

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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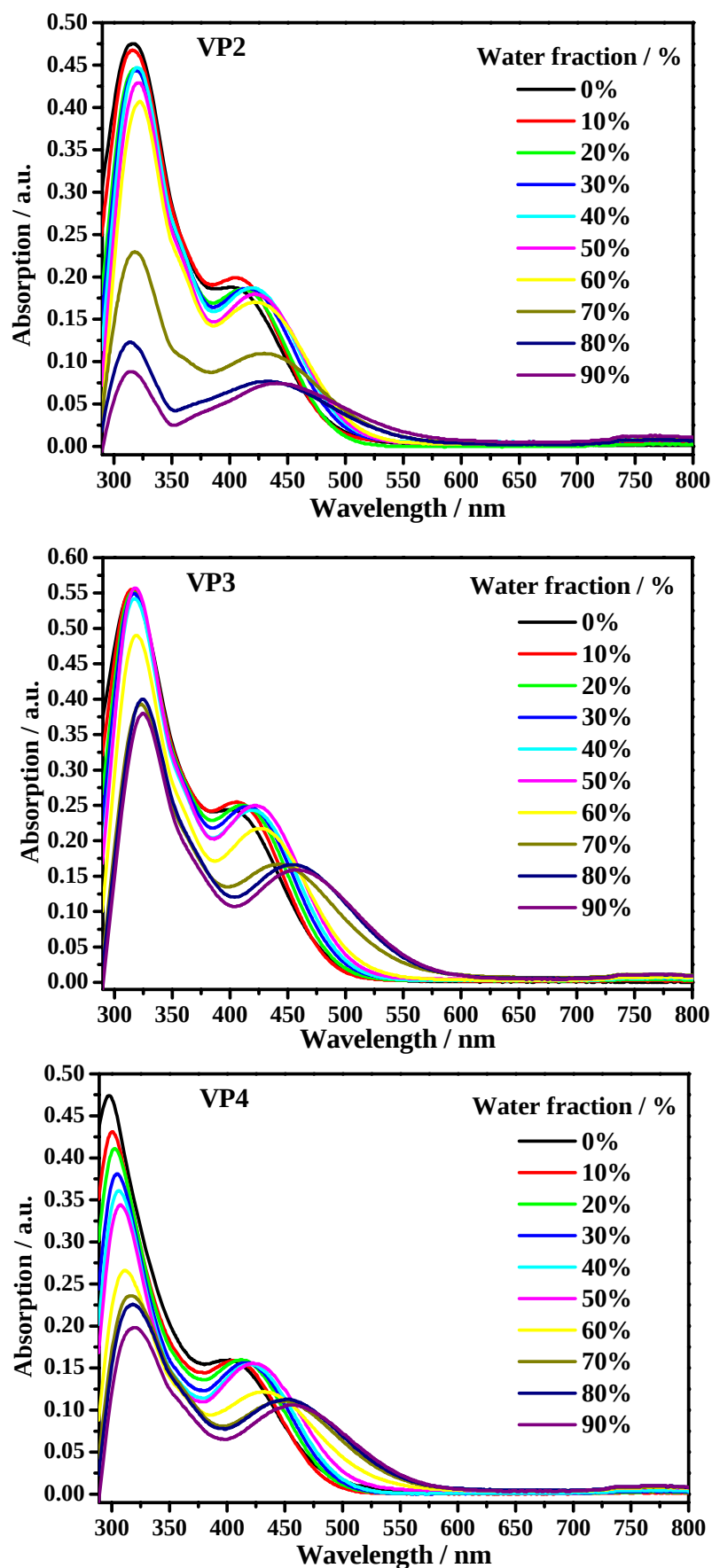


Fig. S1 UV-vis absorption spectra of **VP2**, **VP3**, and **VP4** in DMF-H₂O mixtures.

