Supporting Information

Novel Triphenylamine-Modified Ruthenium(II) Terpyridine Complexes for Nickel Oxide-based Cathodic Dye-sensitized Solar Cells.

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1) NMR spectra for **K1** and **K2**
2) UV-visible absorption spectra of **K1** and **K2**
3) Differential Pulse Voltammetry for **K1** and **K2**
4) FTIR spectra of **K1** and **K2** adsorbed on NiO
5) Emission decay for **K1** in methanol
6) DFT calculations for **K1** and **K2** in methanol
7) *J*-*V* and IPCE data for **K1** with $Co(dtb)_3ClO_{3(2)}$ electrolyte.

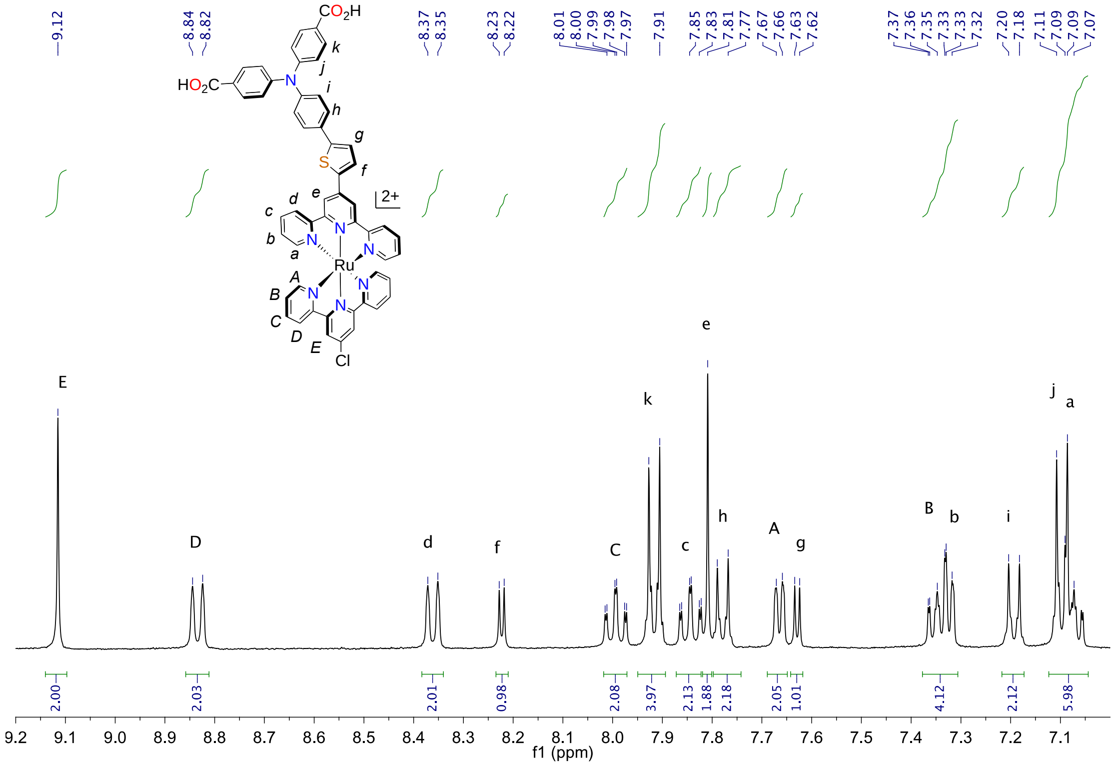


Figure S1. ^{1}H NMR spectrum of **K1** in MeOD with assignments.

