Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.


# Photovoltaic properties of bis(octyloxy)benzo[c][1,2,5]-thiadiazole sensitizers based on *N*,*N*-diphenylthiophen-2-amine donor

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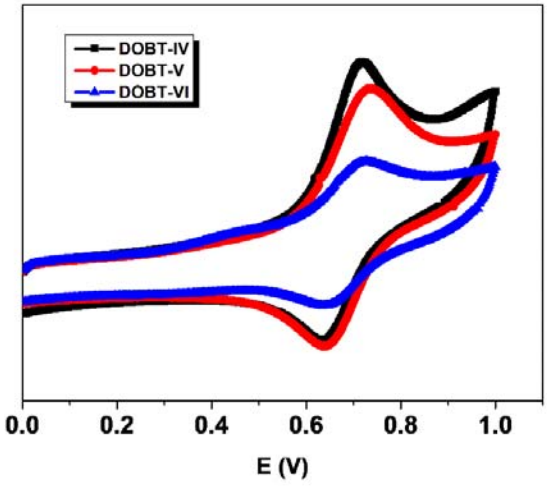



**Fig. S1**. Cyclic voltammetry plots of **DOBT-IV~VI** dyes measured in $CH_2Cl_2$ solution.

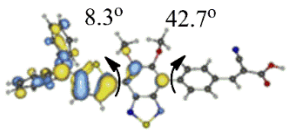
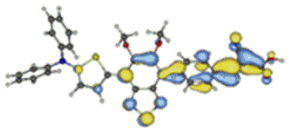
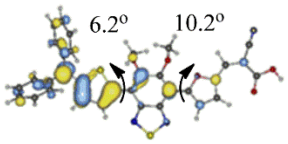
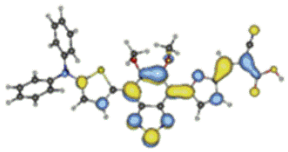
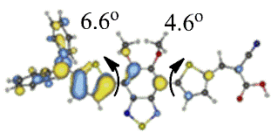
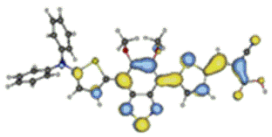
| Dye | HOMO[a] | LUMO |
|---|---|---|
| **DOBT-IV** |   |  |
| **DOBT-V** |   |  |
| **DOBT-VI** |   |  |

**Fig. S2**. The frontier orbitals of **DOBT-IV~VI**, calculated at (isodensity=0.020 a.u.) Hydrogens are omitted for clarity. [a] The dihedral angles between the benzothiadiazole rings and π-spacer near anchoring moiety

**Table S1**. Computed ICT absorption wavelength, oscillator strength, oxidation potential in ground state and excited state, and free energy for electron injection process. For $\lambda_{max}$, experimentally measured values are shown in parentheses for comparison.

| Compound | $\lambda_{max}$ / nm | Osc. Str. | $E_{OX}$(GS) / eV | $E_{OX}$(ES) / eV | $\Delta G^{inject}$ / eV |
|---|---|---|---|---|---|
| **DOBT-IV** | 500 (483) | 1.0755 | 4.95 | 2.47 | -1.53 |
| **DOBT-V** | 582 (525) | 1.4772 | 4.93 | 2.80 | -1.20 |
| **DOBT-VI** | 587 (531) | 1.5849 | 4.93 | 2.82 | -1.18 |

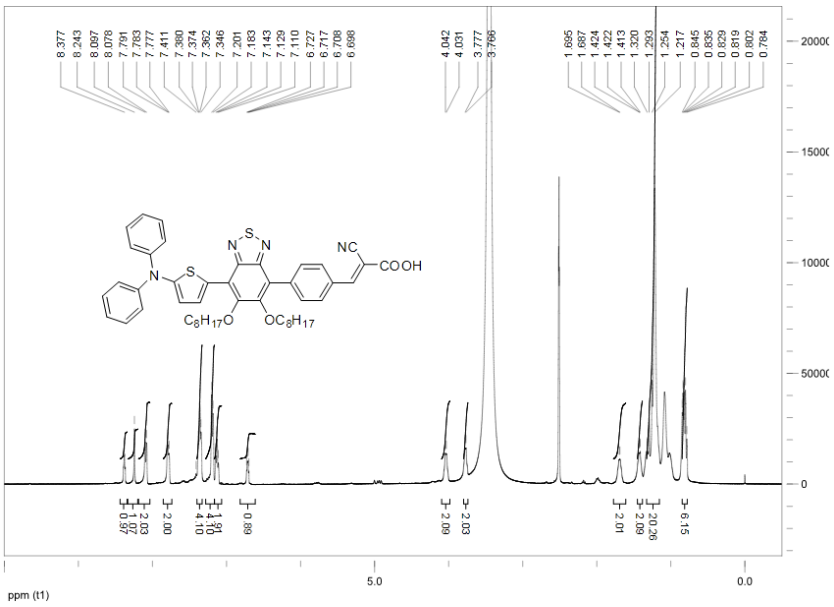
**Table S2**. Computed energy levels of frontier molecular orbitals and HOMO-LUMO energy gap. Shown in parentheses are the computed redox potentials with respect to NHE.

