Supporting Information

Systematic investigations on the roles of the electron acceptor and neighboring ethynylene moiety in porphyrins for dye sensitized solar cells

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Characterization data for the compounds

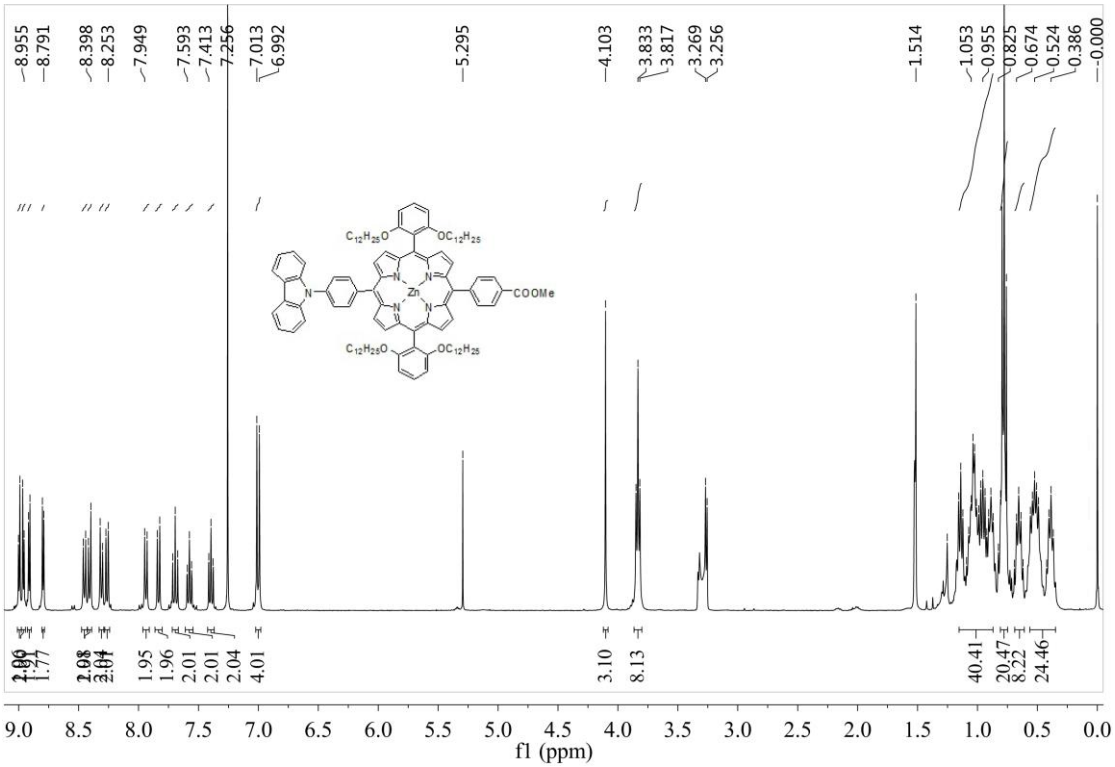

Figure S1. The ^{1}H NMR spectrum of **1s** in $CDCl_3$

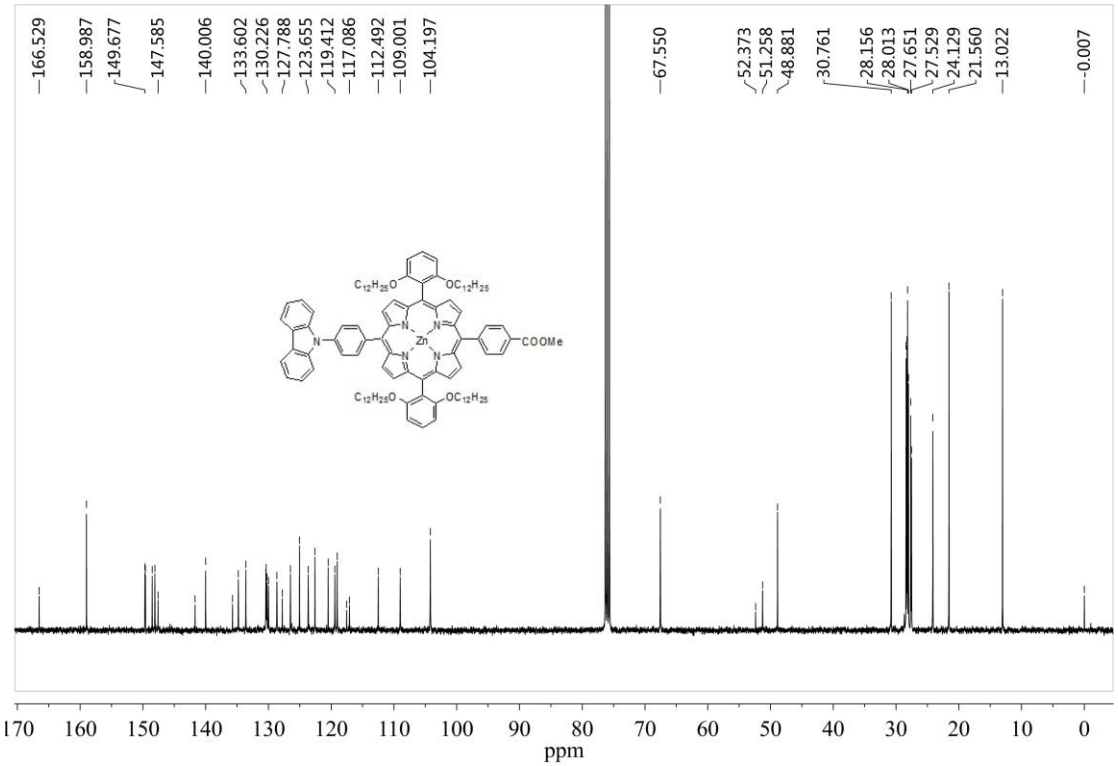

Figure S2. The ^{13}C NMR spectrum of **1s** in $CDCl_3$

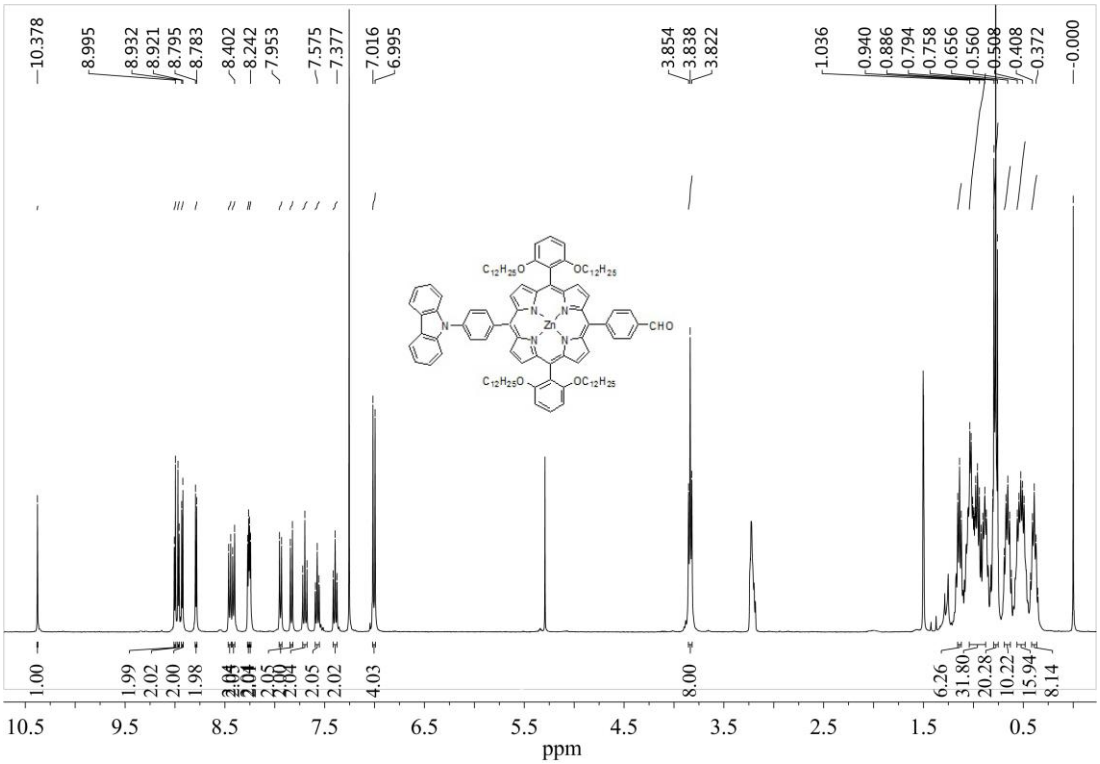