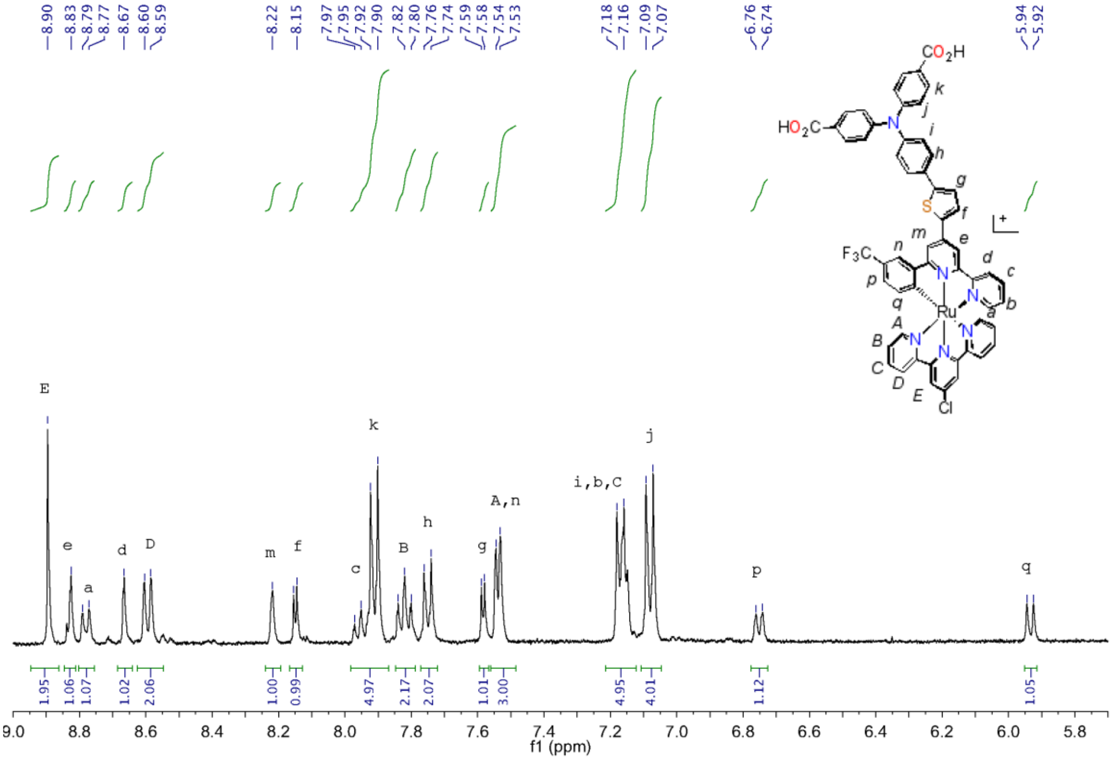


Figure S2. ^{1}H NMR spectrum of **K2** in MeOD/NaOD with assignments.

