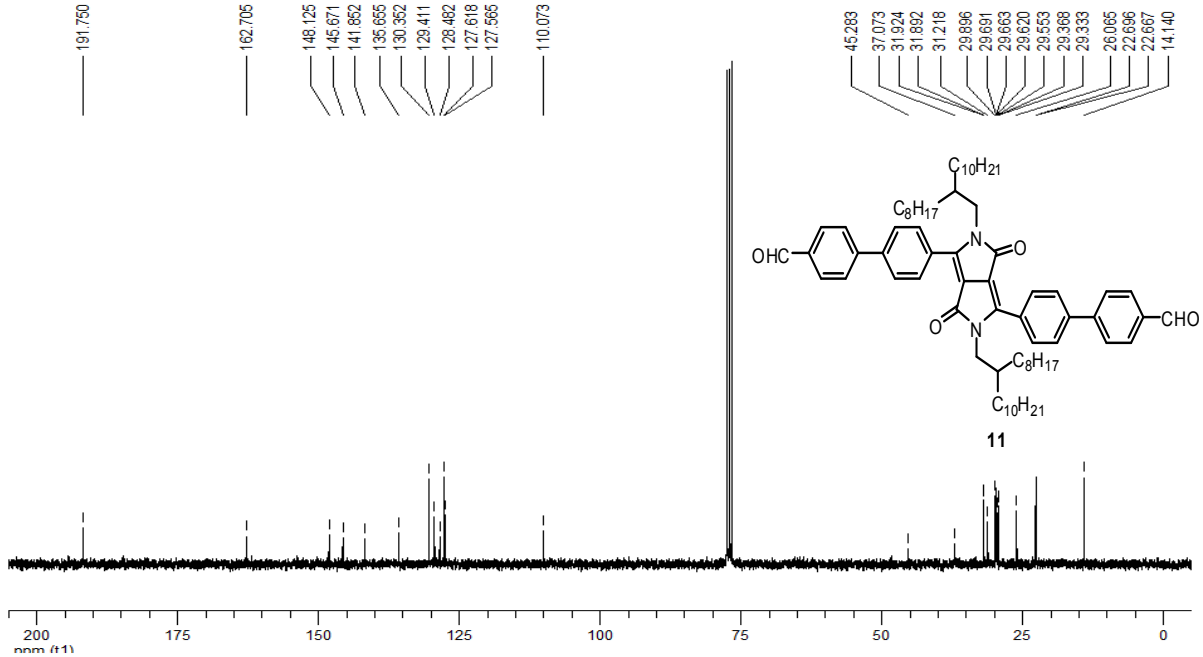
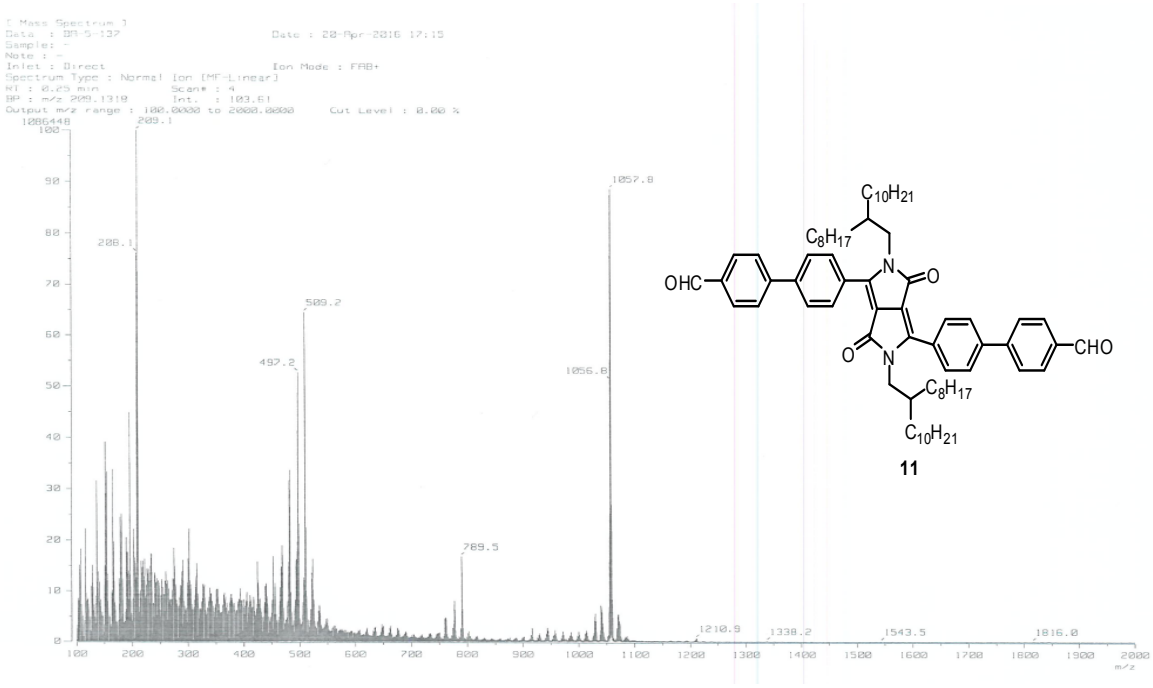