Figure S3. The ^{1}H NMR spectrum of **2s** in $CDCl_3$

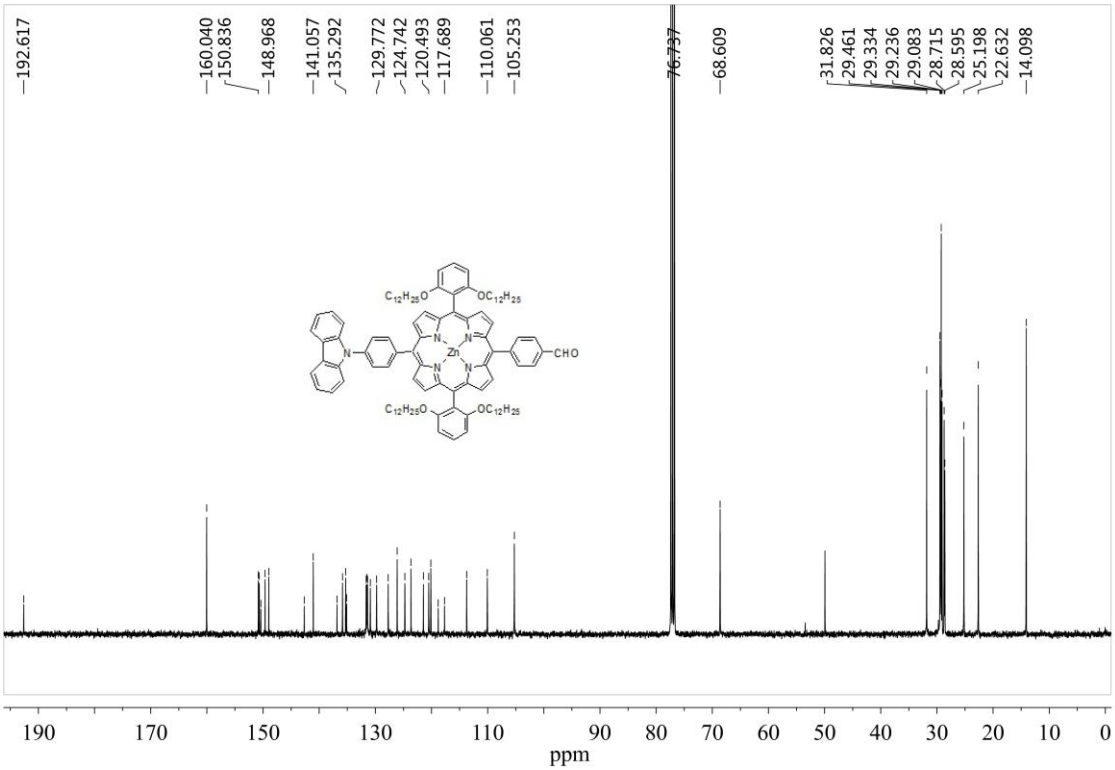

Figure S4. The ^{13}C NMR spectrum of **2s** in $CDCl_3$

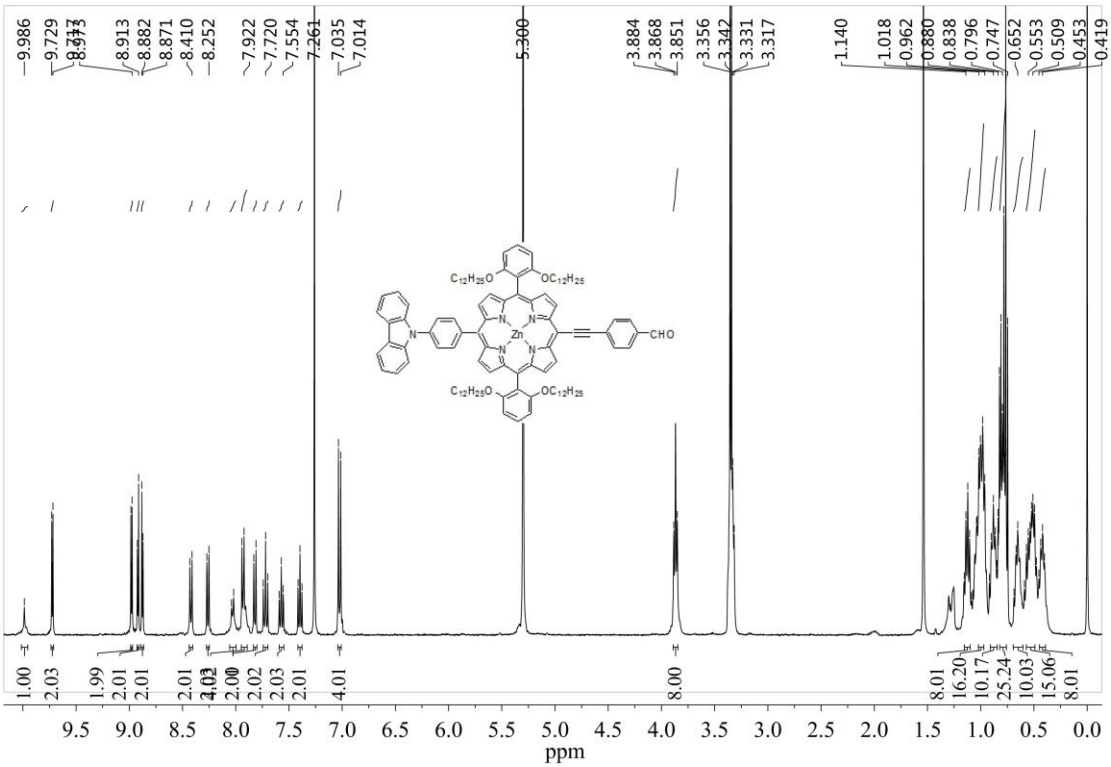

Figure S5. The ^{1}H NMR spectrum of **3s** in $CDCl_3$