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

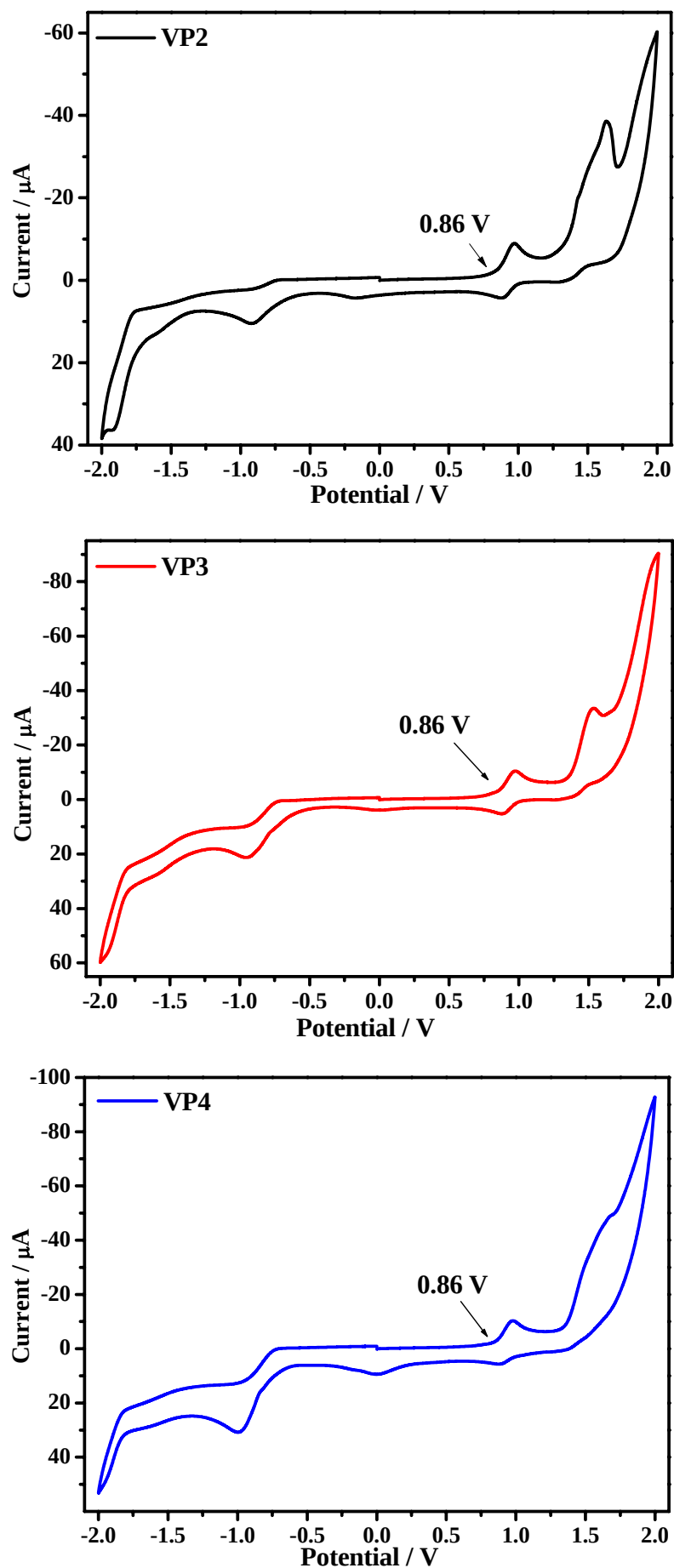


Fig. S2 Cyclic voltammetry curves of **VP2**, **VP3**, and **VP4** in MC of 0.1 mol L⁻¹ *n*-Bu₄NClO₄ electrolyte at a scan rate of 100 mV s⁻¹.

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

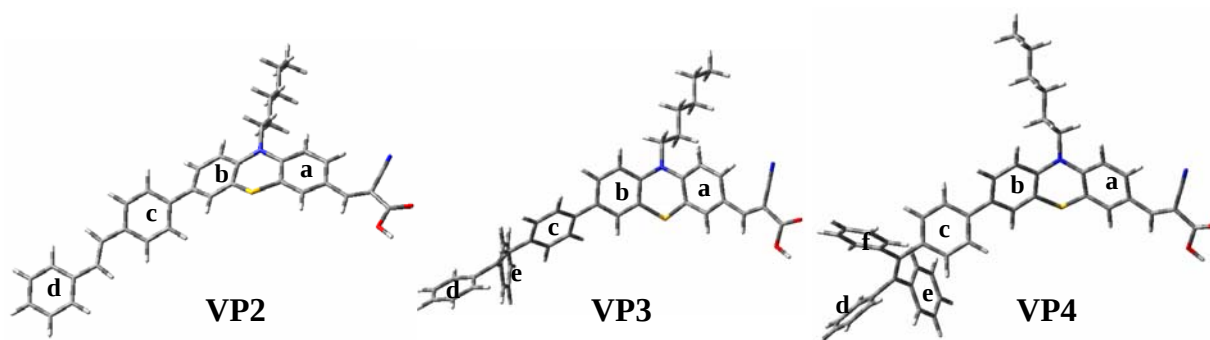


Table S2 Electrochemical properties of the organic dyes and amount of the dyes adsorbed on TiO₂ film

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 CH₂Cl₂ with 0.1 mol/L *n*-Bu₄NClO₄ 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