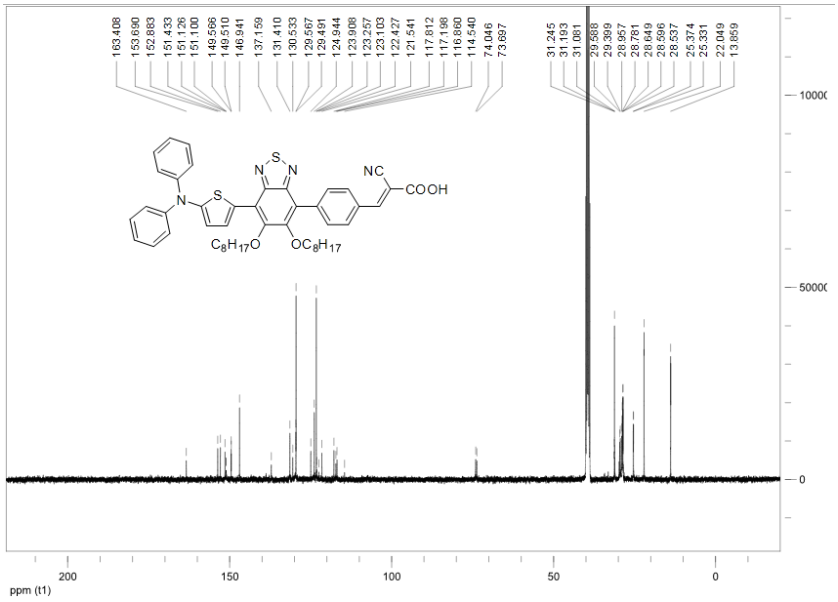
| Compound | HOMO / eV | LUMO / eV | $\Delta E$ / eV |
|---|---|---|---|
| **DOBT-IV** | -5.22 (0.78) | -2.76 (-1.68) | 2.46 |
| **DOBT-V** | -5.21 (0.77) | -2.91 (-1.53) | 2.30 |
| **DOBT-VI** | -5.22 (0.78) | -2.96 (-1.48) | 2.26 |

**Table S3**. The simulated results by using equivalent circuit of R(QR)(QR) for DSSCs with $I^-/I_3^-$ electrolyte and Co(II)/(III) electrolyte.

| Compound | $R_s$ (Ω) | $R_{CE}$ (Ω) | $R_{res}$ (Ω) | $\tau_e$ (ms) |
|---|---|---|---|---|
| **DOBT-IV**-I | 13.77 | 6.71 | 91.22 | 16.58 |
| **DOBT-V**-I | 17.54 | 8.79 | 57.79 | 11.70 |
| **DOBT-VI**-I | 13.69 | 7.47 | 23.18 | 5.35 |
| **DOBT-IV**-Co | 76.65 | 42.39 | 321.20 | 8.06 |
| **DOBT-V**-Co | 62.75 | 42.27 | 164.30 | 5.13 |
| **DOBT-VI**-Co | 16.89 | 64.19 | 42.99 | 0.82 |

# $^{1}$HNMR、 $^{13}$CNMR and HRMS of target compounds



**Elemental Composition Report** **Page 1**

**Single Mass Analysis**
Tolerance = 50.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
97 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-48 H: 0-120 N: 0-4 O: 0-4 S: 0-2

