Electronic supplementary information (ESI)

Effect of Polyphenyl-Substituted Ethylene End-Capped Groups in Metal-Free Organic Dyes on Performance of Dye-Sensitized Solar Cells

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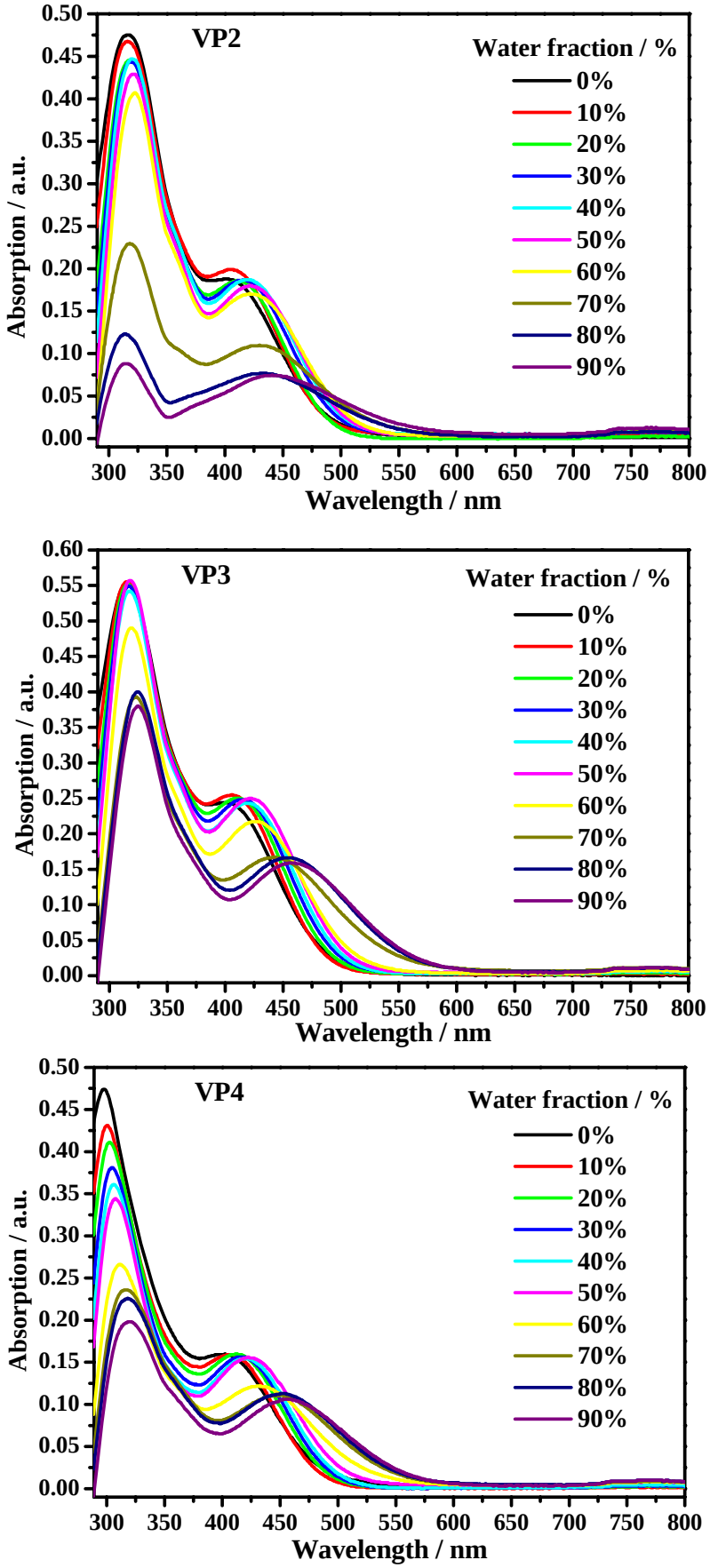

Fig. S1 UV-vis absorption spectra of **VP2**, **VP3**, and **VP4** in DMF-H_2O mixtures.

（Note：generally, *J*-aggregate formation is always accompanied with a bathochromic shift of the UV absorption maximum.[1]）

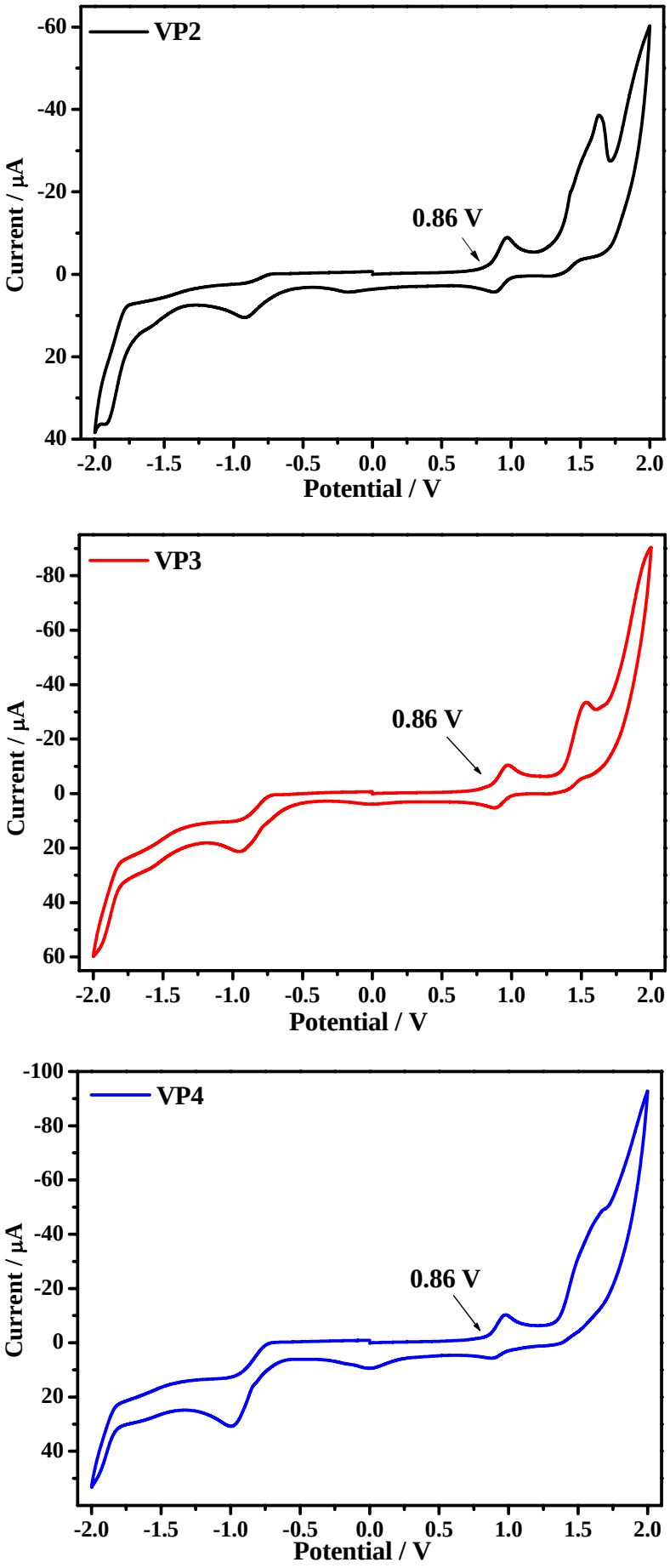

Fig. S2 Cyclic voltammetry curves of **VP2**, **VP3**, and **VP4** in MC of 0.1 mol L^{-1} *n*-Bu_4NClO_4 electrolyte at a scan rate of 100 mV s^{-1}.