**Figure S11.** $^{13}$C-NMR spectrum of compound **11**.

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[ Elemental Composition ]
Data  : BA-5-137-HR                    Date : 21-Apr-2016 17:16
Sample: -
Note : -
Inlet : Direct                         Ion Mode : FAB+
RT : 1.42 min                          Scan#: 18
Elements : C 100/1, H 150/1, N 5/1, O 10/1
Mass Tolerance       : 100ppm, 5mmu if m/z > 50
Unsaturation (U.S.) : 0.0 - 30.0

Observed m/z Int%   Err[ppm / mmu]     U.S.  Composition
 1057.7760     0.5     -2.7 /  -2.8    28.0  C 75 H 99 N 3 O
                       +1.1 /  +1.2    24.0  C 70 H 99 N 5 O 3
                       -0.1 /  -0.1    23.5  C 72 H 101 N 2 O 4
                       +3.7 /  +3.9    19.5  C 67 H 101 N 4 O 6
                       +2.4 /  +2.5    19.0  C 69 H 103 N O 7
                       -4.4 /  -4.7    15.0  C 63 H 103 N 5 O 8
```

**Figure S12.** HRMS (FAB) spectrum of compound **11**.

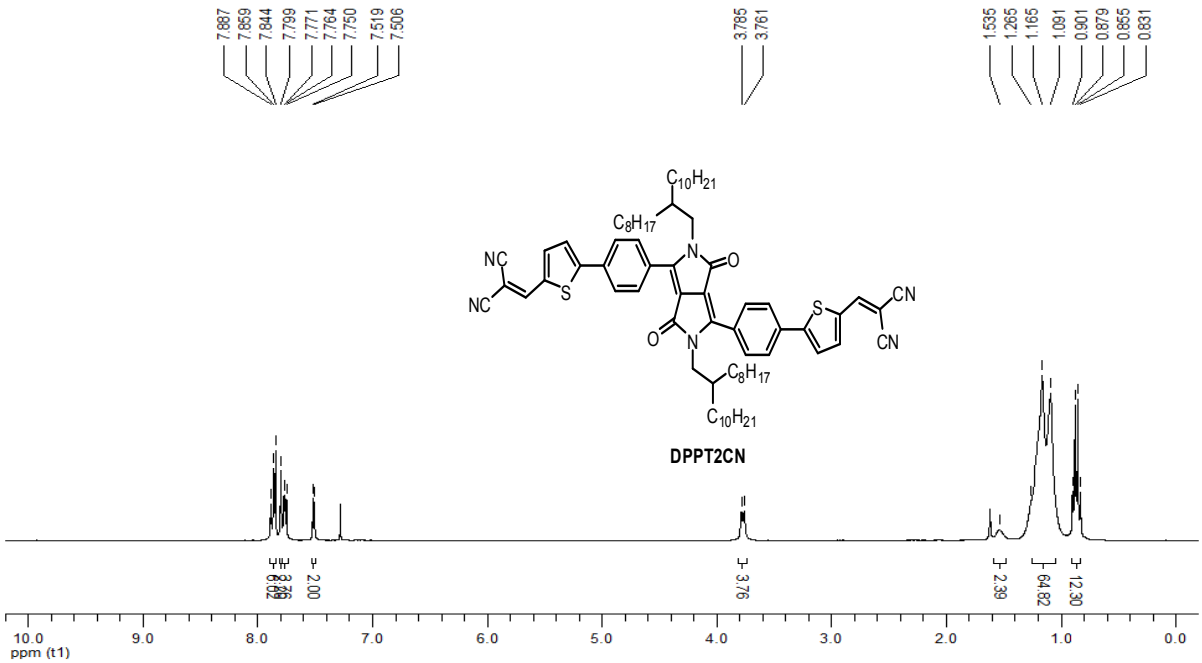