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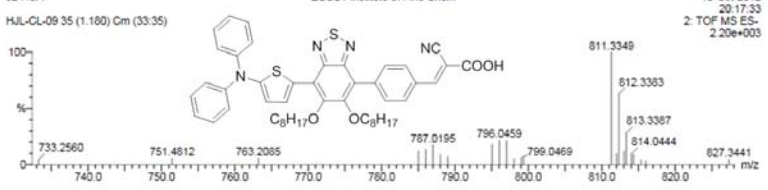
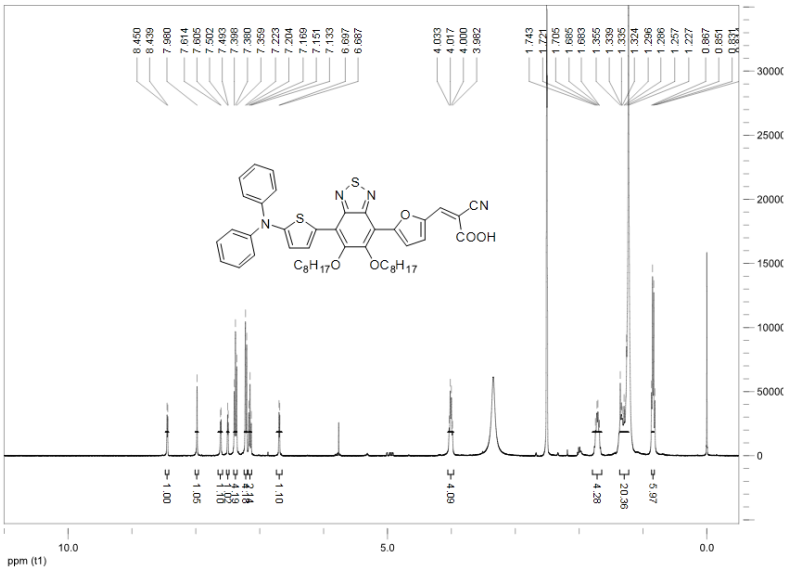
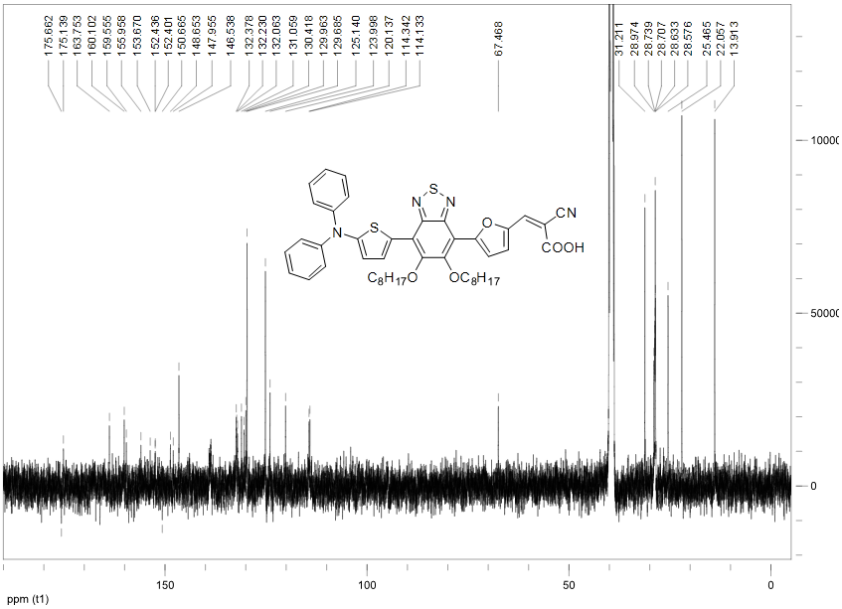



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 50.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 811.3349 | 811.3352 | -0.3 | -0.4 | 25.5 | 20.3 | 0.0 | C48 H51 N4 O4 S2 |



## Single Mass Analysis

Tolerance = 50.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
142 formula(e) evaluated with 3 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-48 H: 0-120 N: 0-4 O: 0-5 S: 0-2