Table S1 Some dihedral angle parameters of **VP2**, **VP3**, and **VP4** at the B3LYP/6-31G level

Dihedral angles	a-b	b-c	c-d
VP2 (deg.)	155	36	6
VP3 (deg.)	142	33	62
VP4 (deg.)	142	36	79

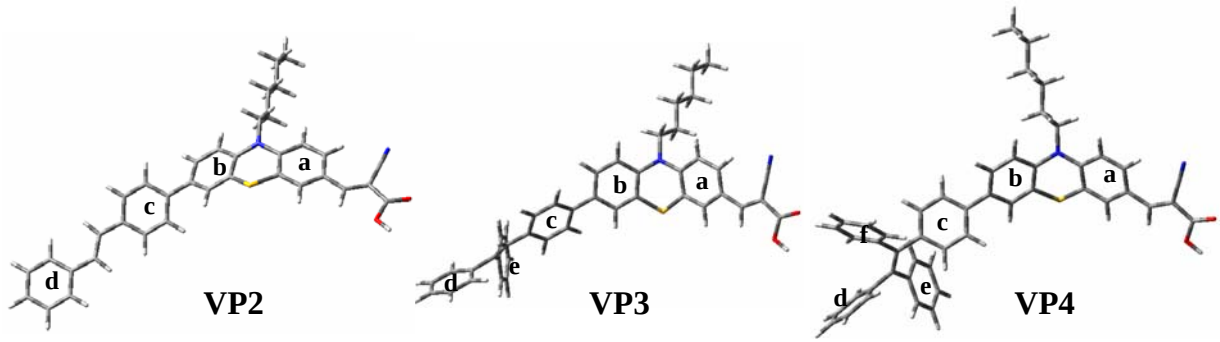

Table S2 Electrochemical properties of the organic dyes and amount of the dyes adsorbed on TiO_2 film

Dye	**VP2**	**VP3**	**VP4**
E_{HOMO}[a]/ eV	-5.12	-5.12	-5.12
$E_{band\ gap}$[b]/ eV	1.94	1.95	1.95
E_{LUMO}[c]/ eV	-3.18	-3.17	-3.17
E_{HOMO}[d]/ eV	-5.31	-5.33	-5.31
E_{LUMO}[d]/ eV	-2.53	-2.50	-2.53
$E_{bandgap}$[d]/ eV	2.78	2.83	2.78
μ[d,e]/ Debye	7.9435	7.9802	7.9882

[a] The HOMO is derived from a comparison with the ionization potential of ferrocene (0.5 mmol/L) in CH_2Cl_2 with 0.1 mol/L *n*-Bu_4NClO_4 as electrolyte (scanning rate, 100 mV/s; working electrode, glassy carbon; counter electrode, Pt disk; and reference electrode, Ag/AgCl). [b] The band gap is calculated from the absorption onset of the absorption spectrum. [c] The LUMO is calculated from the band gap and HOMO value. [d] Calculated at the B3LYP/6-31G level. [e]μ referred to dipole moment.