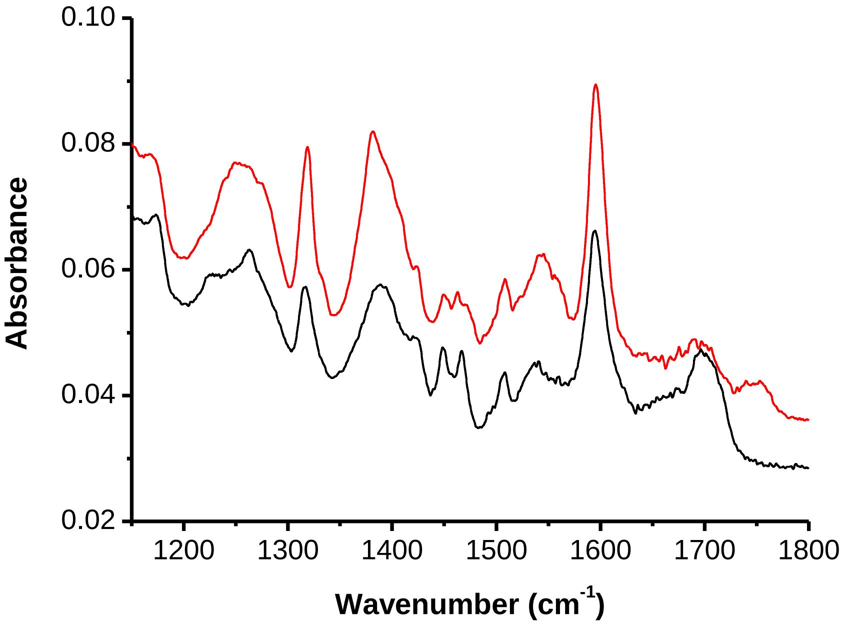


Figure S3. FTIR spectra of **K1** (black) and **K2** (red) adsorbed on NiO.

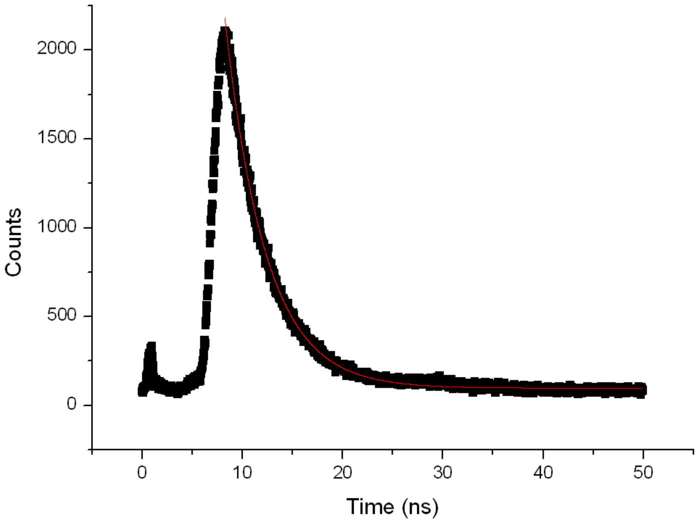


Figure S4 Plot of emission decay of **K1** at 530 nm (excitation at 406 nm). The data was fitted to a single exponential function to give and excited state lifetime of 4.053 (+/- 0.01) ns. This lifetime is considered too close to the instrument response time of the detector to be meaningful.

