Electronic Supplementary Information

Efficient and stable organic DSSC sensitizers bearing quinacridone and furan moiety as a well-planarity π-spacer

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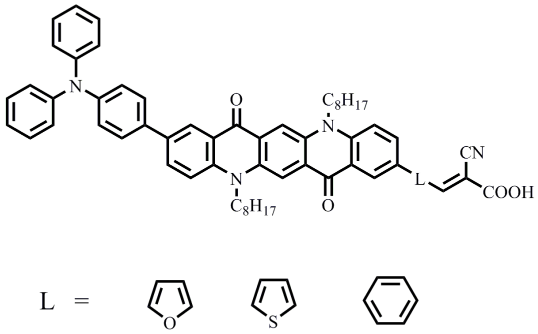


Scheme S1 Molecular structures of **QA** based dyes with different π-spacers

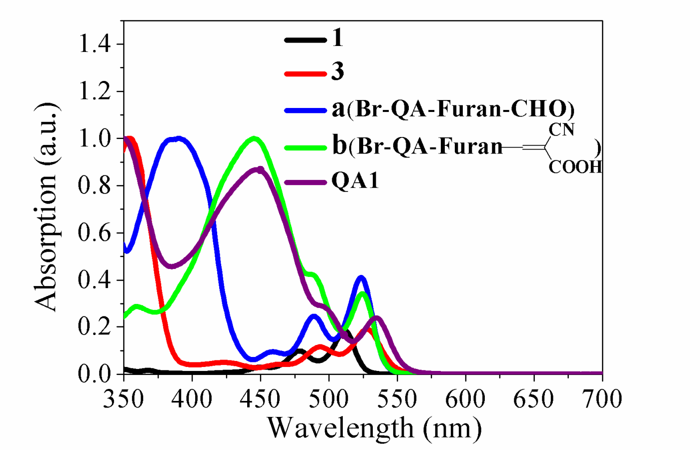


Fig. S1 UV-Vis absorption spectra of **QA1** and intermediates **1**, **3**, **a** and **b** in THF solutions. Note: In the presence of furan ring and terminal cynaoacrylic acid group, the UV-Vis spectra of both **b** and **QA1** shows the absorption peak at around 446 nm, meanwhile that of **1**, **3** and **a** shows no evident peak here. Compared with **b**, the absorption peak of **QA1** at around 446 nm almost gives no shift, which indicates that the triarylamine moiety gives no contribution to the middle band.