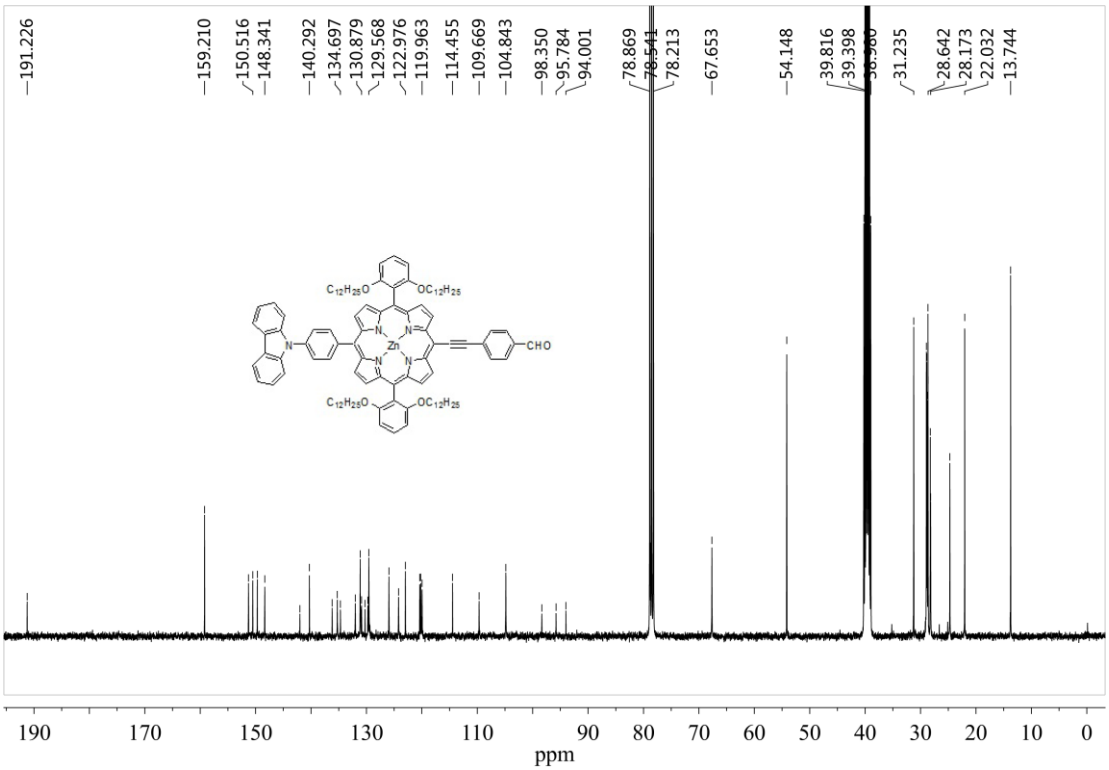

Figure S6. The ^{13}C NMR spectrum of **3s** in $CDCl_3$

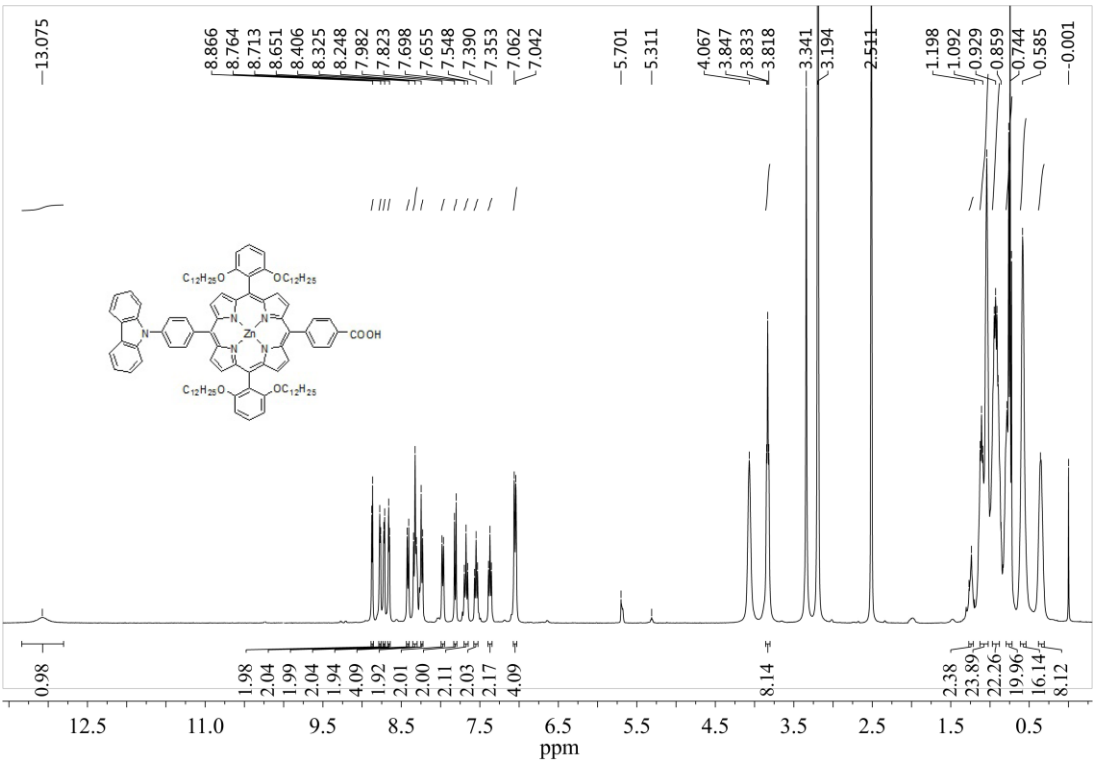

Figure S7. The ^{1}H NMR spectrum of **XW5** in $CDCl_3$:DMSO-d_6 (1 : 3)