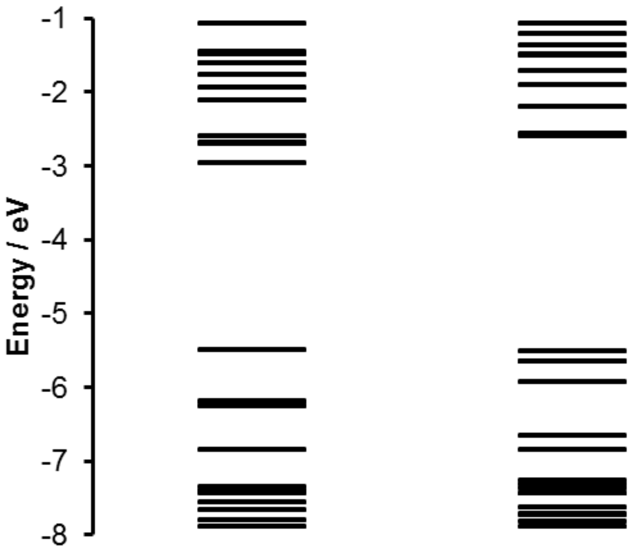
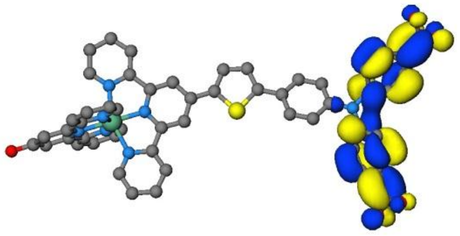
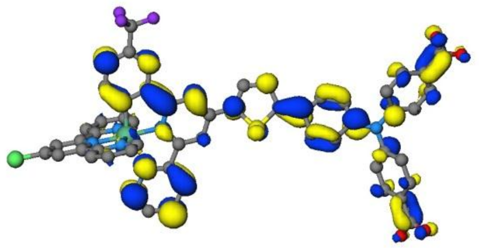
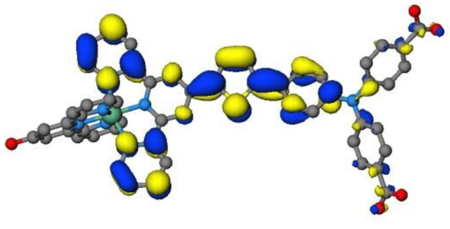
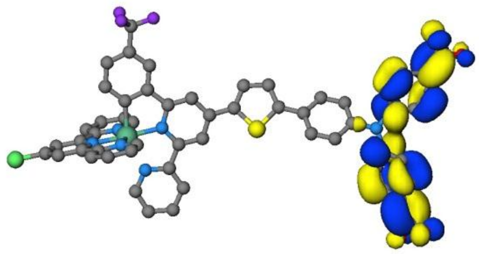
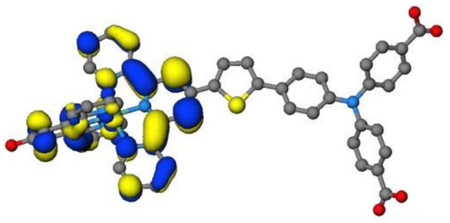
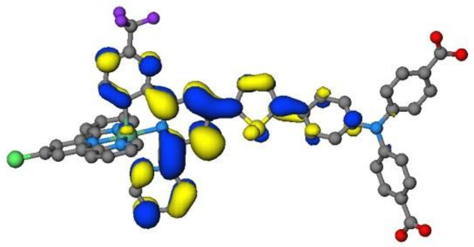
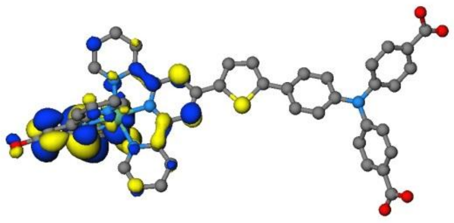
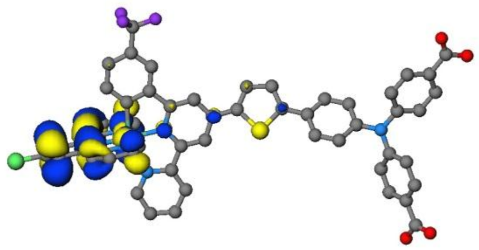
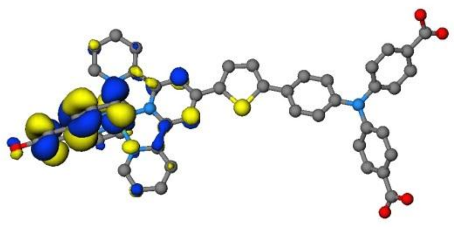
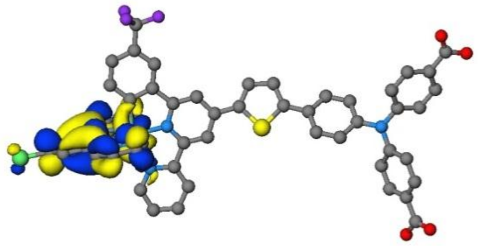


Figure S5. Molecular orbital energy level plot for **K1** (left) and **K2** (right).

	K1	**K2**
LUMO+5	-1.93	-1.72
LUMO+4	-2.11	-1.91
LUMO+3	-2.60	-2.19
LUMO+2	-2.68	-2.57
LUMO+1	-2.70	-2.58
LUMO	-2.97	-2.61
HOMO	-5.49	-5.52
HOMO-1	-6.19	-5.65
HOMO-2	-6.20	-5.66
HOMO-3	-6.25	-5.93
HOMO-LUMO	2.52	2.91

Table S6. Energies of frontier orbitals.