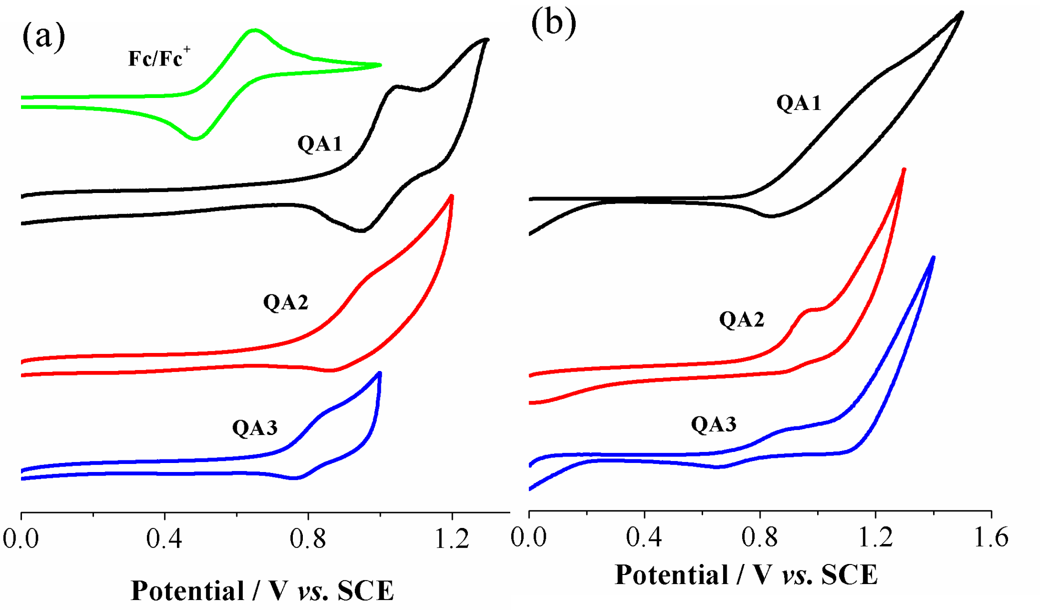


Fig. S2 Cyclic voltammetry plots of **QA1-3** measured in THF solution (a) and on nanocrystalline TiO_2 film deposited on conducting FTO glass (b) with $TBAPF_6$ (0.1M) as the electrolyte.

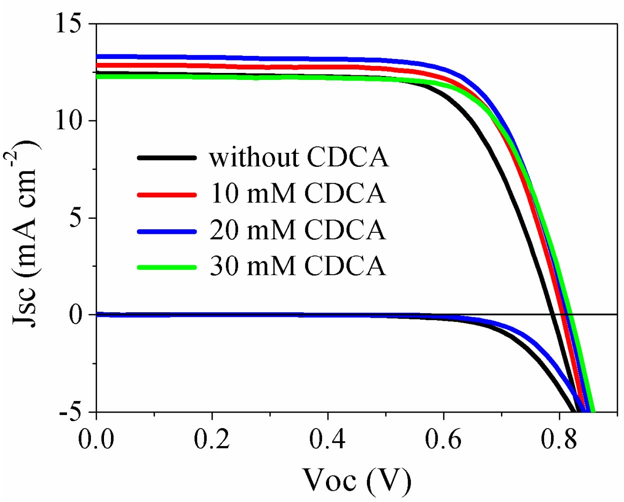


Fig. S3 I-V curves for untreated and CDCA with different concentrations of 10 mM, 20 mM and 30 mM co-adsorbed DSSCs based on dye **QA1** under light (100 mW cm^{-2} simulated AM 1.5 solar light).

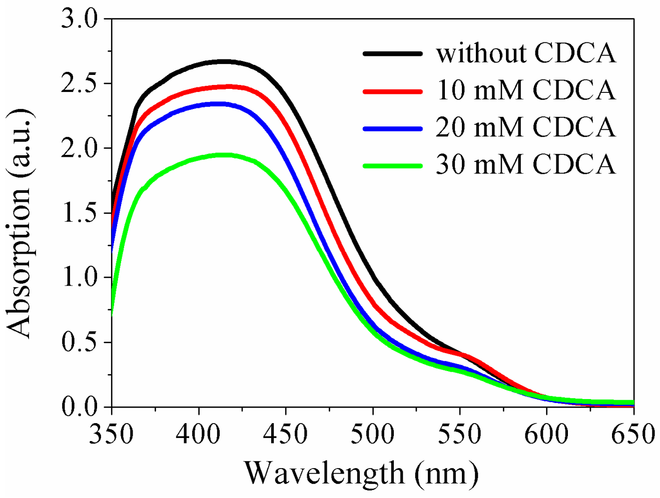


Fig. S4 UV-Vis absorption spectra of TiO_2 electrodes sensitized by **QA1** containing 0, 10, 20, 30 mM CDCA after adsorption for 12 h.