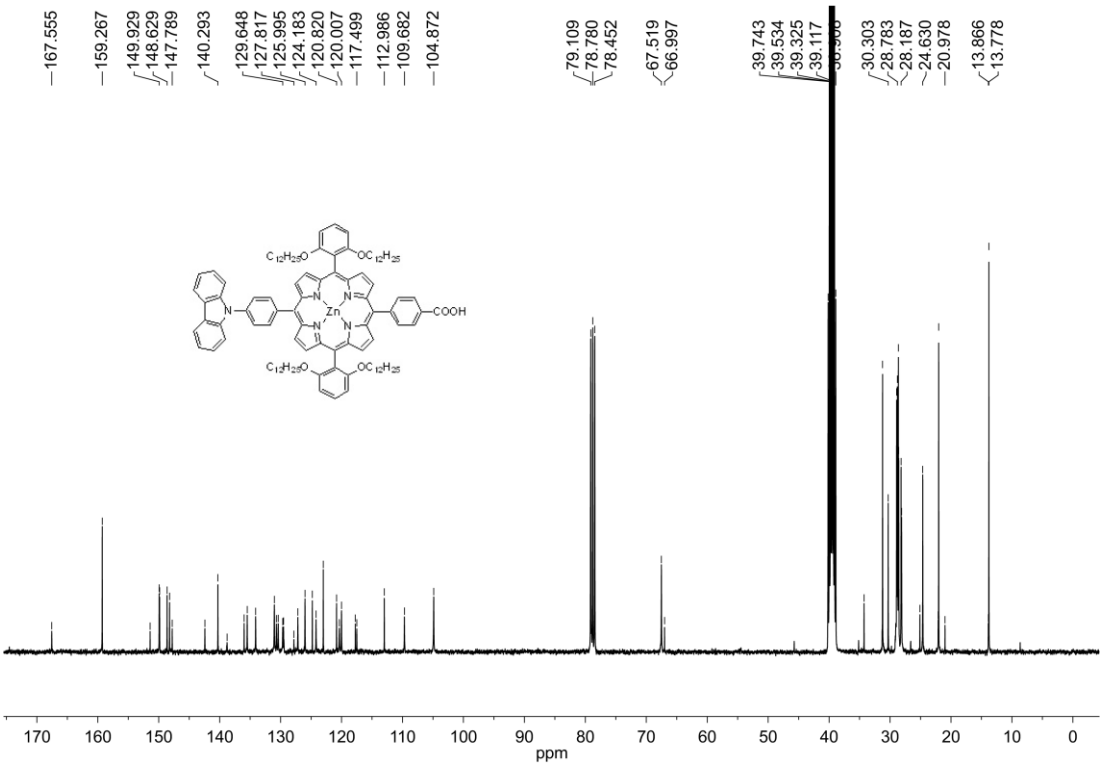

Figure S8. The ^{13}C NMR spectrum of **XW5** in $CDCl_3$:DMSO-d_6 (1 : 3)

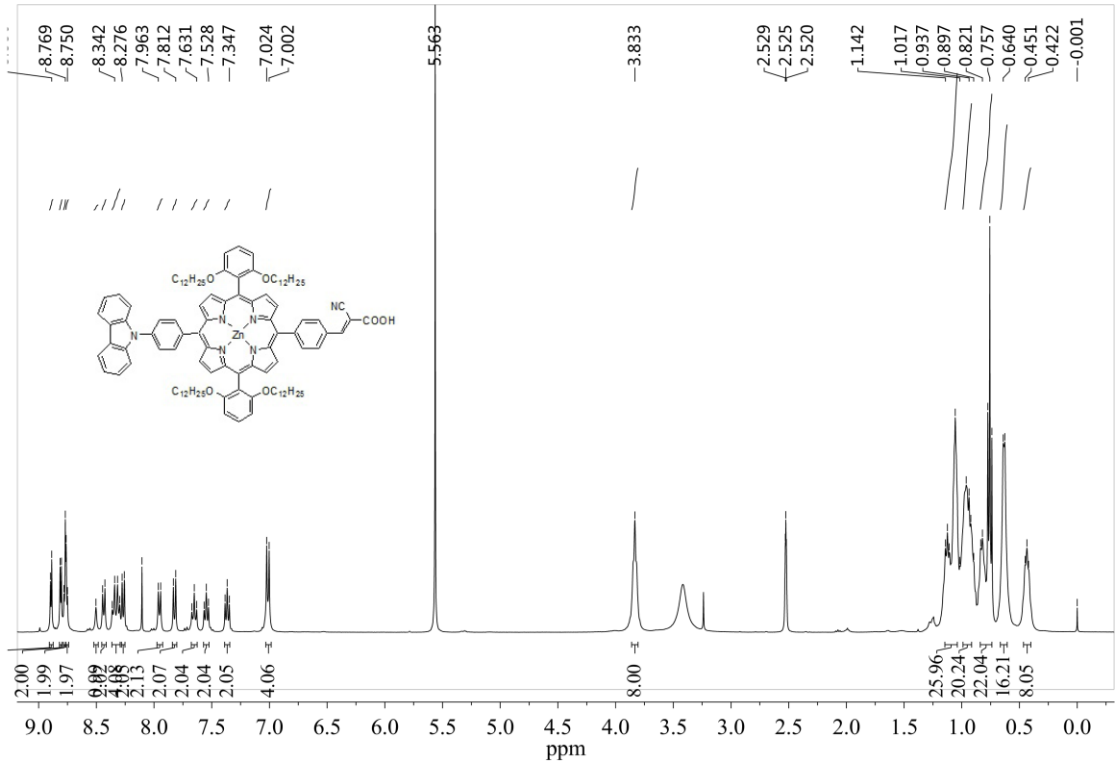

Figure S9. The ^{1}H NMR spectrum of **XW6** in $CDCl_3$:DMSO-d_6 (1 : 3)