NMR and MS spectra

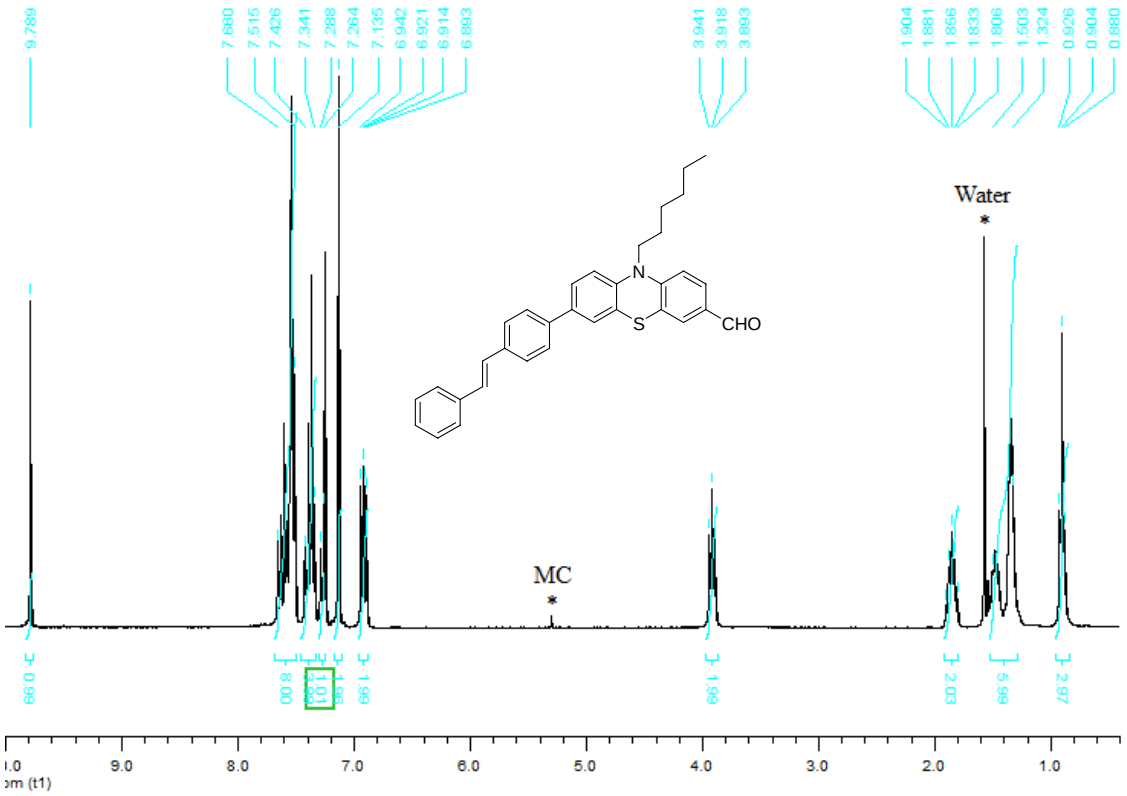

Fig. S3 ^{1}H NMR spectrum of **VP2A**

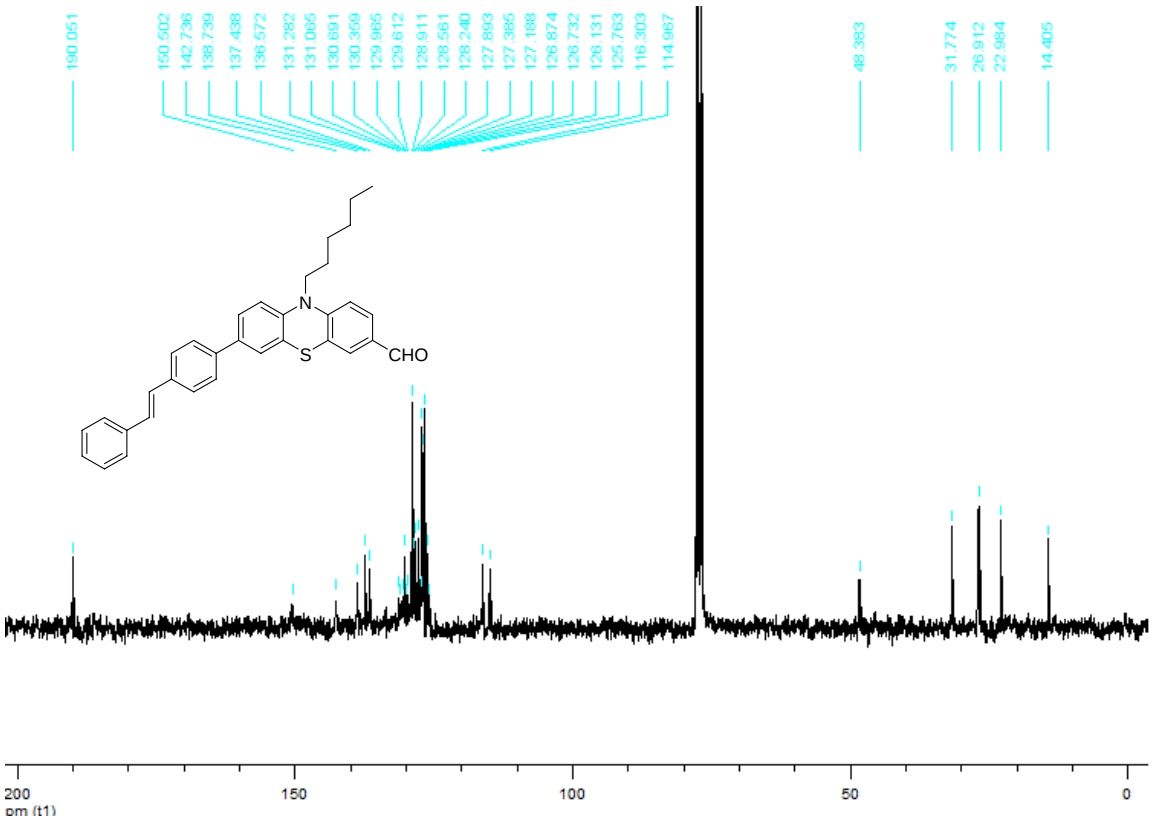

Fig. S4 ^{13}C NMR spectrum of **VP2A**

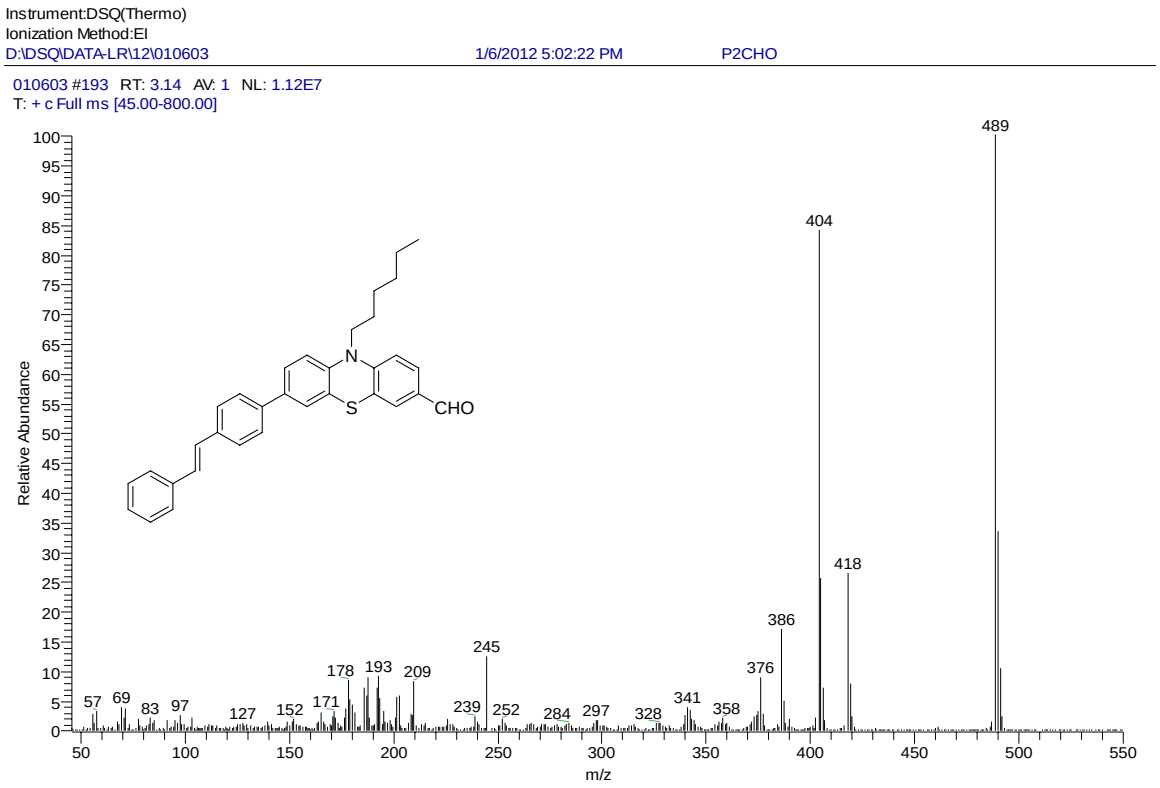

Fig. S5 MS spectrum of **VP2A**