**Figure S13.** $^{1}$H-NMR spectrum of **DPPT2CN**.

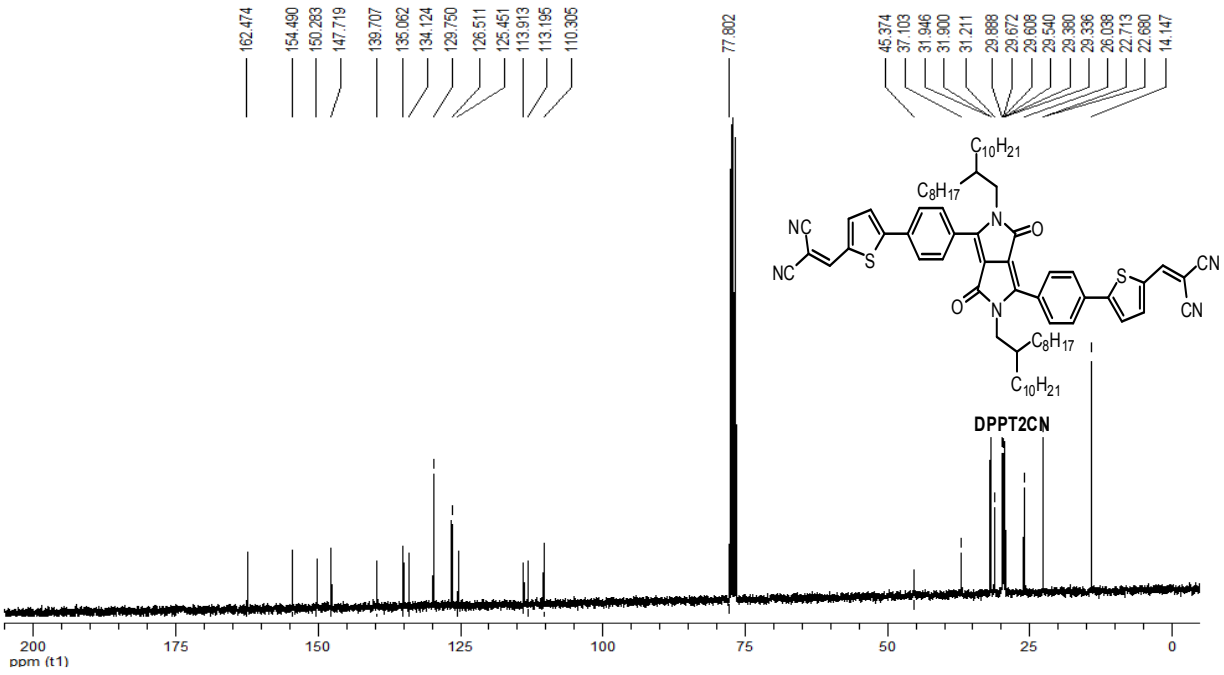
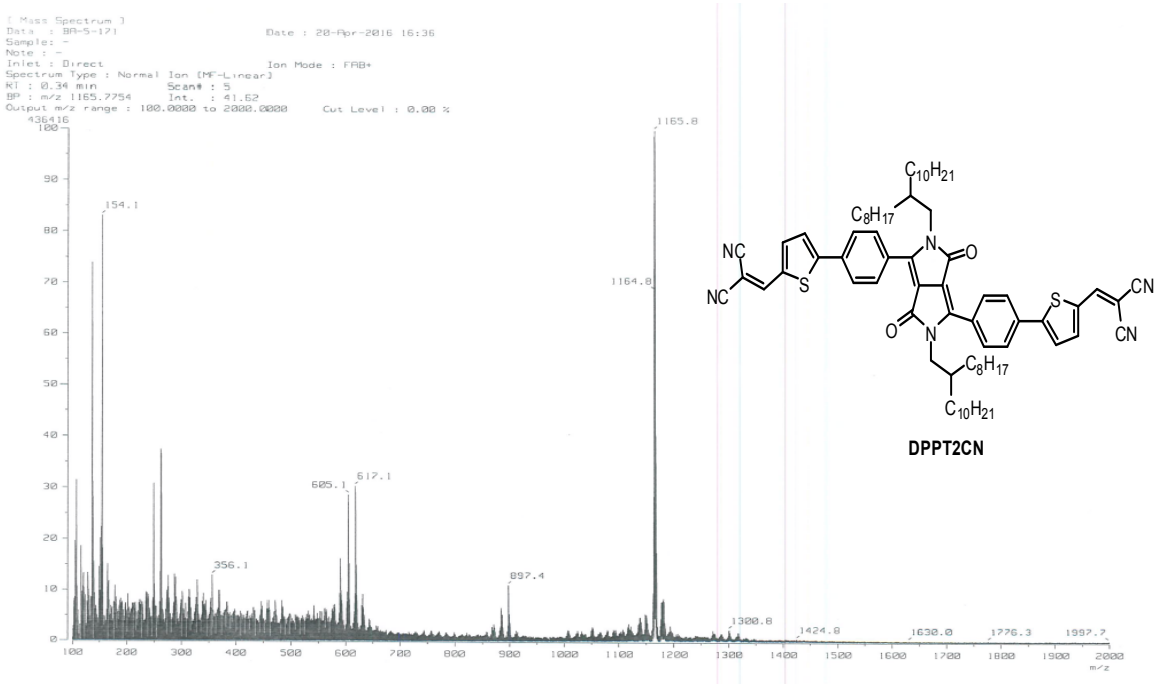



**Figure S14.** $^{13}$C-NMR spectrum of **DPPT2CN**.




```
[ Elemental Composition ]
Data  : BA-5-171-HR                    Date : 21-Apr-2016 15:55
Sample: -
Note : -
Inlet : Direct                         Ion Mode : FAB+
RT : 3.00 min                          Scan#: 37
Elements : C 100/1, H 150/1, N 10/1, O 4/1, S 4/1
Mass Tolerance       : 100ppm, 3mmu if m/z > 30
Unsaturation (U.S.) : 0.0 - 40.0

Observed m/z Int%   Err[ppm / mmu]    U.S.  Composition
 1165.7128    2.0      -0.6 /  -0.7   39.0  C 84 H 95 N O S
                       -2.2 /  -2.5   31.5  C 71 H 93 N 10 O 3 S
                       +2.3 /  +2.7   32.0  C 72 H 95 N 9 O S 2
                       +1.1 /  +1.3   31.5  C 74 H 97 N 6 O 2 S 2
                       +0.0 /  +0.0   31.0  C 76 H 99 N 3 O 3 S 2
                       -0.6 /  -0.7   28.0  C 69 H 99 N 9 O S 3
                       -1.8 /  -2.0   27.5  C 71 H 101 N 6 O 2 S 3
                       +1.7 /  +2.0   23.5  C 66 H 101 N 8 O 4 S 3
                       +1.5 /  +1.8   27.5  C 74 H 105 N 2 O S 4
                       -1.2 /  -1.4   19.5  C 63 H 105 N 8 O 4 S 4
```