	K1	**K2**
LUMO+5		
LUMO+4		
LUMO+3		
LUMO+2		
LUMO+1		

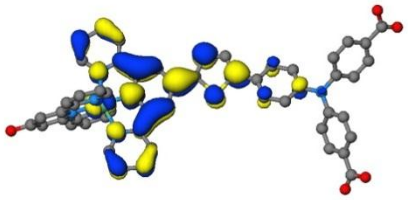
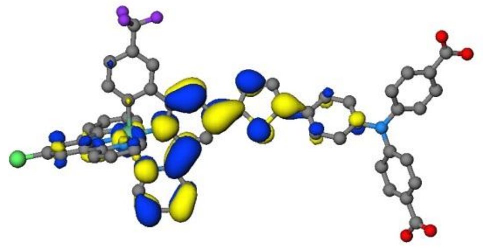
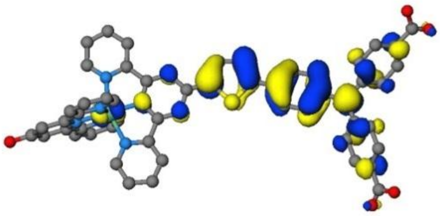
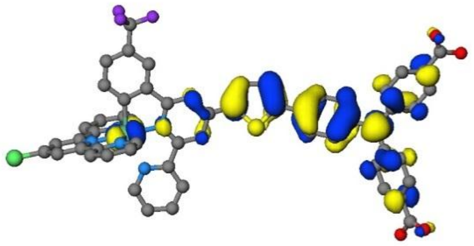
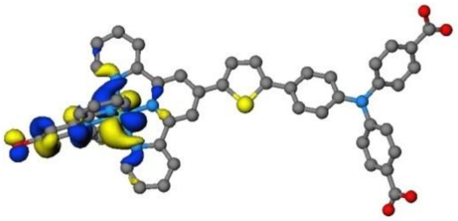
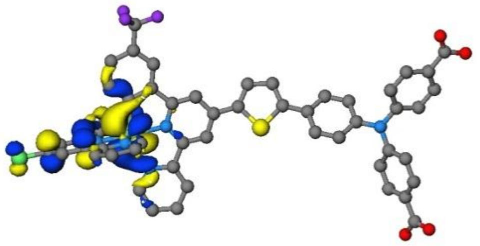
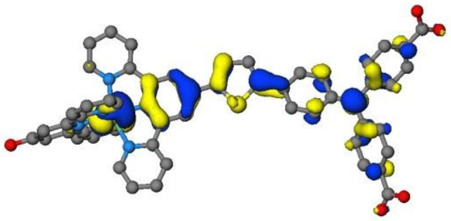
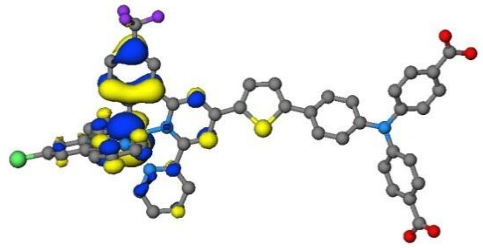
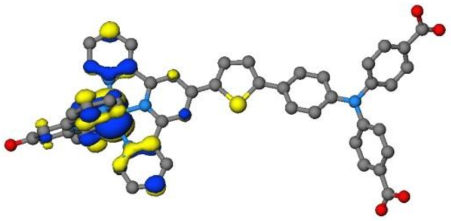
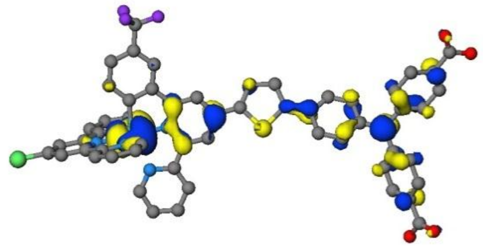
LUMO		
HOMO		
HOMO-1		
HOMO-2		
HOMO-3		

Table S2.Electron distribution in the frontier orbitals.