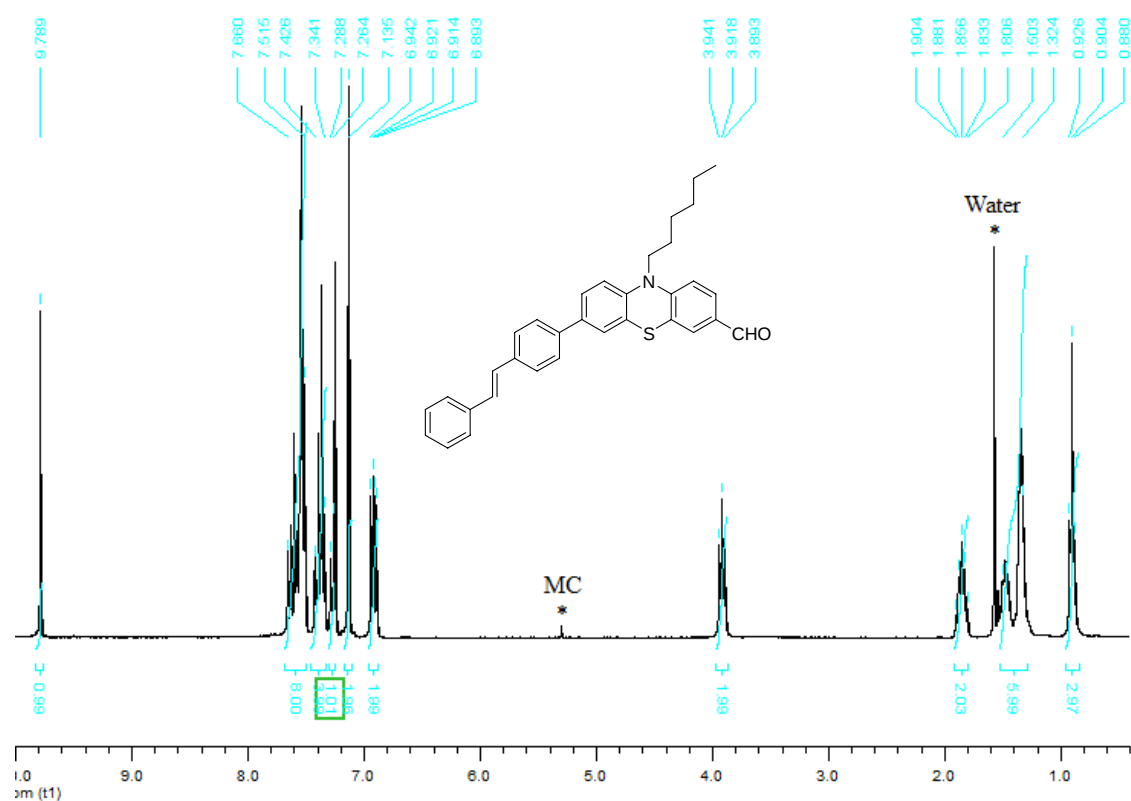


Fig. S3 ¹H NMR spectrum of VP2A

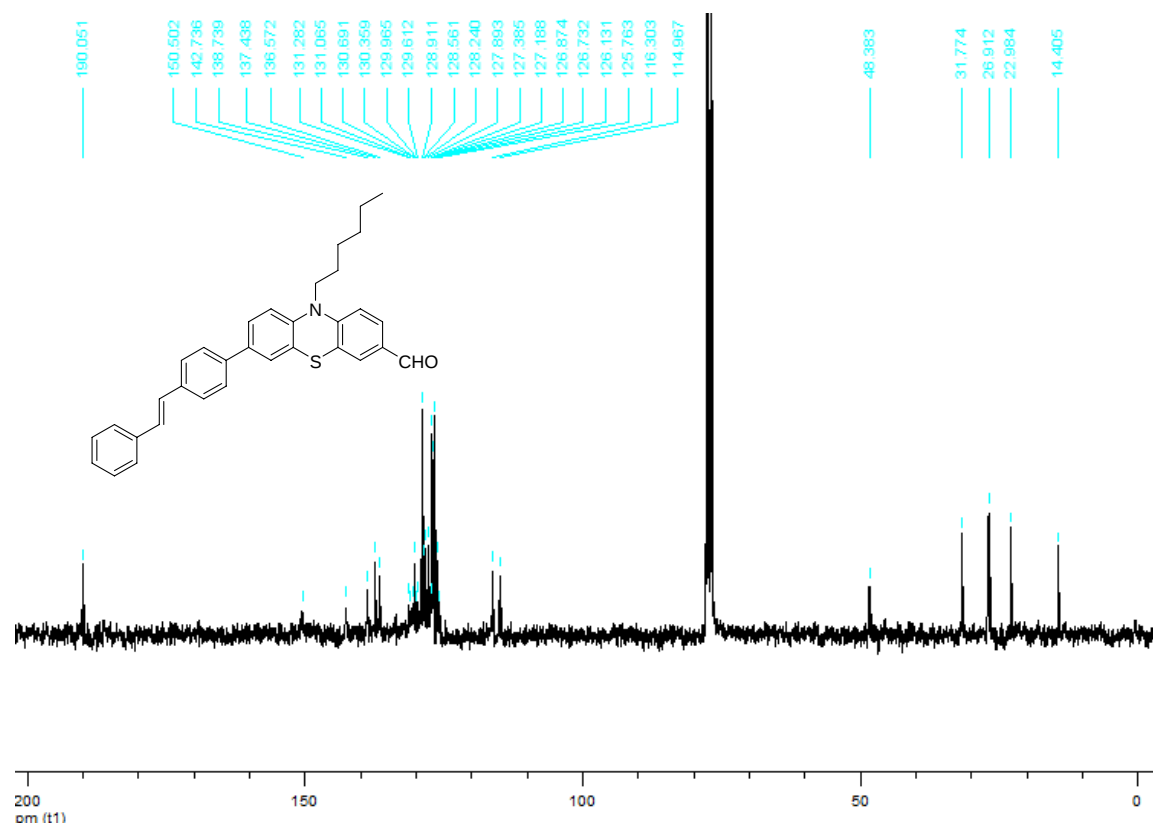


Fig. S4 ¹³C NMR spectrum of VP2A

Fig. S6 ^1H NMR spectrum of VP3A

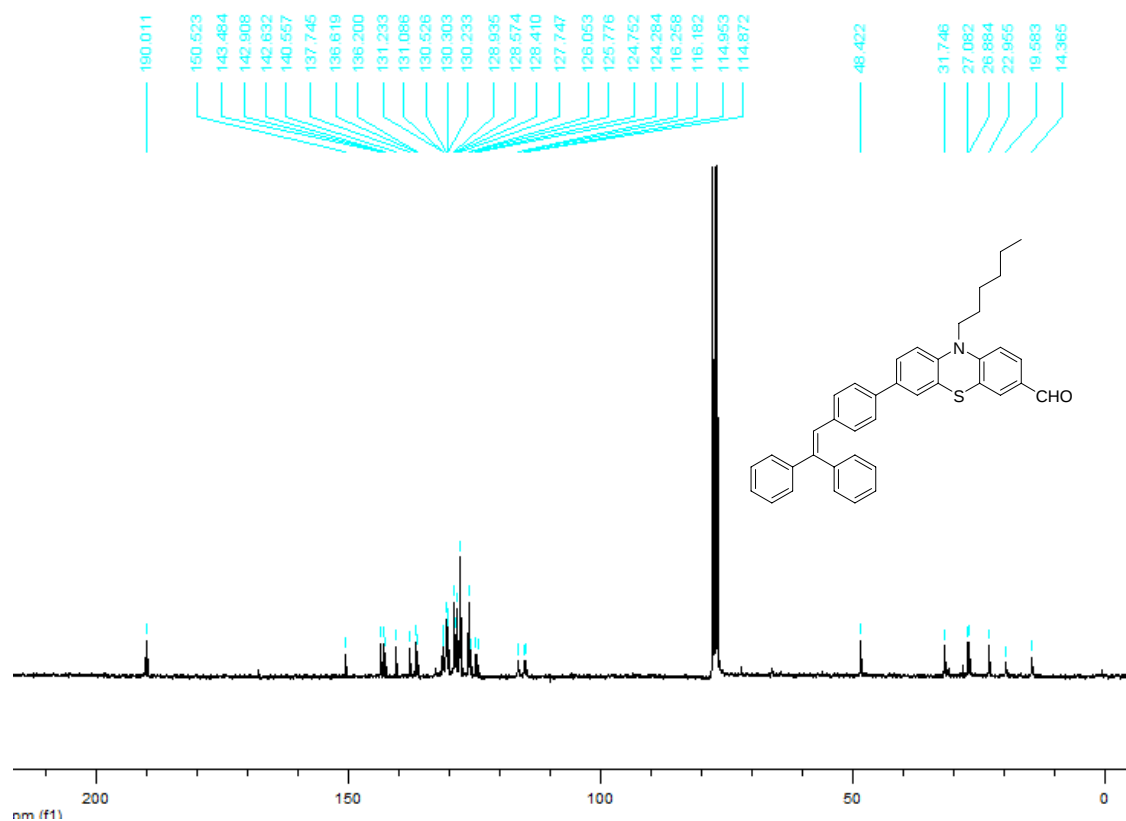


Fig. S7 ¹³C NMR spectrum of VP3A

Instrument:DSQ(Thermo)