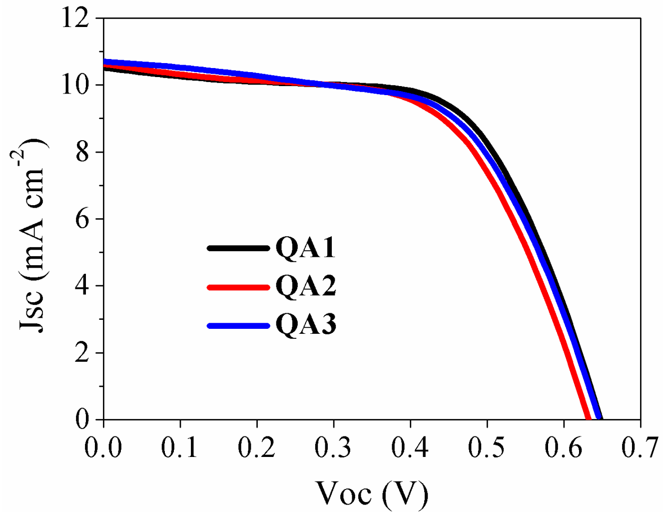


Fig. S5 I-V curves for 20 mM CDCA co-adsorbed DSSCs based on dyes **QA1-3** using ionic-liquid electrolyte.

Table S1 TD-DFT parameters (composition in terms of molecular orbital contributions, excitation energies (*E*) and wavelengths (λ) for the lowest transitions, and oscillator strengths (*f*))

Dye	State	Composition	*E*/eV, λ/nm	*f*
QA1	S_1	H-0 -> L+0 (73%), H-0 -> L+1 (17%)	2.37 eV, 522 nm	0.2812
	S_2	H-0 -> L+0 (16%), H-0 -> L+1 (75%)	2.50 eV, 495 nm	0.0950
	S_3	H-1 -> L+0 (83%)	2.65 eV, 468 nm	0.5034
QA2	S_1	H-0 -> L+0 (79%), H-0 -> L+1 (14%)	2.27 eV, 546 nm	0.2908
	S_2	H-0 -> L+0 (15%), H-0 -> L+1 (79%)	2.40 eV, 515 nm	0.0459
	S_3	H-1 -> L+0 (86%)	2.63 eV, 470 nm	0.7152
QA3	S_1	H-0 -> L+0 (84%), H-0 -> L+1 (13%)	2.18 eV, 568 nm	0.1163
	S_2	H-0 -> L+0 (13%), H-0 -> L+1 (83%)	2.31 eV, 536 nm	0.0078
	S_3	H-1 -> L+0 (90%)	2.58 eV, 481 nm	0.6925

Table S2 The electron distribution in HOMO-1 and LUMO levels of dyes in THF solution

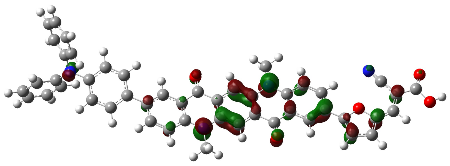
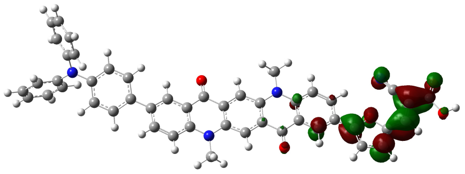
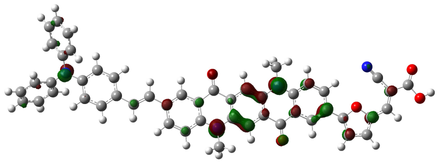
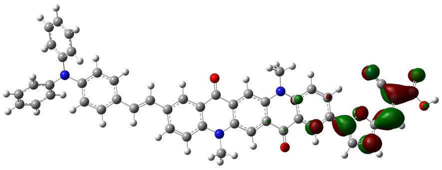
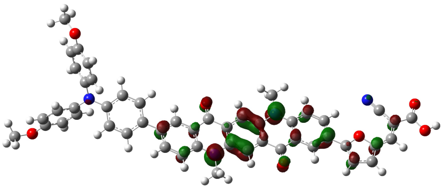
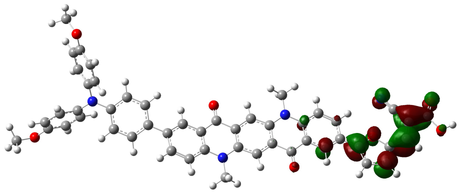
Dye	HOMO-1	LUMO
QA1		
QA2		
QA3		