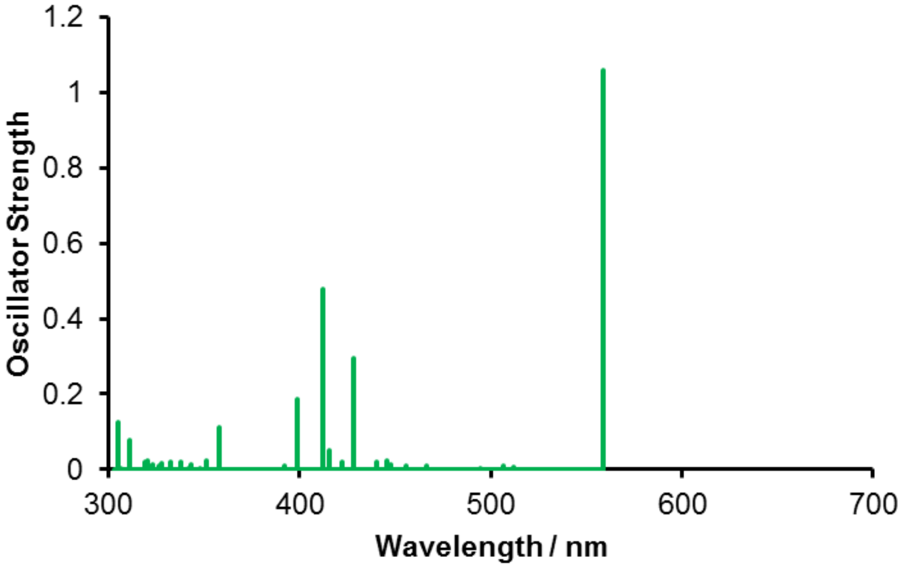


Figure S7. Calculated TD-DFT optical absorption spectrum for **K1**

Table S3. Wavelengths, oscillator strengths (*f*) and predominant compositions or selected major transitions for **K1**.

State	λ / nm	*f*	Composition
S_1	559	1.058	HOMO→LUMO
S_{13}	428	0.256	HOMO-3→LUMO+1 & HOMO-3→LUMO+2
S_{16}	412	0.477	HOMO→LUMO+4
S_{17}	398	0.188	HOMO→LUMO+5
S_{21}	358	0.113	HOMO-4→LUMO & HOMO→LUMO+7

