Oligo(3-hexylthiophene)-Functionalized Dicyano-ethylene Substituted Quinacridone Derivatives: Synthesis, Characterizations and Applications as Acceptors in Photovoltaic Devices

Chenguang Wang,^{*a*} Weiping Chen,^{*a*} Shanyong Chen,^{*a*} Shanshan Zhao,^{*a*} Jingying Zhang,^{*a*} Dengli Qiu,^{*b*} and Yue Wang^{*a*}

^a State Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University, Changchun 130012, P. R. China
 ^b Bruker AXS GmbH Beijing Representative Office, Bruker Nano Inc., Beijing 100081, P. R. China

* To whom correspondence should be addressed. E-mail: yuewang@jlu.edu.cn

Figure S1. Cyclic voltammograms of DCN-Tn-QA (n = 1-3). 2

 Table S1. The photovoltaic performances of [ITO/PEDOT:PSS/P3HT:DCN-T2-QA/LiF/Al]
 3

 spin-coated from different solvent under AM 1.5 G, 100 mW cm⁻².
 Table S2. The photovoltaic performances of [ITO/PEDOT:PSS/P3HT:DCN-T2-QA/LiF/Al]
 3
 at different annealing temperature under AM 1.5 G, 100 mW cm $^{-2}$.

 Table S3. The photovoltaic performances of [ITO/PEDOT:PSS/P3HT:DCN-T2-QA/LiF/Al]
 4

 at different ratio of donor/acceptor under AM 1.5 G, 100 mW cm $^{-2}$. Figure S2. ¹H NMR spectra of 1 recorded in CDCl₃ (300 M Hz). 5 Figure S3. ¹H NMR spectra of 2 recorded in CDCl₃ (300 M Hz). 6 Figure S4. ¹³C NMR spectra of 2 recorded in CDCl₃ (75 M Hz). 7 Figure S5. ¹H NMR spectra of 3 recorded in CDCl₃ (300 M Hz). 8 Figure S6. ¹H NMR spectra of 4 recorded in CDCl₃ (300 M Hz). 9 Figure S7. ¹³C NMR spectra of 4 recorded in CDCl₃ (75 M Hz). 10 **Figure S8.**¹H NMR spectra of **5** recorded in CDCl₃ (300 M Hz). 11 Figure S9. ¹³C NMR spectra of 5 recorded in CDCl₃ (75 M Hz). 12 **Figure S10.** ¹H NMR spectra of **6** recorded in CDCl₃ (300 M Hz). 13 Figure S11. ¹³C NMR spectra of 6 recorded in CDCl₃ (75 M Hz). 14 **Figure S12.** ¹H NMR spectra of **7** recorded in CDCl₃ (300 M Hz). 15 Figure S13. ¹³C NMR spectra of 7 recorded in CDCl₃ (75 M Hz). 16 **Figure S14.** ¹H NMR spectra of **8** recorded in CDCl₃ (500 M Hz). 17 Figure S15. ¹³C NMR spectra of 8 recorded in CDCl₃ (75 M Hz). 18 Figure S16. ¹H NMR spectra of DCN-T1-OA recorded in CDCl₃ (500 M Hz). 19 Figure S17. ¹³C NMR spectra of DCN-T1-OA recorded in CDCl₃ (75 M Hz). 20 Figure S18. ¹H NMR spectra of DCN-T2-QA recorded in CDCl₃ (500 M Hz). 21 Figure S19. ¹³C NMR spectra of DCN-T2-QA recorded in CDCl₃ (75 M Hz). 22 Figure S20. ¹H NMR spectra of DCN-T3-QA recorded in CDCl₃ (500 M Hz). 23 Figure S21. ¹³C NMR spectra of DCN-T3-OA recorded in CDCl₃ (75 M Hz). 24



Figure S1. Cyclic voltammograms of DCN-Tn-QA (n = 1–3) in CH₂Cl₂ solution, measured with TBAPF (0.1 M) as a supporting electrolyte at a scan rate of 100 mV $^{s-1}$.