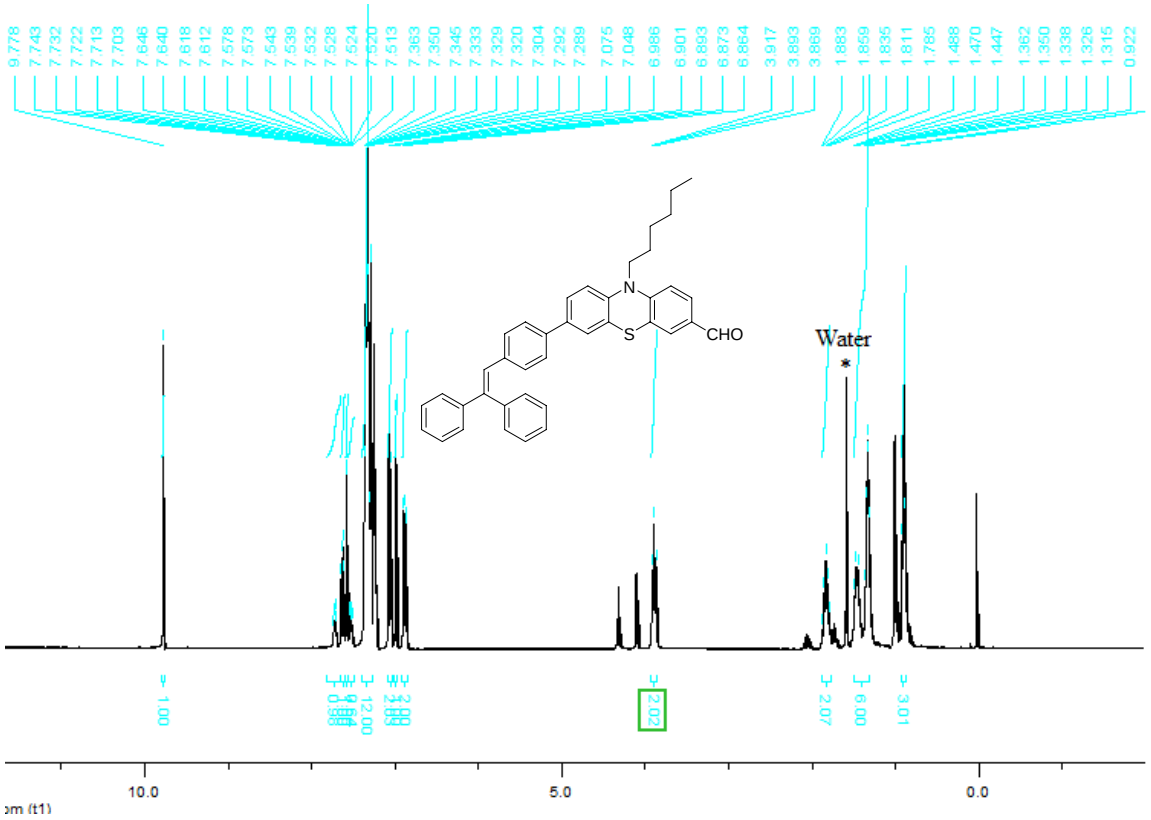

Fig. S6 ^{1}H NMR spectrum of **VP3A**

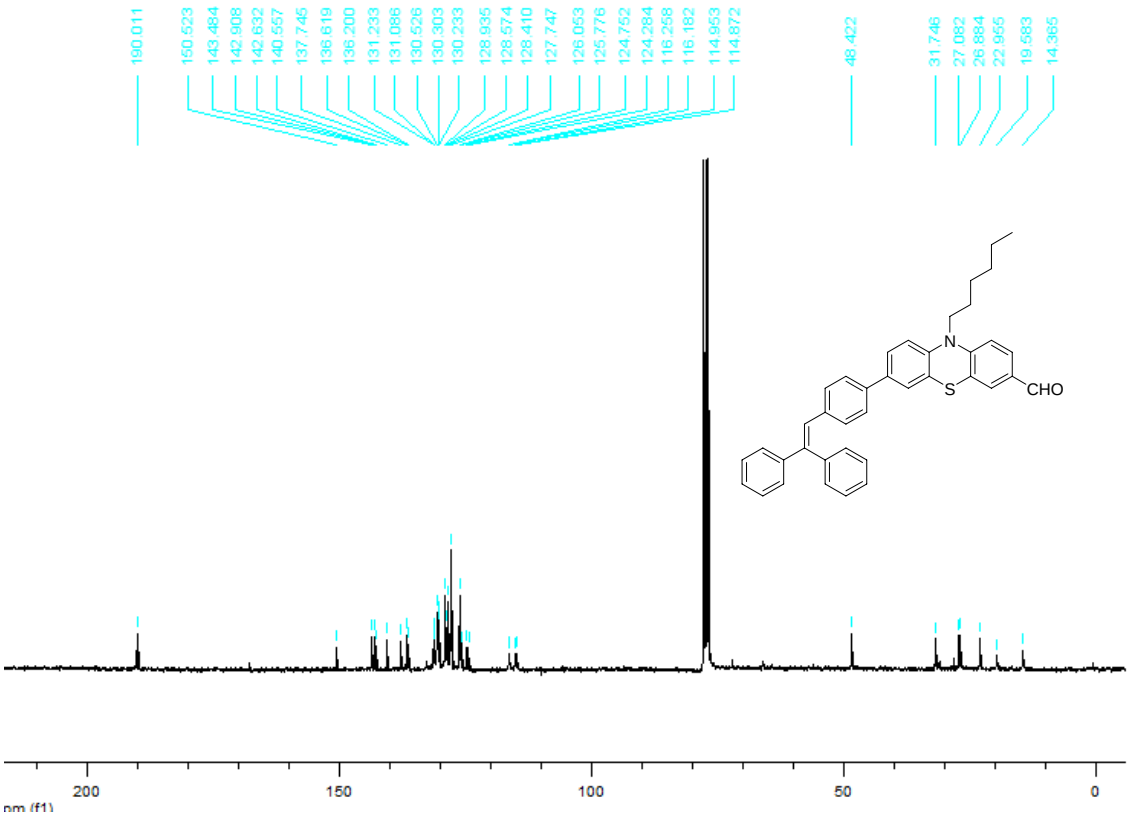

Fig. S7 ^{13}C NMR spectrum of **VP3A**

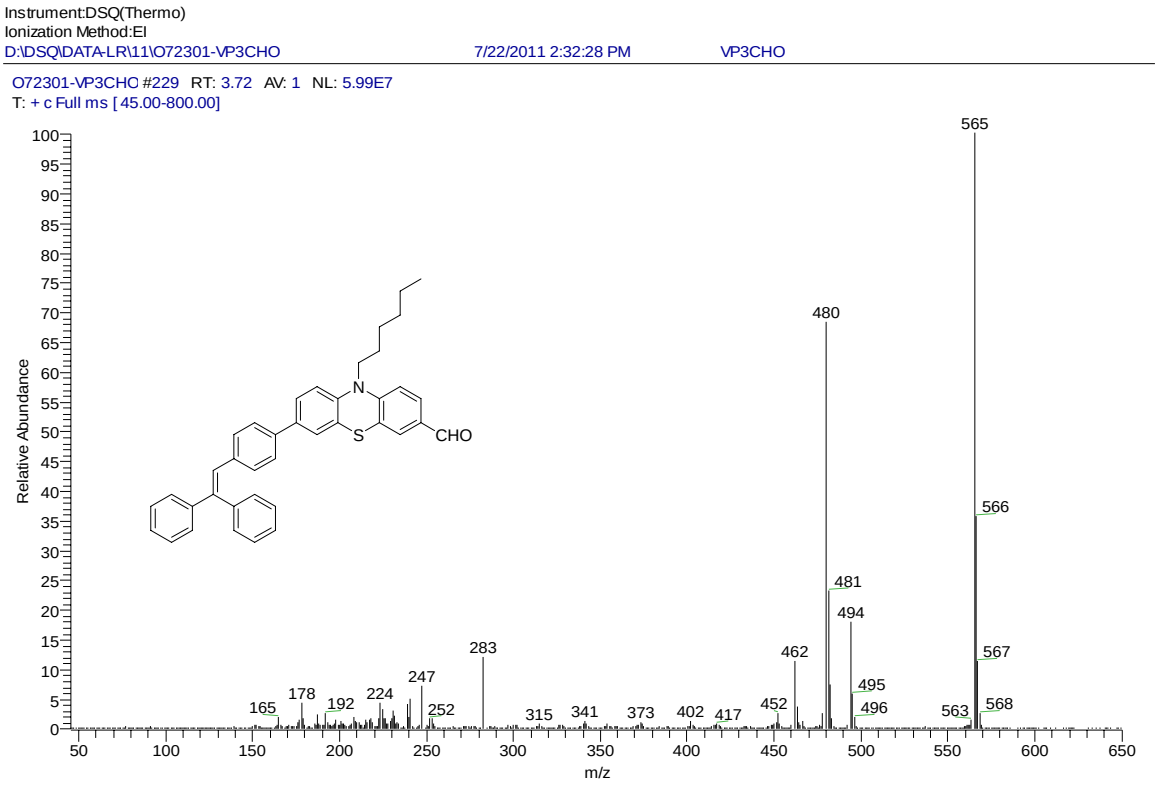

Fig. S8 MS spectrum of **VP3A**

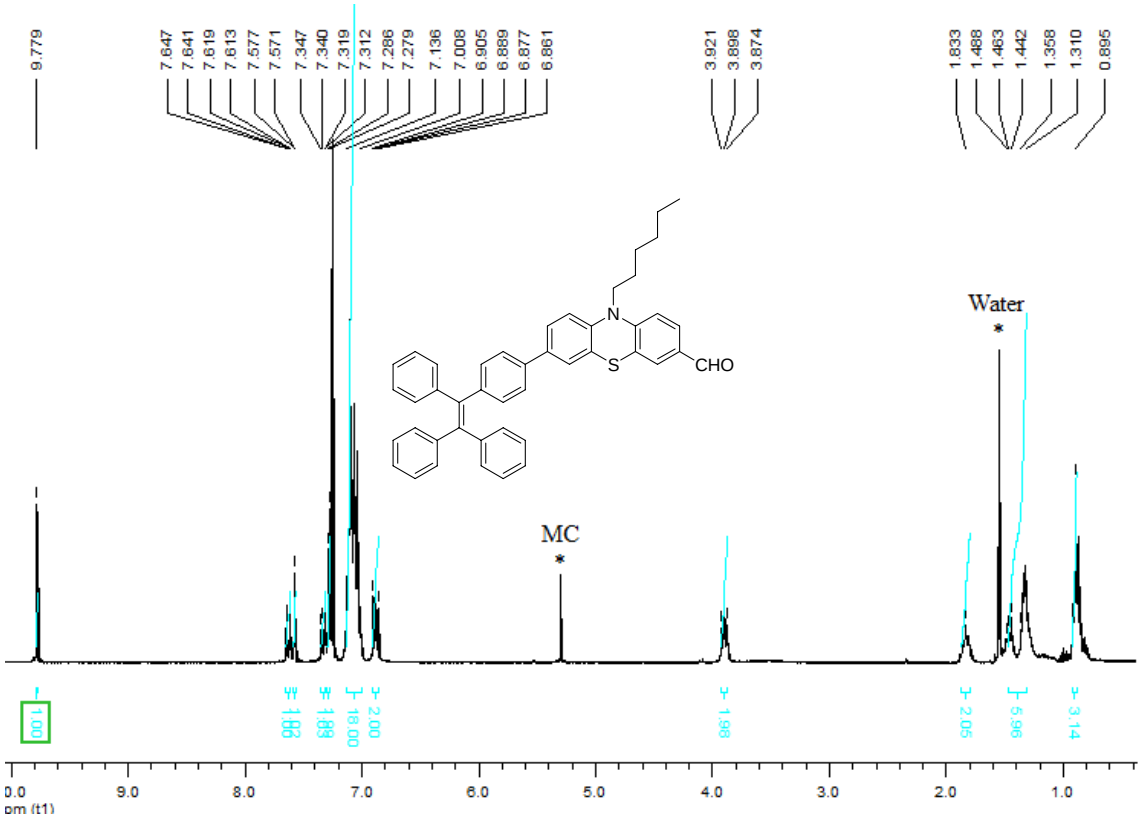