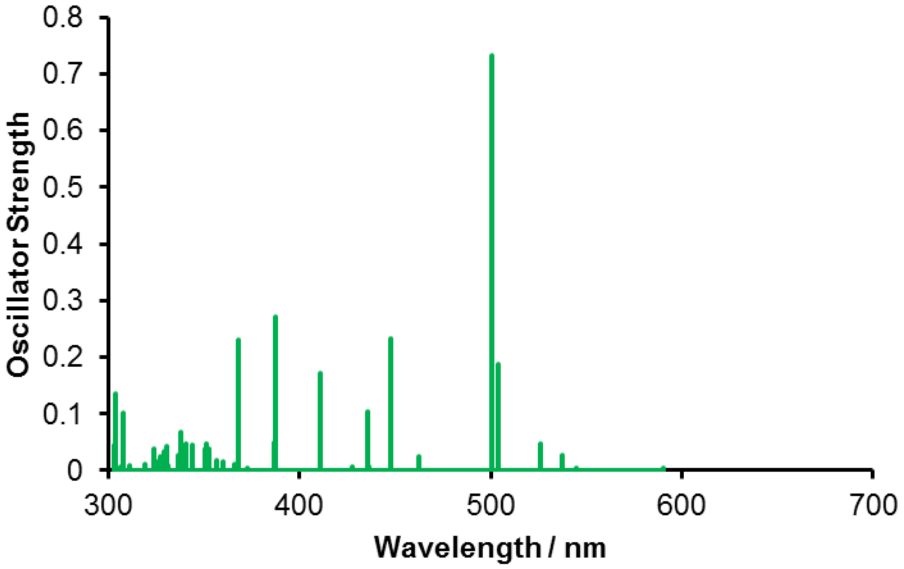


Figure S8. Calculated TD-DFT optical absorption spectrum for **K2**

Table S.4. Wavelengths, oscillator strengths (*f*) and predominant compositions or selected major transitions for **K2**.

State	λ / nm	*f*	Composition
S_1	590	0.0053	HOMO-2→LUMO+1
S_7	504	0.187	HOMO→LUMO & HOMO→LUMO+2
S_8	501	0.733	HOMO→LUMO & HOMO→LUMO+2
S_{10}	447	0.234	HOMO-1→LUMO+1 & HOMO-2→LUMO+2
S_{13}	435	0.104	HOMO→LUMO+3
S_{15}	411	0.171	HOMO-3→LUMO & HOMO-2→LUMO+3
S_{16}	387	0.272	HOMO→LUMO+4
S_{19}	368	0.230	HOMO→LUMO+5

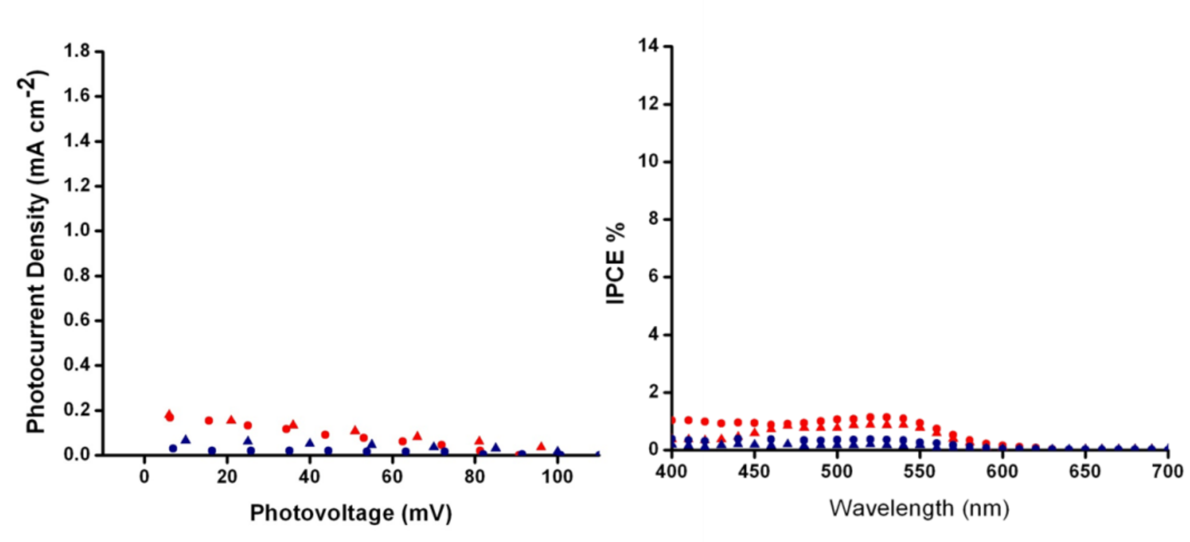


Figure S9. IV and IPCE characterisation of **K1** DSCs incorporating 0.1M $Co(dtb)_3(ClO_4)_{3(2)}$ in propylene carbonate (bottom) showing measurements at 0 hours (circles) and 12 hours (triangles) with 1 hour ‘light soaking’ (red) and kept in the dark (blue).