Table S1. The photovoltaic performances of

[ITO/PEDOT:PSS/P3HT:DCN-T2-QA/LiF/A1] spin-coated from different solvent under AM 1.5 G, 100 mW cm $^{-2}$

	$V_{ m oc}$	$J_{ m sc}$	FF	PCE
Solvent (V:V)	(V)	(mAcm^{-2})	(%)	(%)
o-DCB : CHCl ₃ 1 : 1	0.46	2.80	40	0.51
o-DCB : CHCl ₃ 2 : 1	0.44	2.51	43	0.47
o-DCB	0.46	1.86	46	0.40

The weight ratio of P3HT : DCN-T2-QA is 1 : 1 and the annealing temperature is 60 $\,^{\circ}$ C (10 min) and the active layer is about 110 nm.

Table S2. The photovoltaic performances of

[ITO/PEDOT:PSS/P3HT:DCN-T2-QA/LiF/Al] at different annealing temperature under AM 1.5 G, 100 mW cm⁻²

	$V_{ m oc}$	$J_{ m sc}$	FF	PCE
Annealing temperature	(V)	$(\mathrm{mA\ cm}^{-2})$	(%)	(%)
Without annealing	0.54	1.52	29	0.24
60 °C for 10 min	0.46	2.80	40	0.51
80 °C for 10 min	0.44	2.03	37	0.33

The weight ratio of P3HT : DCN-T2-QA is 1 : 1 and the solvent is o-DCB/CHCl₃ (1 : 1, V : V) and the active layer is about 110 nm.

Table S3. The photovoltaic performances of

[ITO/PEDOT:PSS/P3HT:DCN-T2-QA/LiF/A1] at different ratio of donor/acceptor under AM 1.5 G, 100 mW cm $^{-2}$

	V _{oc}	$\overline{J}_{ m sc}$	FF	PCE
P3HT:DCN-T2-QA (w:w)	(V)	(mAcm^{-2})	(%)	(%)
1.0 : 1.5	0.46	2.13	44	0.43
1.0 : 1.0	0.46	2.80	40	0.51
1.5 : 1.0	0.42	1.86	42	0.33

The annealing temperature is 60 °C (10 min) and the solvent is o-DCB/CHCl₃ (1 : 1, V : V) and the active layer is about 110 nm.



Figure S2. ¹H NMR spectra of **1** recorded in CDCl₃ (300 M Hz).



Figure S3. ¹H NMR spectra of **2** recorded in CDCl₃ (300 M Hz).



Figure S4. ¹³C NMR spectra of **2** recorded in CDCl₃ (75 M Hz).

Electronic Supplementary Material (ESI) for New Journal of Chemistry This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2012



Figure S5. ¹H NMR spectra of **3** recorded in CDCl₃ (300 M Hz).







Figure S6. ¹H NMR spectra of **4** recorded in CDCl₃ (300 M Hz).



Figure S7. ¹³C NMR spectra of **4** recorded in CDCl₃ (75 M Hz).







Figure S8. ¹H NMR spectra of **5** recorded in CDCl₃ (300 M Hz).



Figure S9. ¹³C NMR spectra of **5** recorded in CDCl₃ (75 M Hz).







Figure S10. ¹H NMR spectra of **6** recorded in CDCl₃ (300 M Hz).



Figure S11. ¹³C NMR spectra of **6** recorded in CDCl₃ (75 M Hz).







Figure S12. ¹H NMR spectra of **7** recorded in CDCl₃ (300 M Hz).



Figure S13. ¹³C NMR spectra of 7 recorded in CDCl₃ (75 M Hz).

Electronic Supplementary Material (ESI) for New Journal of Chemistry This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2012



Figure S14. ¹H NMR spectra of **8** recorded in CDCl₃ (500 M Hz).



Figure S15. ¹³C NMR spectra of 8 recorded in CDCl₃ (75 M Hz).







Figure S16. ¹H NMR spectra of **DCN-T1-QA** recorded in CDCl₃ (500 M Hz).



Figure S17. ¹³C NMR spectra of DCN-T1-QA recorded in CDCl₃ (75 M Hz).



Figure S18. ¹H NMR spectra of DCN-T2-QA recorded in CDCl₃ (500 M Hz).



Figure S19. ¹³C NMR spectra of DCN-T2-QA recorded in CDCl₃ (75 M Hz).



Figure S20. ¹H NMR spectra of DCN-T3-QA recorded in CDCl₃ (500 M Hz).



Figure S21. ¹³C NMR spectra of **DCN-T3-QA** recorded in CDCl₃ (75 M Hz).