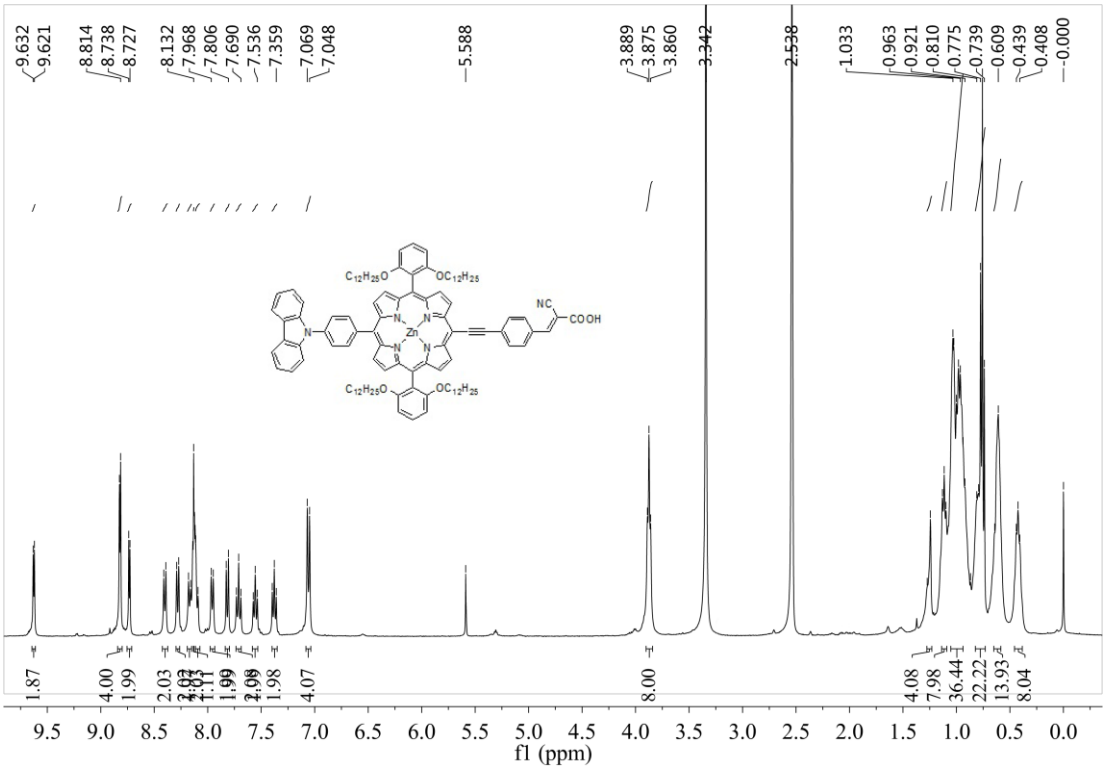

Figure S10. The ^{1}H NMR spectrum of **XW7** in $CDCl_3$: DMSO-d_6 (1 : 3)

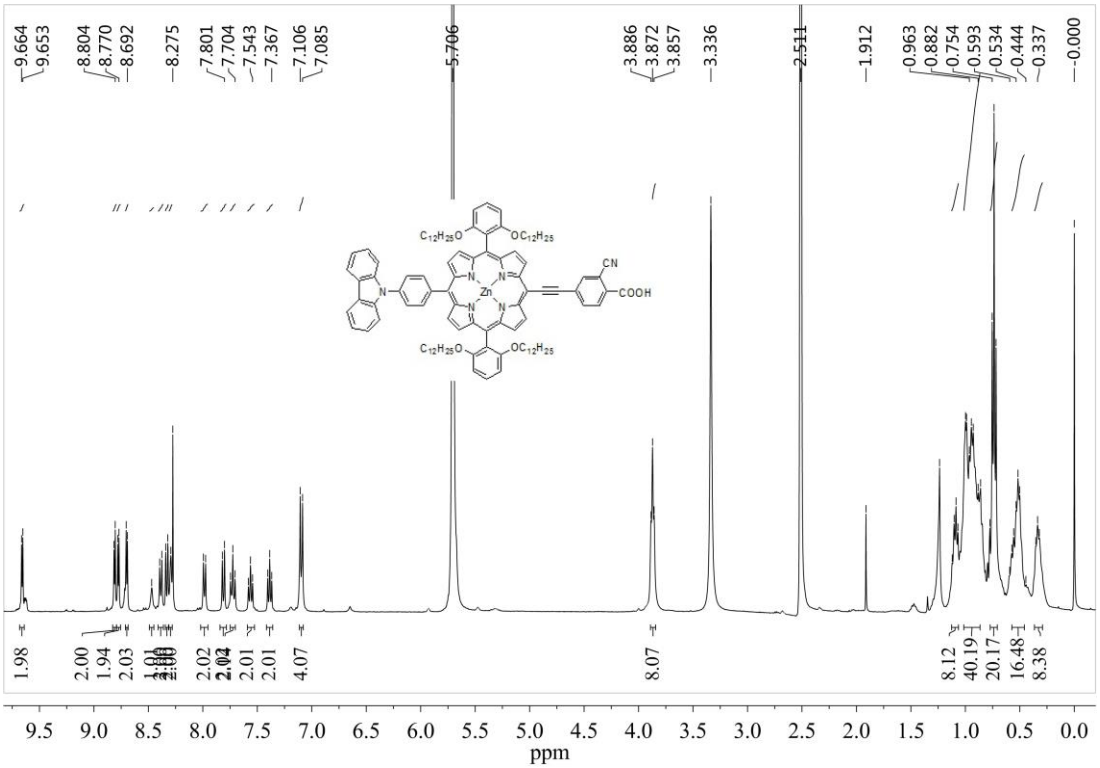

Figure S11. The ^{1}H NMR spectrum of **XW8** in $CDCl_3$: DMSO-d_6 (1 : 3)

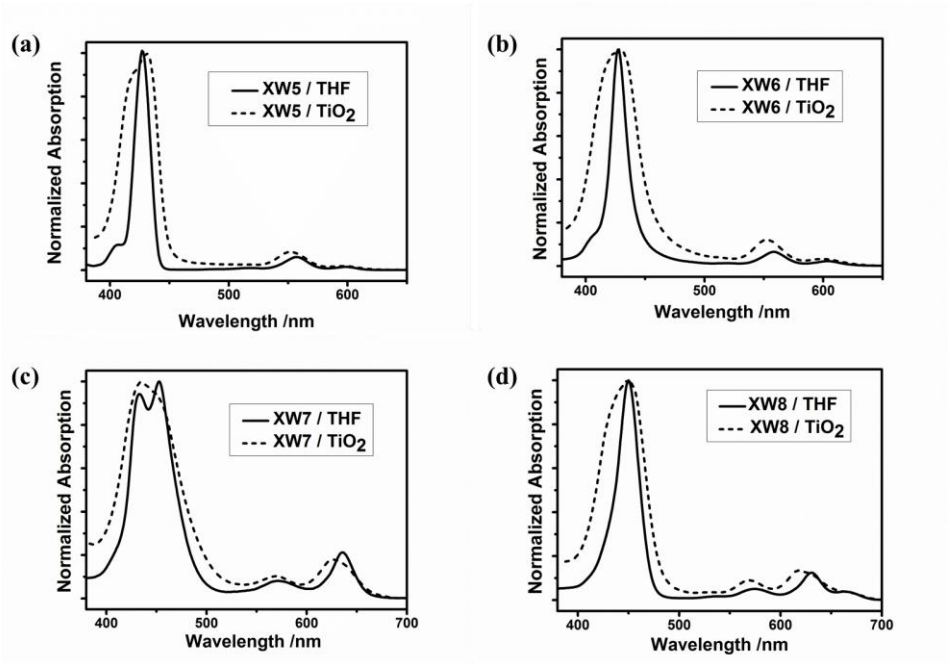

Figure S12 Normalized UV-visible spectra of the porphyrins in THF and on the TiO_2 films (5 μm).