Ionization Method:EI

D:\DSQDATA-LR\11\072301-VP3CHO

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VP3CHO

072301-VP3CHO #229 RT: 3.72 AV: 1 NL: 5.99E7

T: + c Full ms [45.00-800.00]

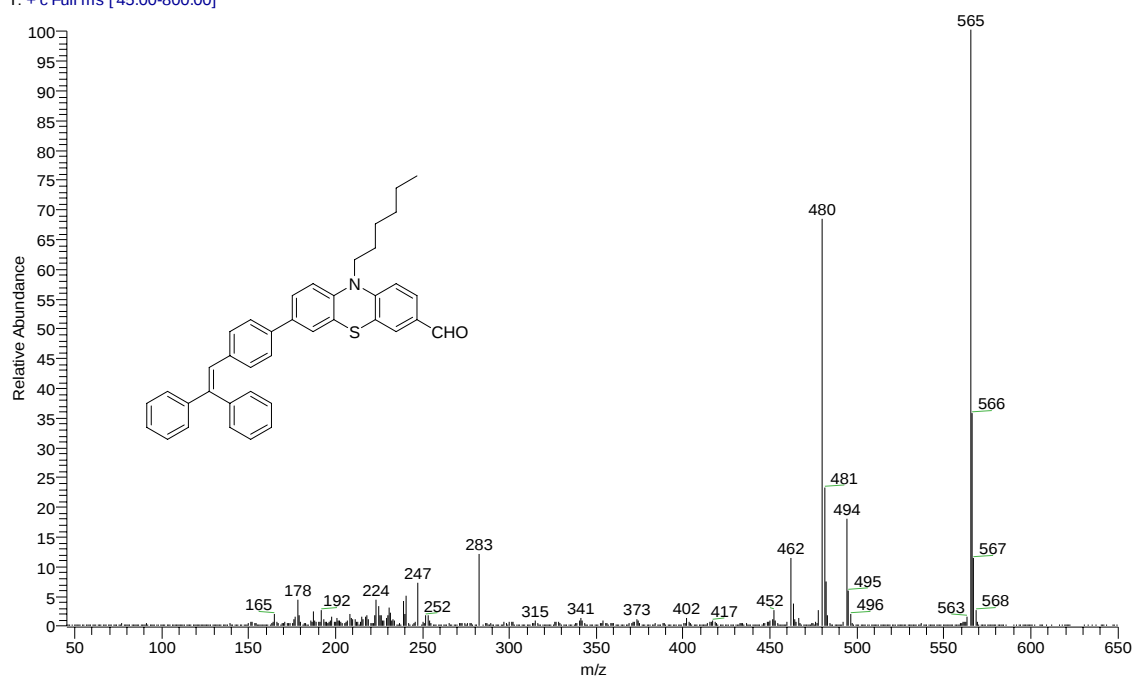
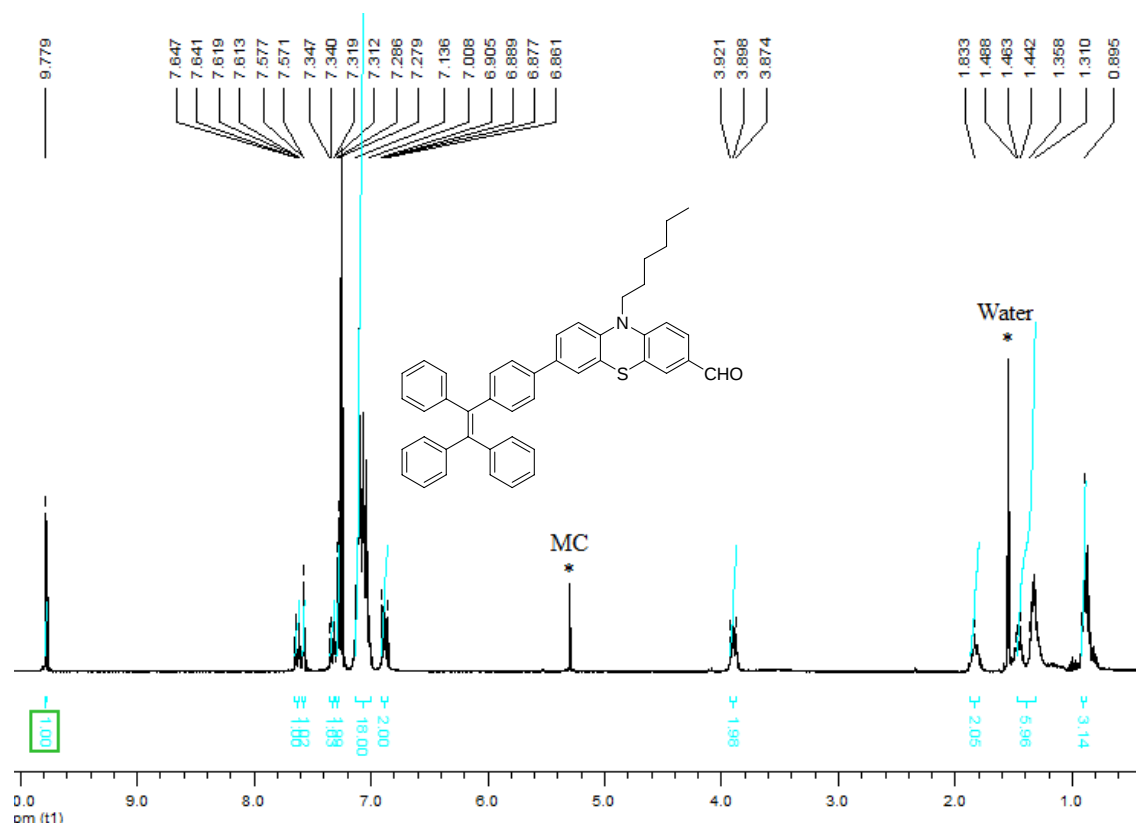