Fig. S9 ^{1}H NMR spectrum of **VP4A**

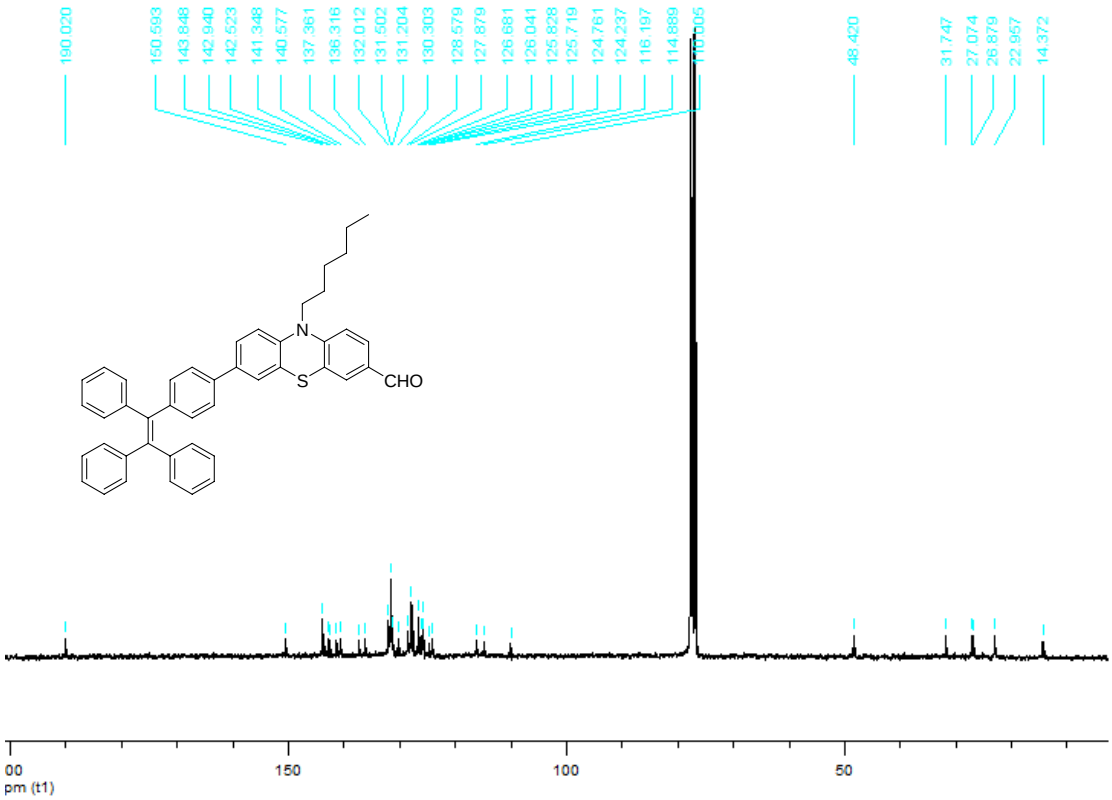

Fig. S10 ^{13}C NMR spectrum of **VP4A**

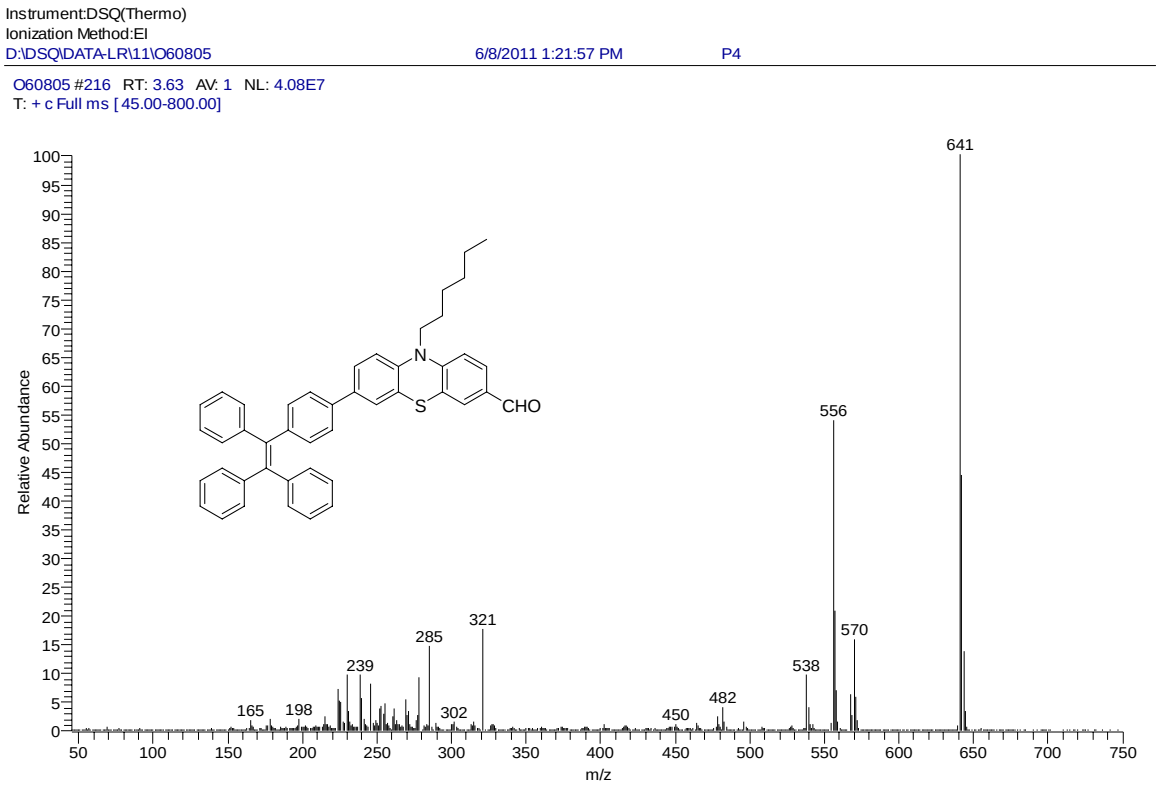

Fig. S11 MS spectrum of **VP4A**

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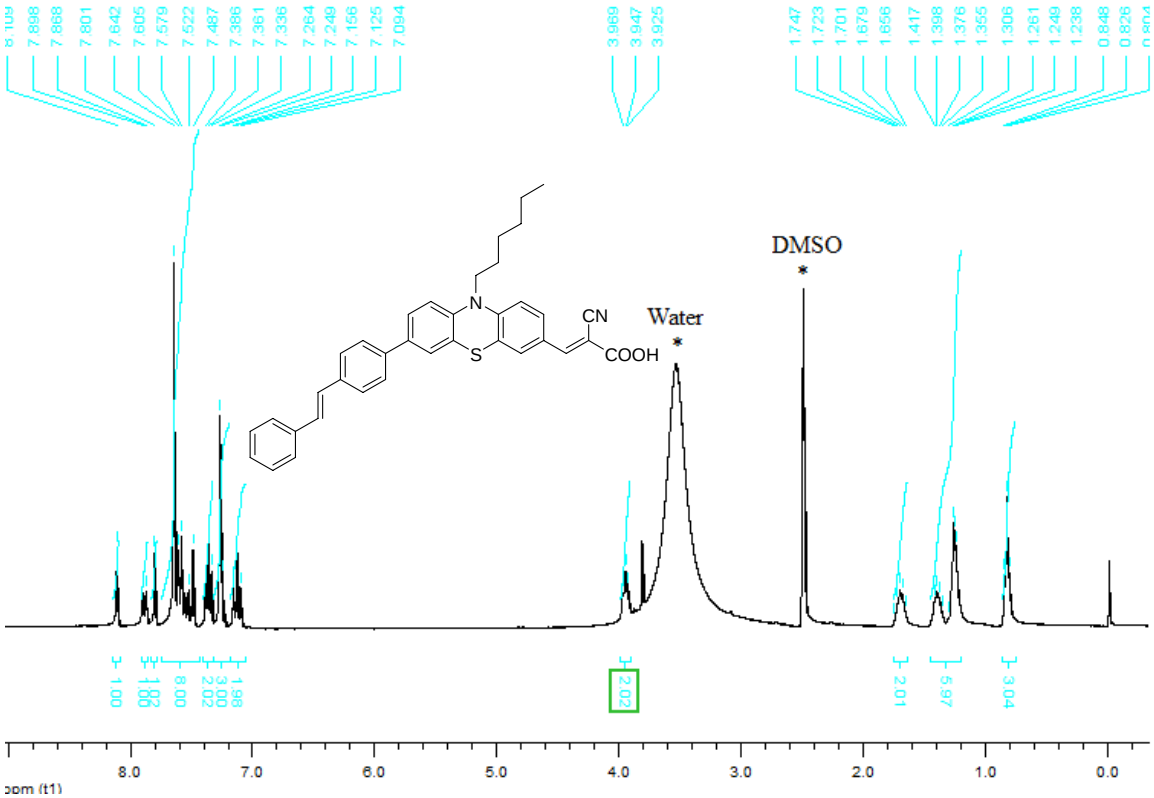