Table S1. Calculated excitation energies, wavelengths, oscillator strengths and molecular orbital compositions for the lowest excited states.

Compound	Excited state	Excitation energy	Oscillator strength	MO composition
XW1	S_1	2.11 eV, 587 nm	0.306	H-0→L+0 (71%) H-1→L+1 (26%)
XW5	S_1	2.22 eV, 557 nm	0.031	H-0→L+0 (57%) H-1→L+1 (41%)
XW6	S_1	2.15 eV, 577 nm	0.167	H-0→L+0 (63%) H-1→L+1 (24%) H-0→L+2 (11%)
XW7	S_1	2.02 eV, 613 nm	0.767	H-0→L+0 (78%) H-1→L+1 (15%)
XW8	S_1	2.10 eV, 591 nm	0.382	H-0→L+0 (73%) H-1→L+1 (24%)

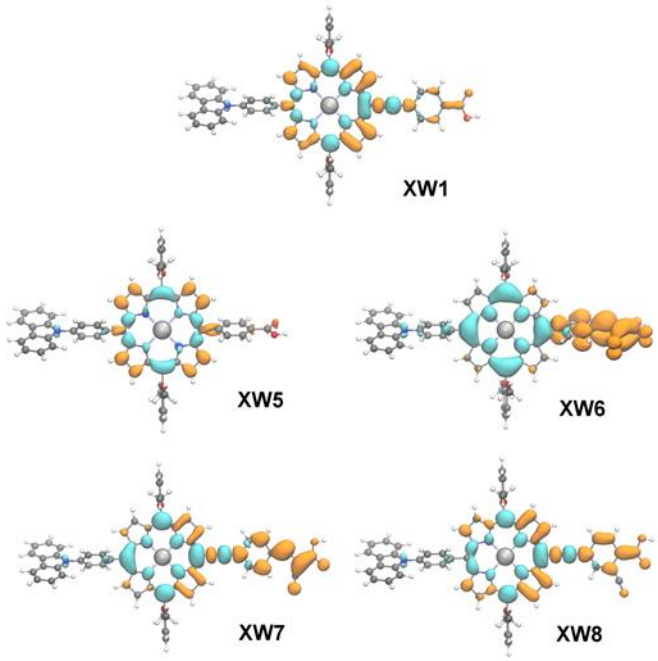

Figure S13. Electron density difference contours for the lowest excited states of the sensitizer dyes. Electron detachment and attachment are shown in cyan and orange color, respectively.

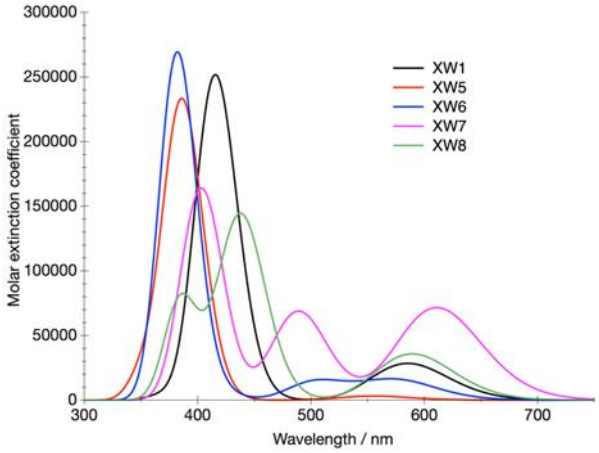

Figure S14. Simulated absorption spectra.

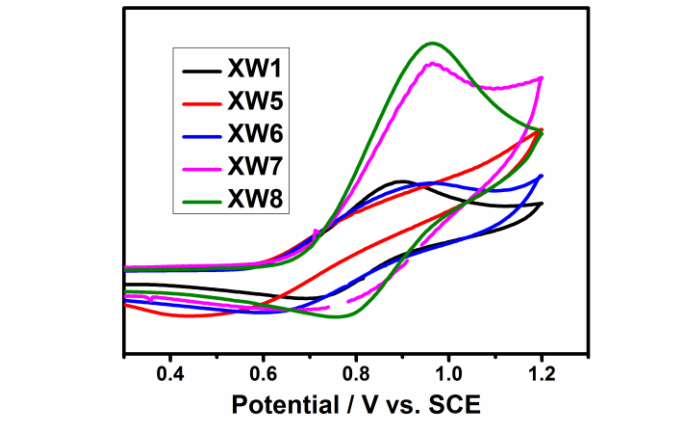

Figure S15. The cyclic voltammetry curves of the dyes adsorbed to a nanocrystalline TiO_2 film deposited on conducting FTO glass.