Fig. S8 MS spectrum of VP3A



Instrument:DSQ(Thermo)
Ionization Method:EI
D:\DSQDATA-LR\11\O60805

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P4

O60805 #216 RT: 3.63 AV: 1 NL: 4.08E7
T: + c Full ms [45.00-800.00]

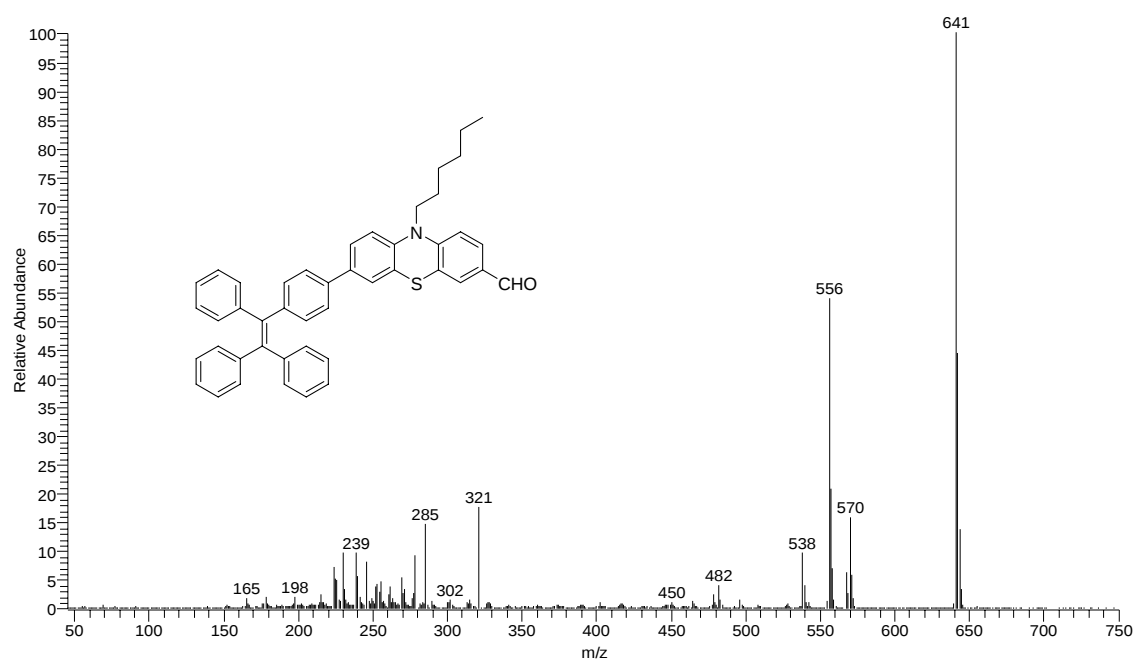


Fig. S11 MS spectrum of VP4A

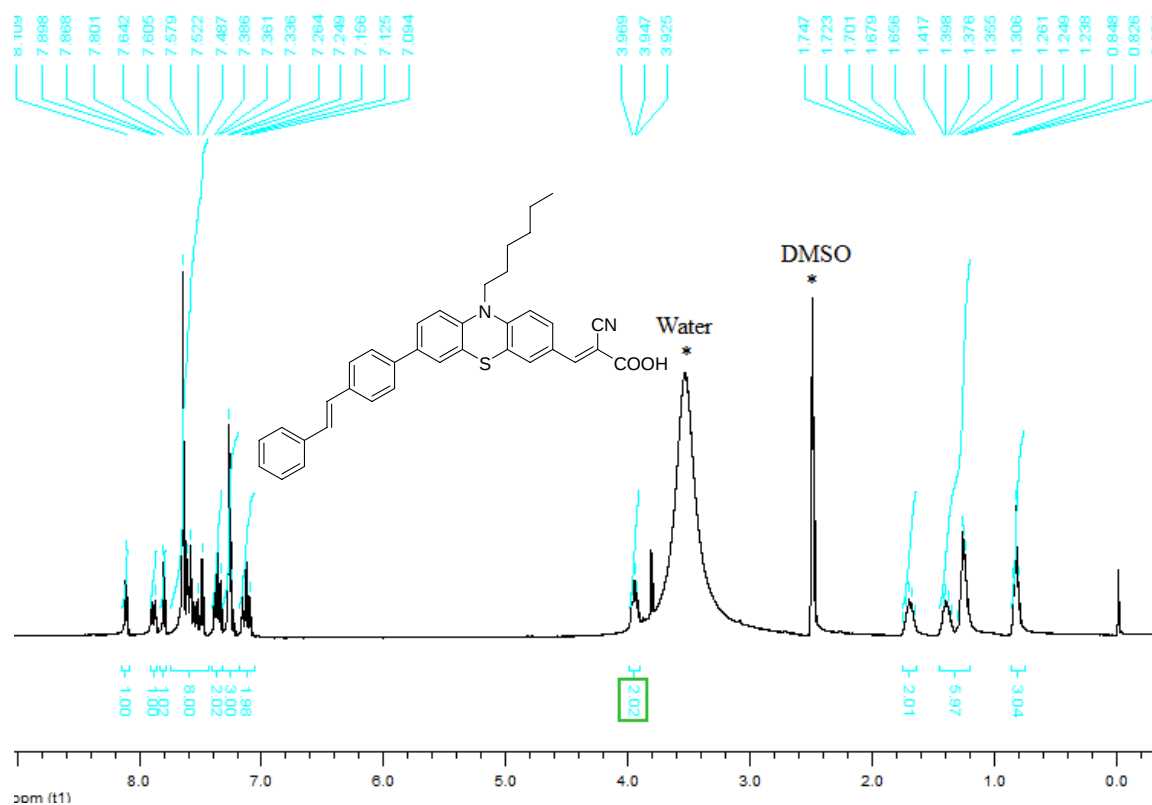


Fig. S12 ¹H NMR spectrum of VP2