Fig. S12 ^{1}H NMR spectrum of **VP2**

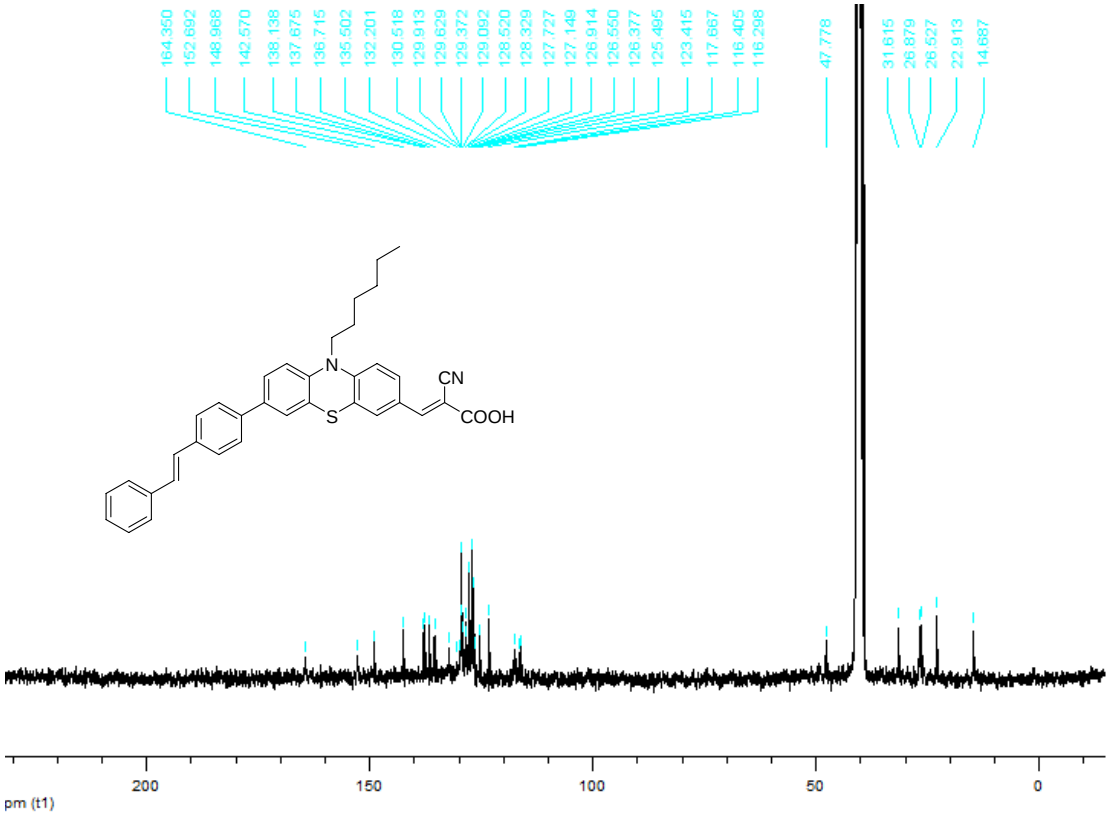

Fig. S13 ^{13}C NMR spectrum of **VP2**

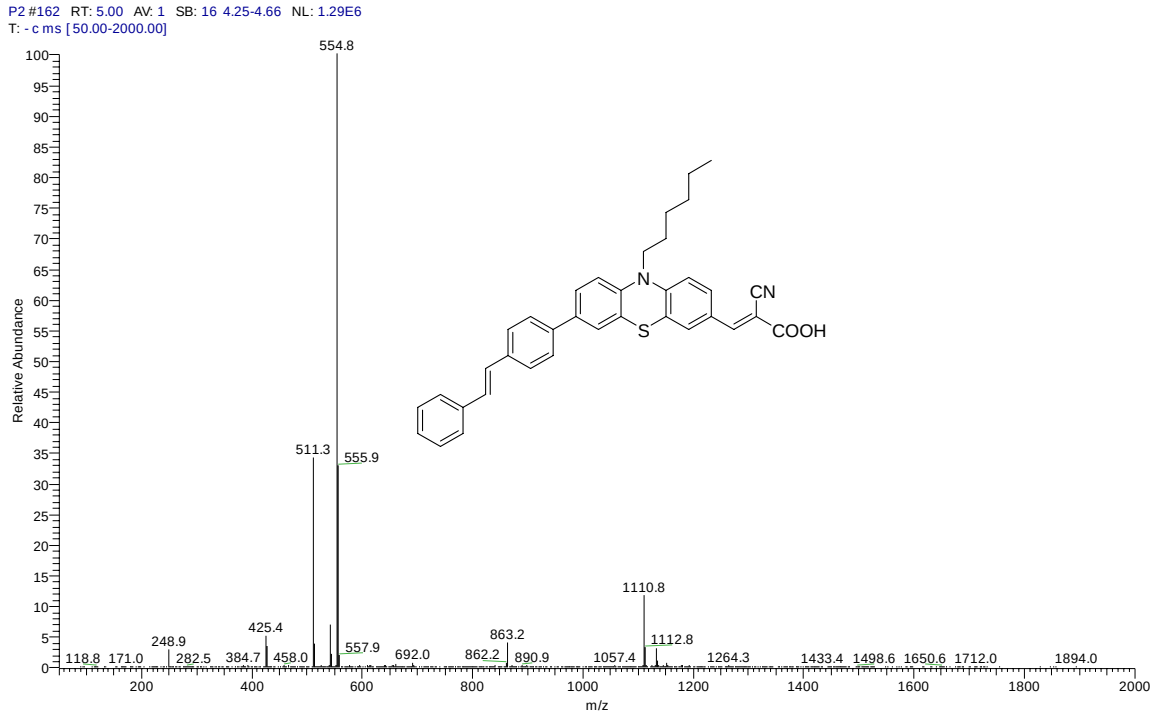

Fig. S14 MS spectrum of **VP2**

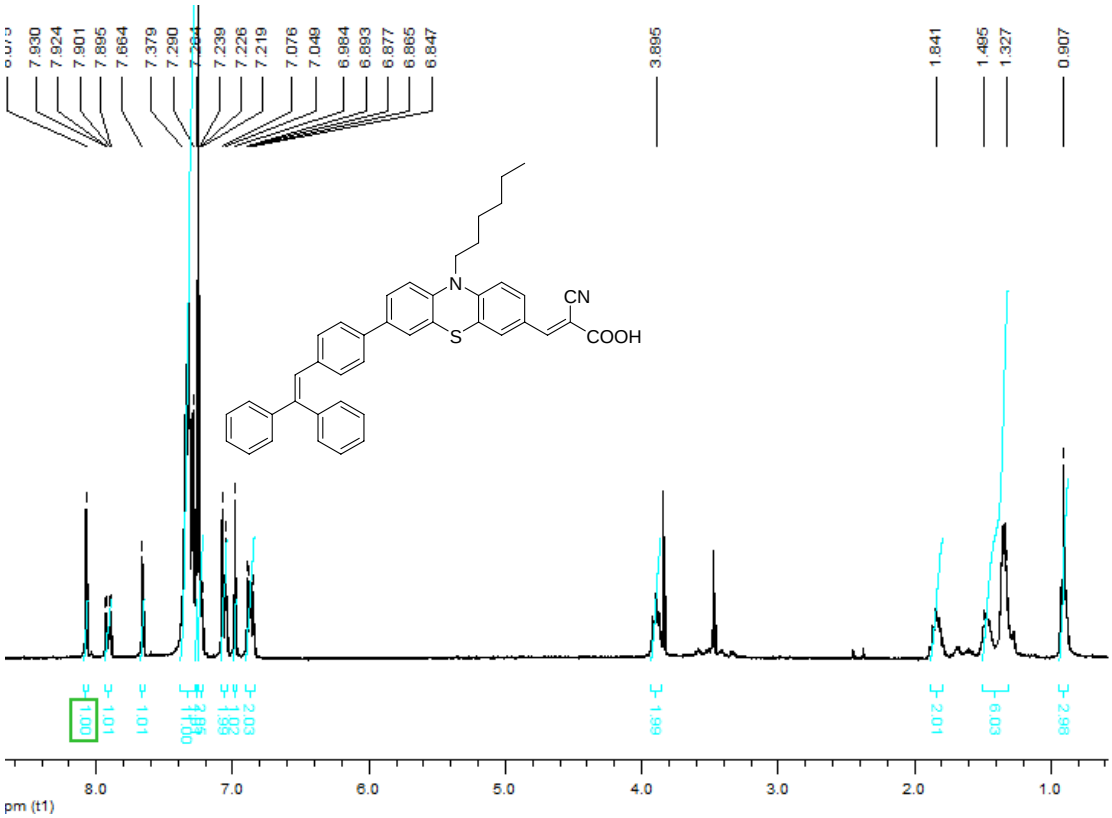