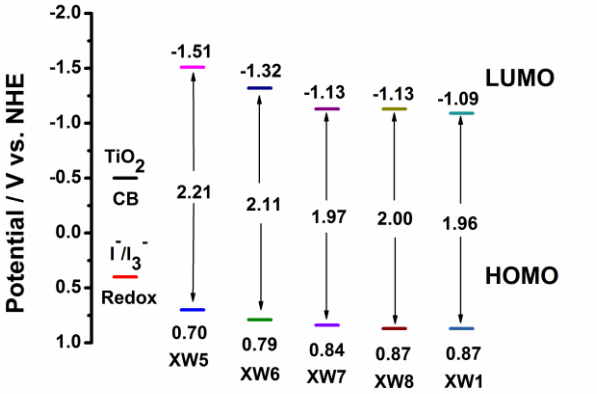

Figure S16. Schematic energy-level diagram of XW5–XW8 and XW1.

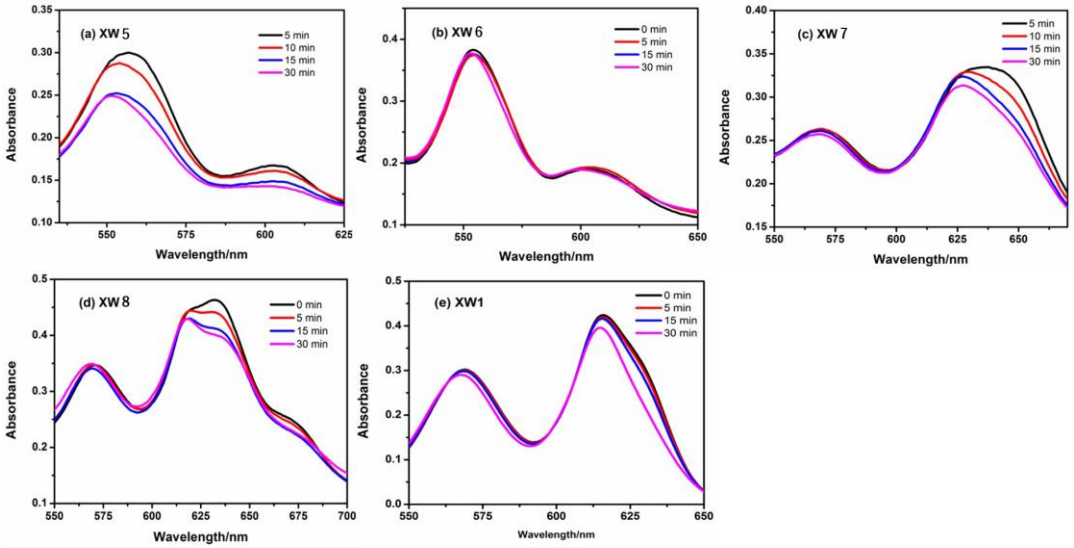

Figure S17. Absorption spectra of (a) XW5, (b) XW6, (c) XW7, (d) XW8 and (e) XW1 adsorbed onto TiO_2 films after irradiation for 0, 5, 15 and 30 min.

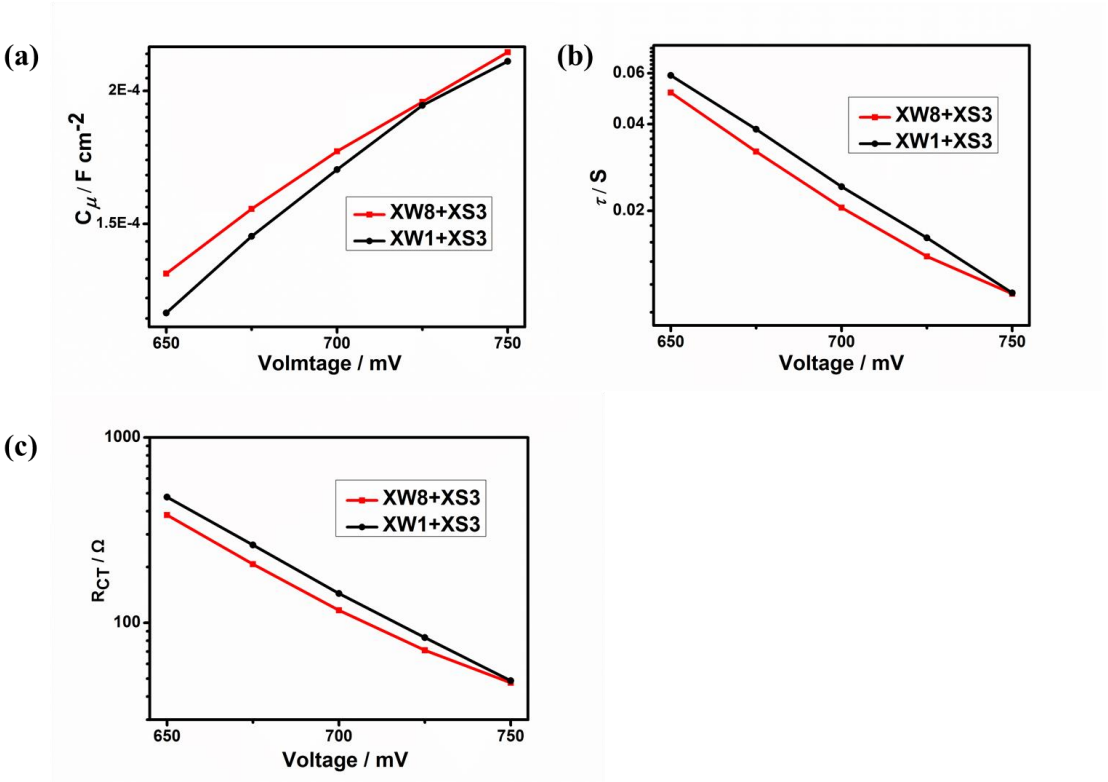

Figure S18. Chemical capacitance Cμ (a), electron lifetime τ (b), and interfacial charge transfer resistance R_{CT} (c) of the co-sensitized DSSC.