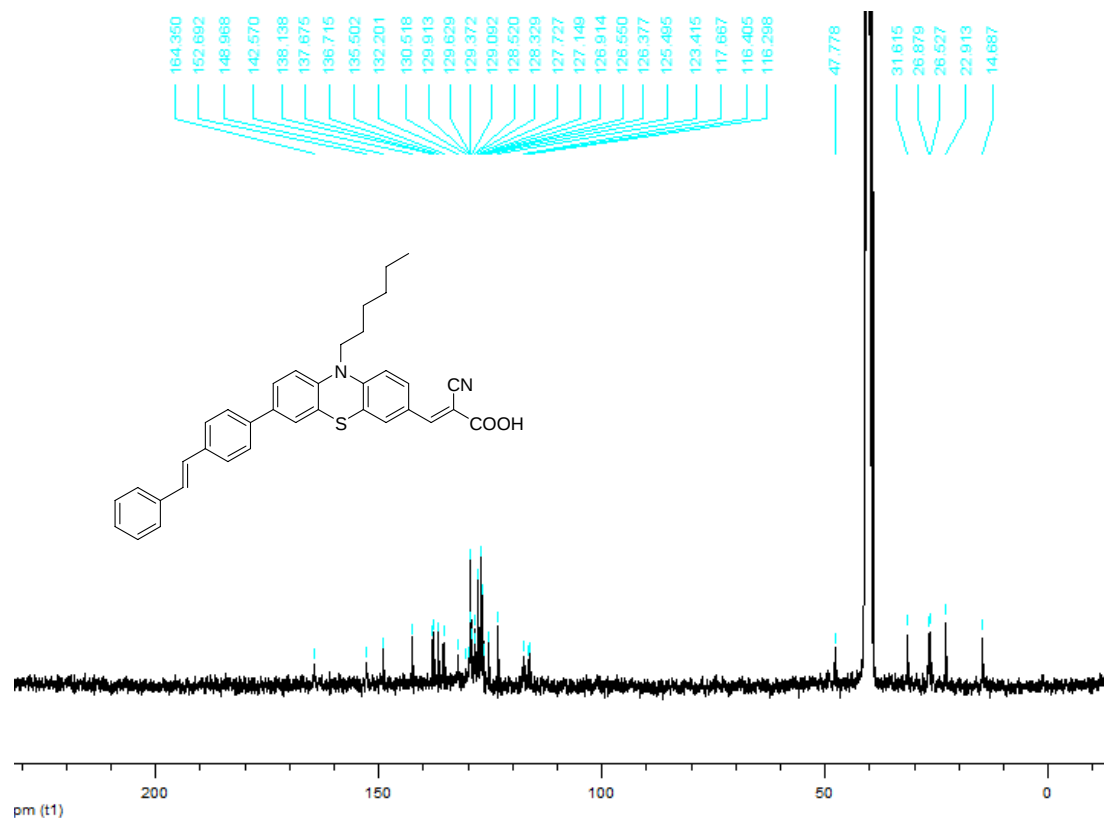


Fig. S13 ^{13}C NMR spectrum of VP2

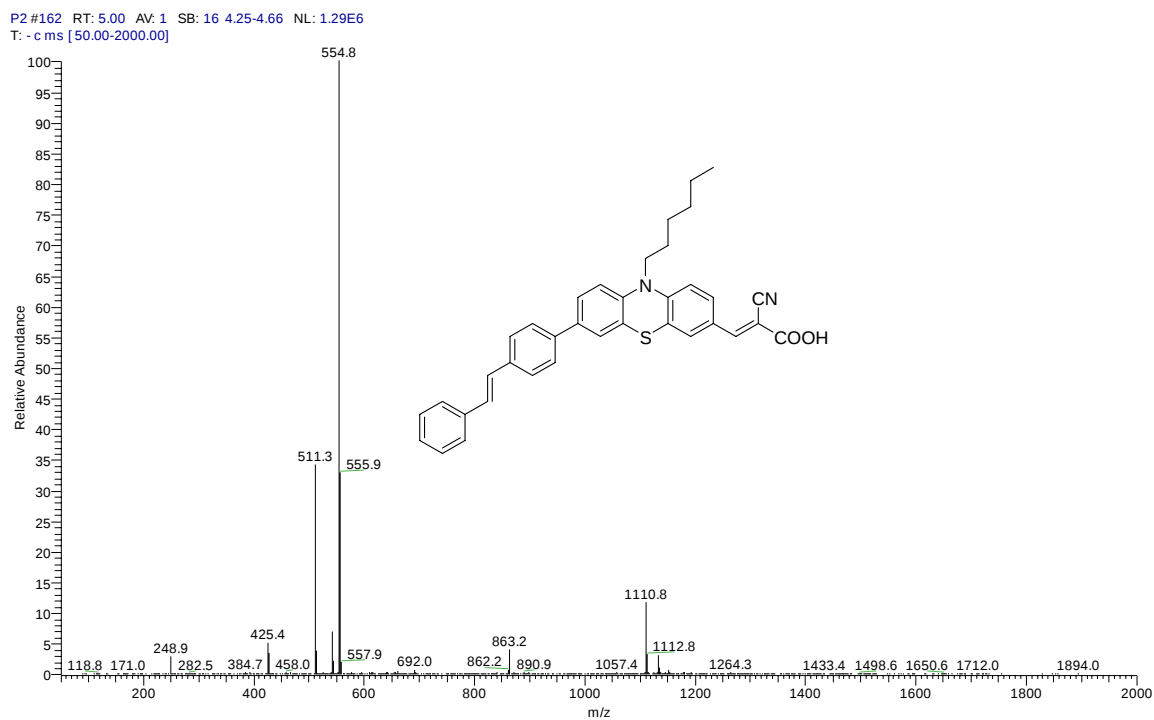
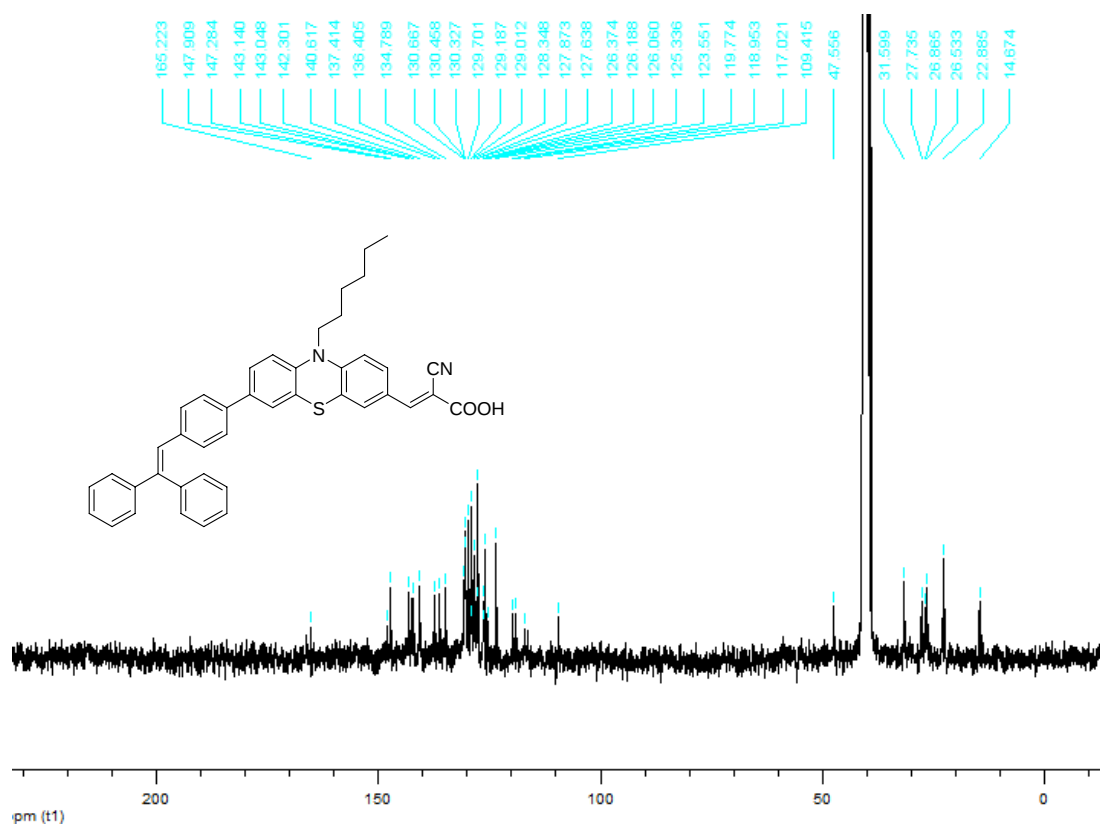


Fig. S14 MS spectrum of VP2



Mass spectrum of compound 10. The x-axis represents the mass-to-charge ratio (m/z) from 100 to 1500, and the y-axis represents the relative abundance from 0 to 100. The base peak is at m/z 587.2. Other significant peaks are labeled at m/z 145.1, 155.1, 222.9, 248.9, 252.9, 256.8, 363.5, 384.9, 412.7, 458.0, 501.3, 532.9, 631.0, 631.9, 707.9, 716.7, 790.6, 814.6, 848.6, 908.6, 980.1, 1048.5, 1168.7, 1271.8, 1305.0, 1325.0, 1392.1, and 1413.0. The chemical structure of compound 10 is shown as an inset.