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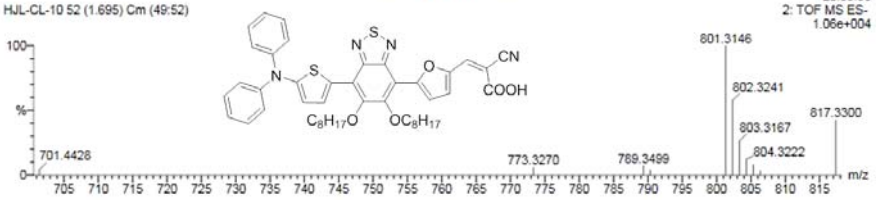
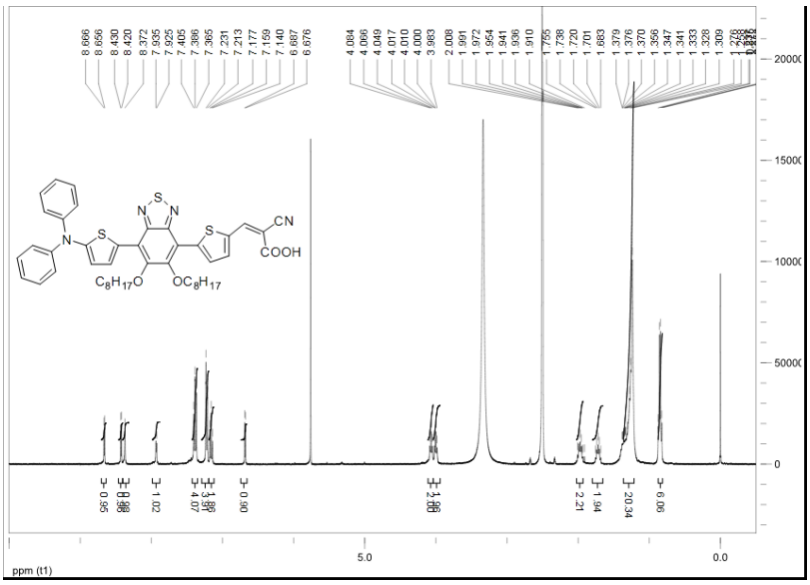
HJL-CL-10 52 (1.695) Cm (49:52) 2: TOF MS ES- 1.06e+004

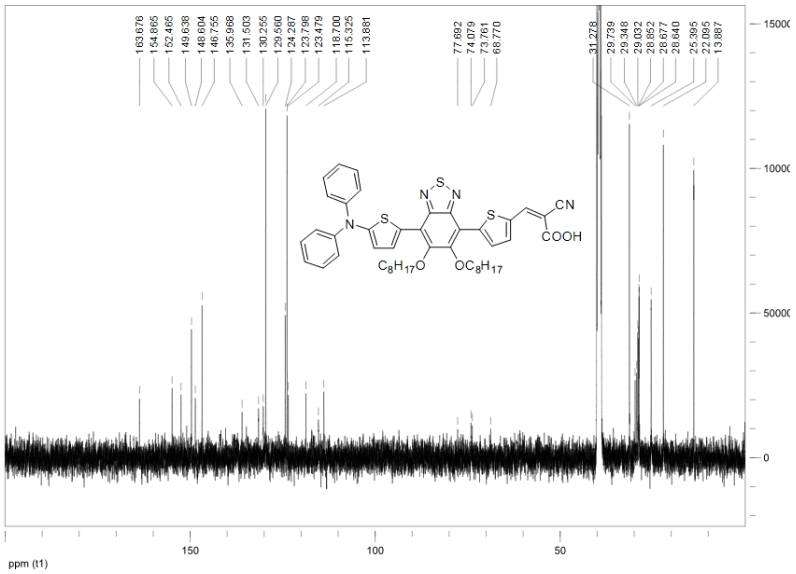






| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | 50.0 | 50.0 | -1.5 | | | |
| Maximum: | | | | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 801.3146 | 801.3144 | 0.2 | 0.2 | 24.5 | 14.2 | 0.0 | C46 H49 N4 O5 S2 |




**Elemental Composition Report** **Page 1**

**Single Mass Analysis**
Tolerance = 50.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
96 formula(e) evaluated with 8 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-50 H: 0-67 N: 0-4 O: 0-4 S: 0-3

JL-HUAN ECUST institute of Fine Chem 27-Jun-2012 22:42:49

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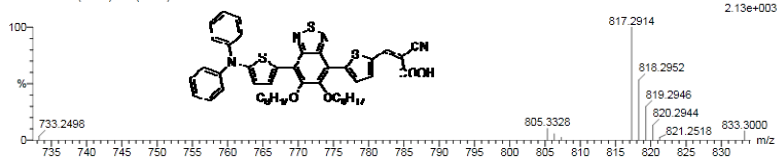


| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 50.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 817.2914 | 817.2916 | -0.2 | -0.2 | 24.5 | 8.8 | 0.0 | C46 H49 N4 O4 S3 |