Fig. S15 ^{1}H NMR spectrum of **VP3**

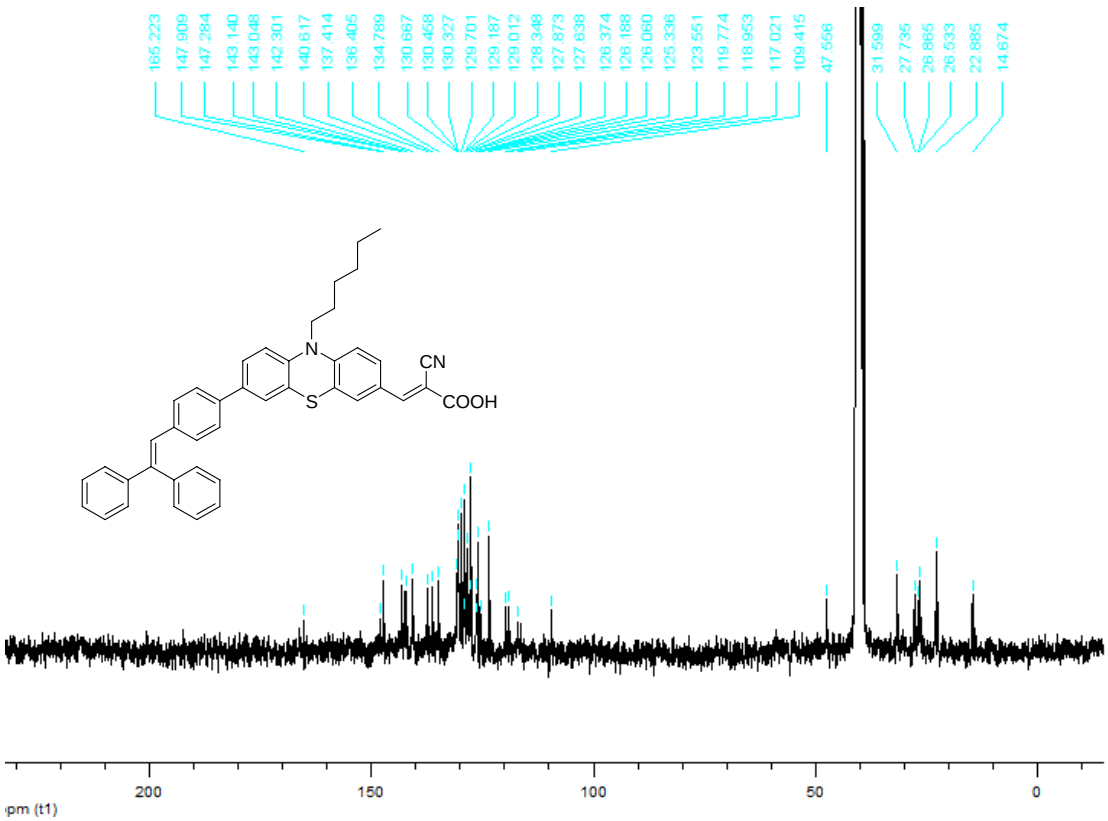

Fig. S16 ^{13}C NMR spectrum of **VP3**

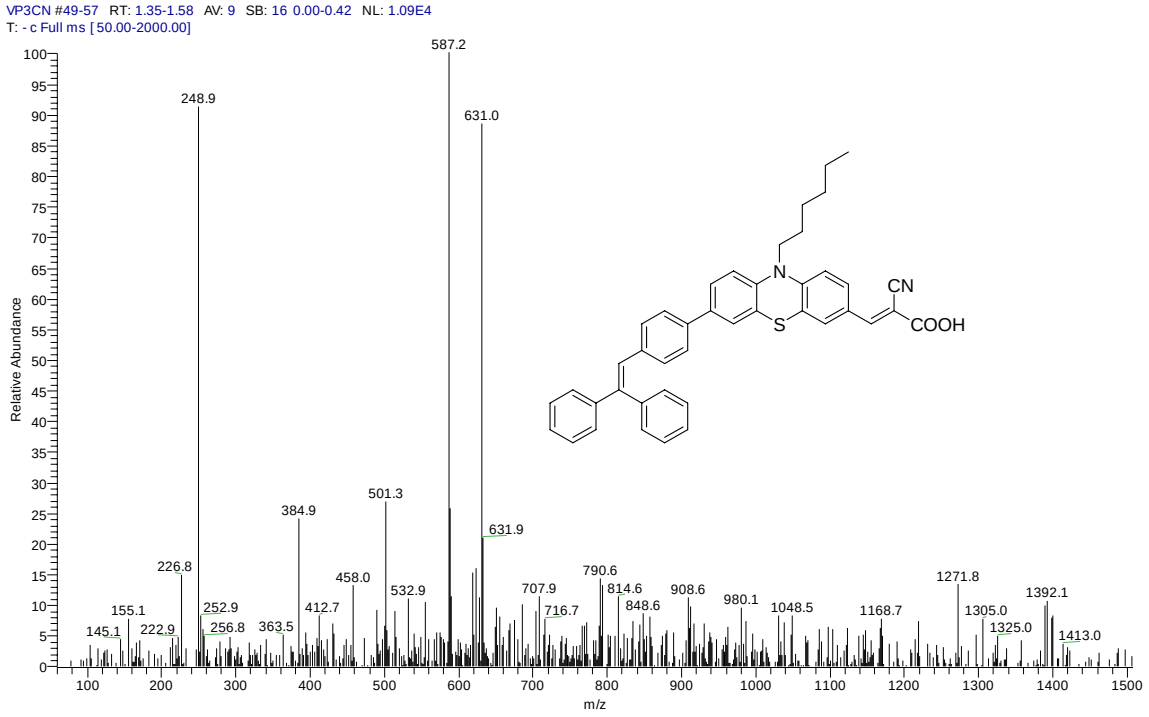

Fig. S17 MS spectrum of **VP3**

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