Table S3 The optimized structures and the dihedral angles between the quinacridone moiety and furan ring of dyes

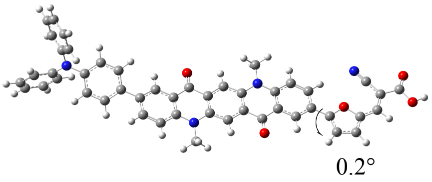
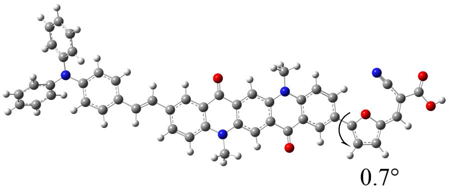
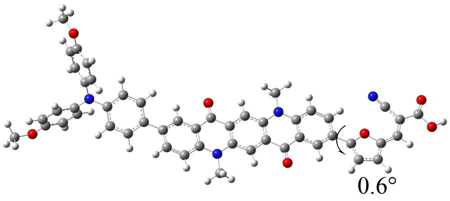
Dye	Optimized structure [a]
QA1	
QA2	
QA3	

Table S4 The electron distribution in HOMO and LUMO levels of dyes in gas phase

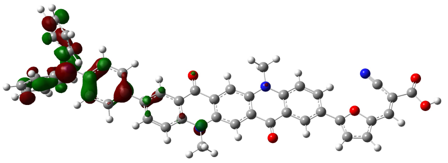
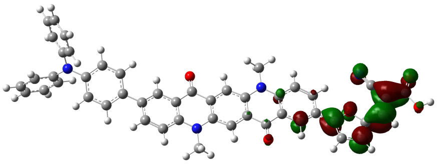
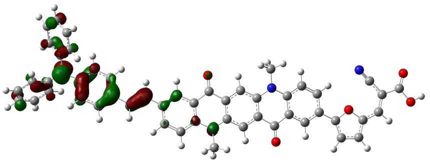
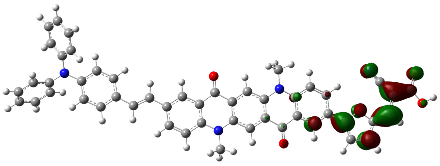
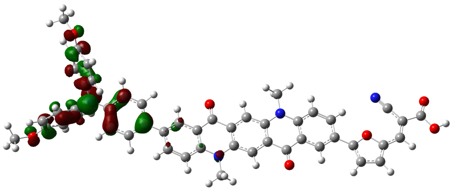
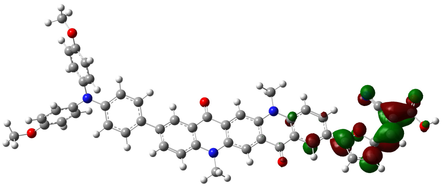
Dye	HOMO	LUMO
QA1		
QA2		
QA3		

Table S5 Photovoltaic performance of 20 mM CDCA co-adsorbed DSSCs based on dyes **QA1-3** using ionic-liquid electrolyte. [a]

Dye	J_{sc}/mA cm^{-2}	V_{oc}/mV	*ff*	η (%)
QA1[b]	10.60	640	0.63	4.28
QA2[b]	10.74	624	0.60	4.04
QA3[b]	10.86	641	0.60	4.15

[a] Measured under irradiation of AM 1.5 G simulated solar light (100 mW cm^{-2}) at room temperature, 11 μm film thickness, 0.28 cm^2 working area, electrolyte containing: 0.1 M I_2, 0.1 M LiI, 0.45 M BI in PMII. [b] The concentration of **QA** dyes is 3 × 10^{-4} M in THF.