**Figure S15.** HRMS (FAB) spectrum of **DPPT2CN**.

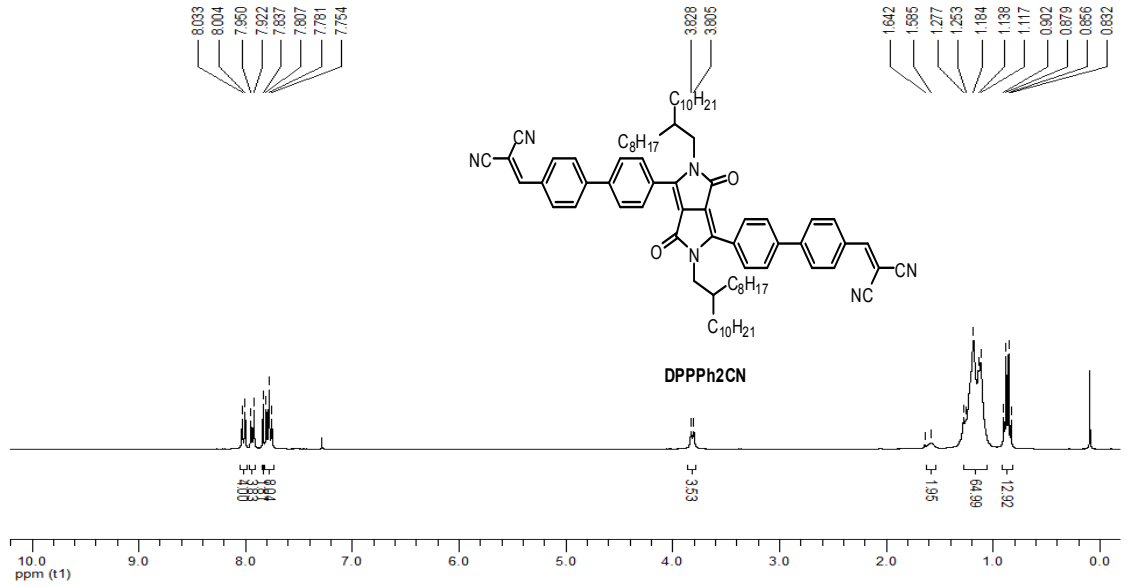



**Figure S16.** [1]H-NMR spectrum of **DPPPh2CN**.

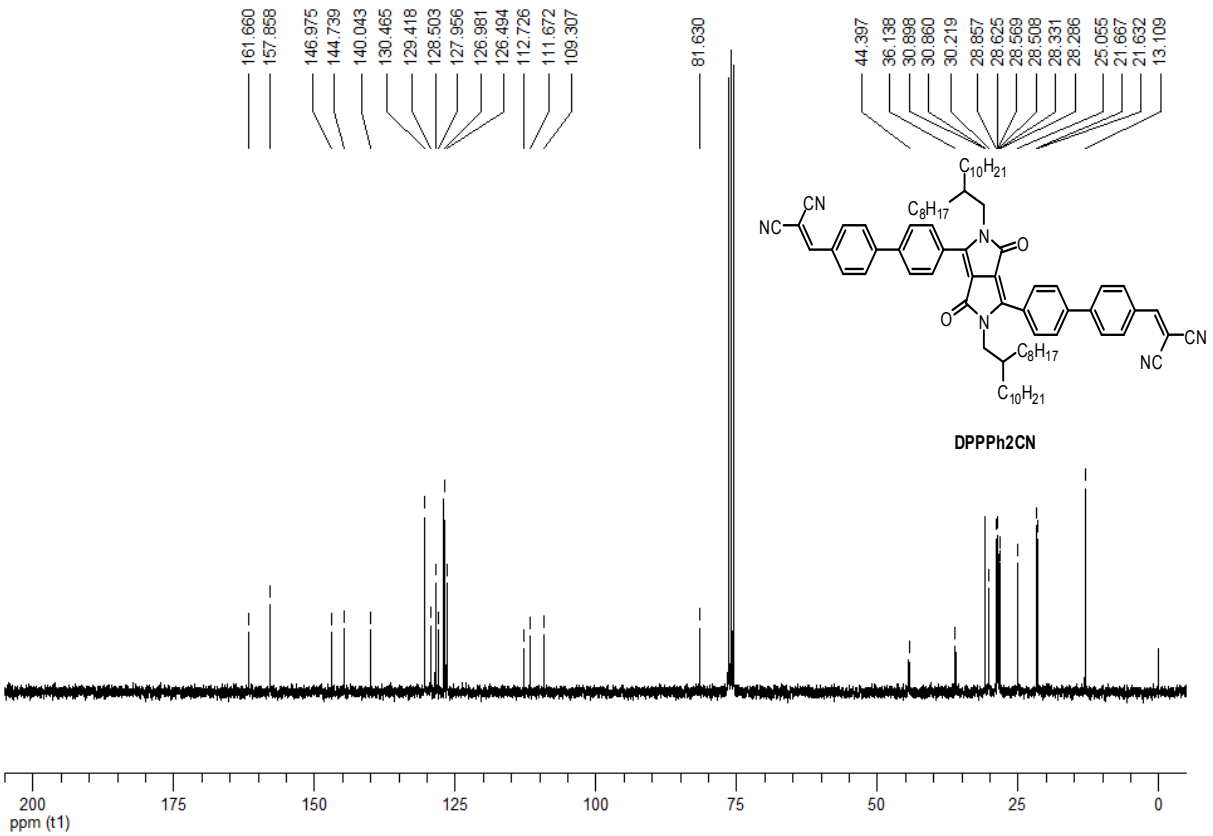
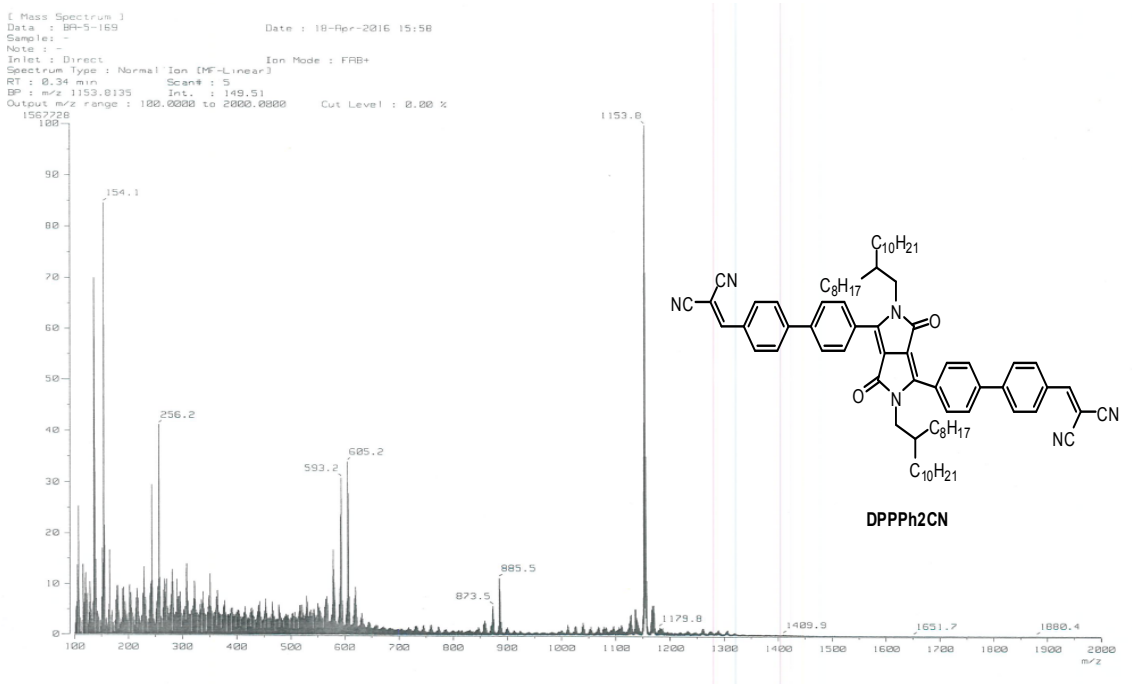



**Figure S17.** [13]C-NMR spectrum of **DPPPh2CN**.




```
[ Elemental Composition ]
Data  : BA-5-169-HR                    Date : 18-Apr-2016 16:19
Sample: -
Note : -
Inlet : Direct                         Ion Mode : FAB+
RT : 0.34 min                          Scan#: 5
Elements : C 100/1, H 150/1, N 10/1, O 5/1
Mass Tolerance       : 100ppm, 5mmu if m/z > 50
Unsaturation (U.S.) : 0.0 - 50.0

Observed m/z Int%   Err[ppm / mmu]     U.S.  Composition
 1153.7999     0.1     -3.5 /  -4.0    35.0  C 85 H 103 N O
                       +2.3 /  +2.7    32.0  C 76 H 99 N 9 O
                       +1.1 /  +1.3    31.5  C 78 H 101 N 6 O 2
                       +0.0 /  +0.0    31.0  C 80 H 103 N 3 O 3
                       +3.5 /  +4.0    27.0  C 75 H 103 N 5 O 5
```

**Figure S18.** HRMS (FAB) spectrum of **DPPPh2CN**.