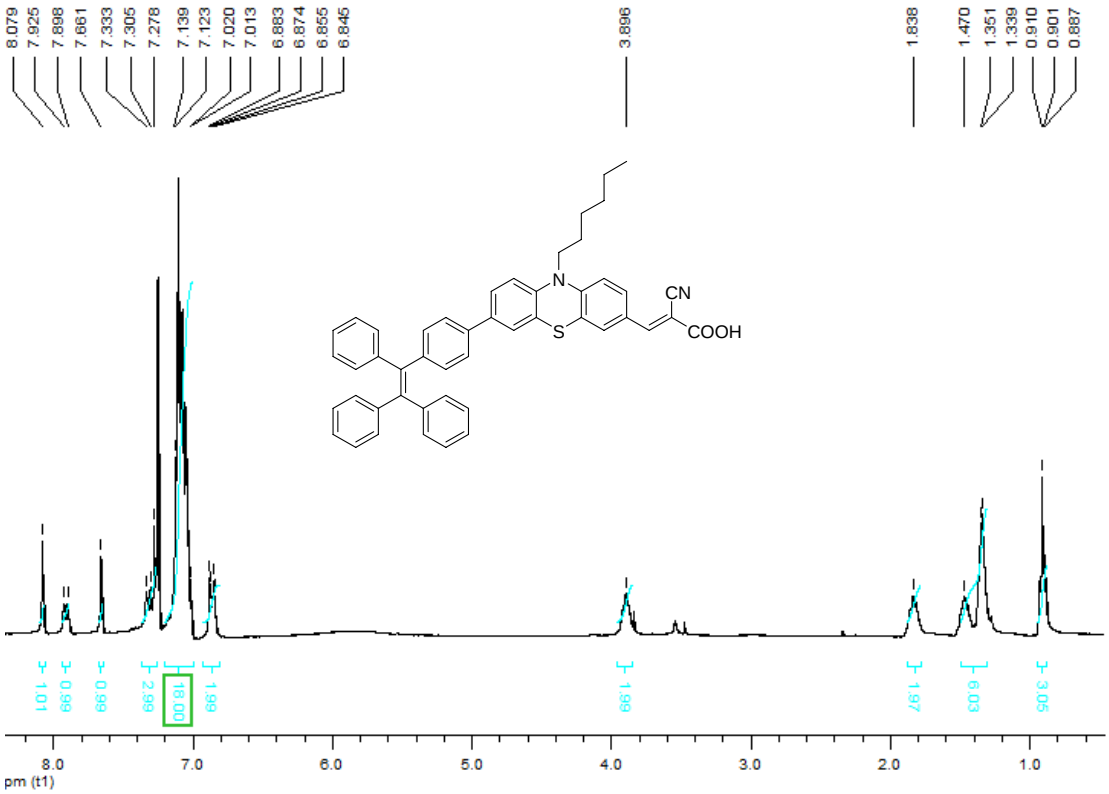

Fig. S18 ^{1}H NMR spectrum of **VP4**

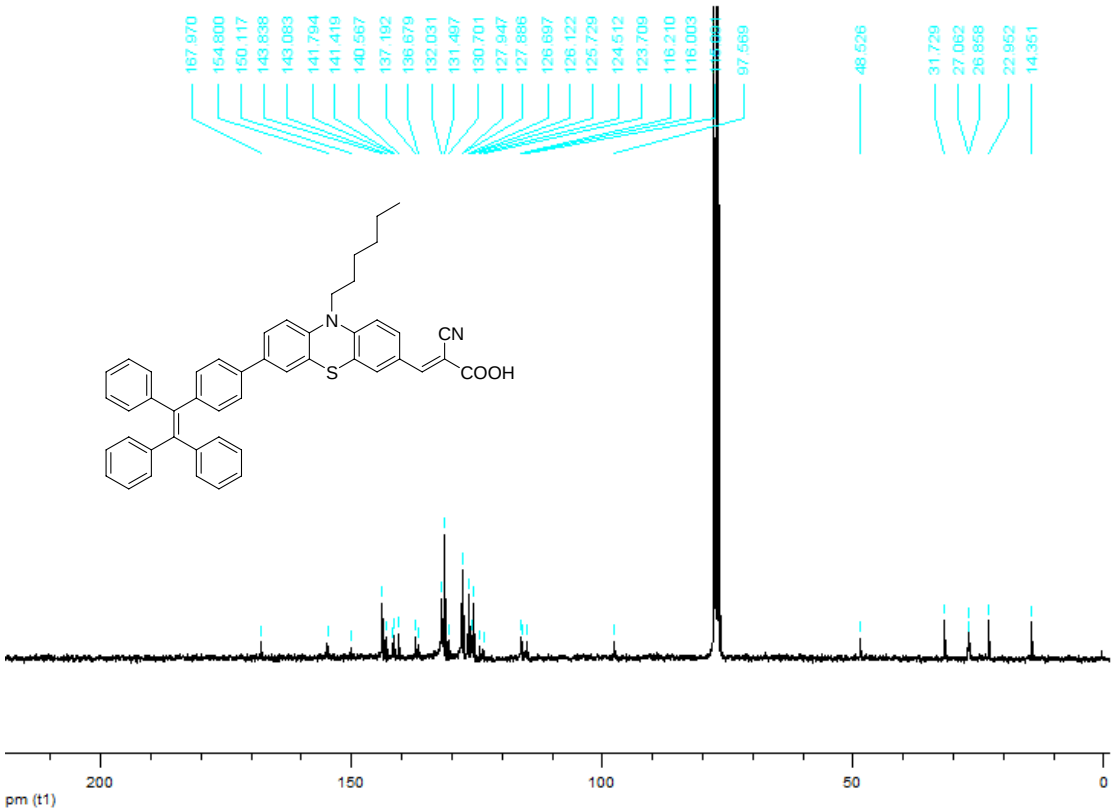

Fig. S19 ^{13}C NMR spectrum of **VP4**

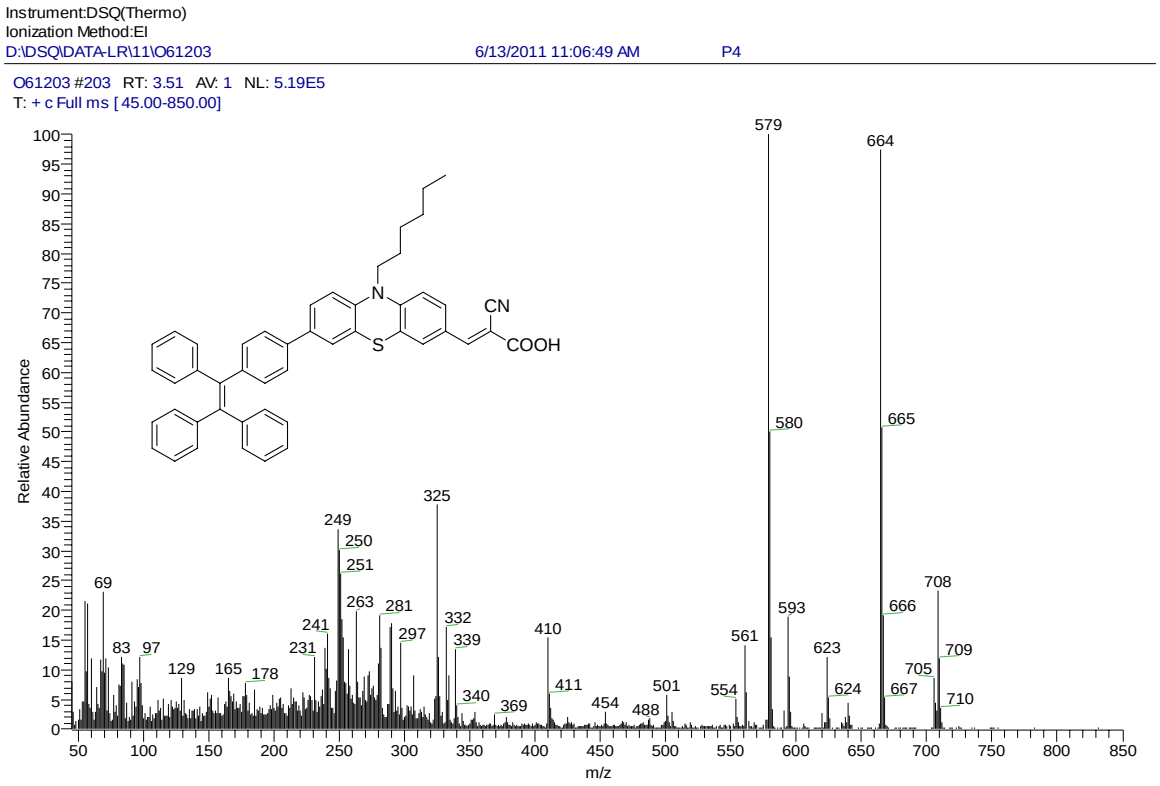

Fig. S20 MS spectrum of **VP4**