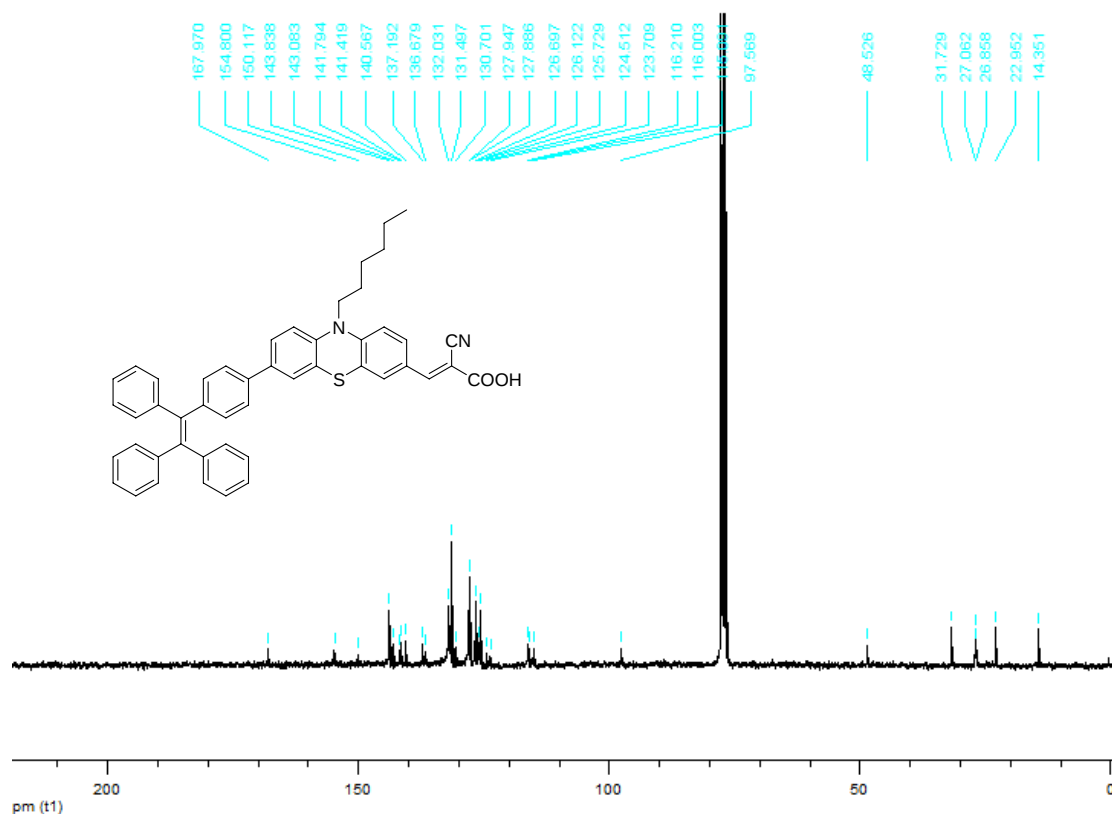


Fig. S19 ¹³C NMR spectrum of VP4

Instrument:DSQ(Thermo)

Ionization Method:EI

D:\DSQDATA-LR\11\O61203

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O61203 #203 RT: 3.51 AV: 1 NL: 5.19E5

T: + c Full ms [45.00-850.00]

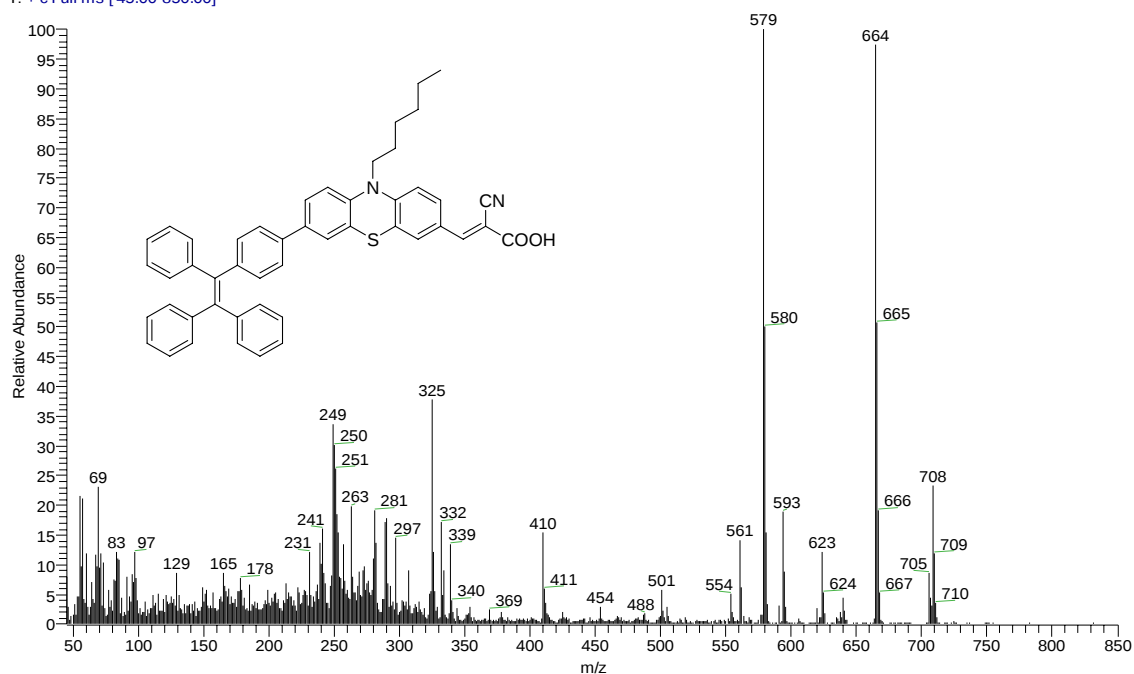


Fig. S20 MS spectrum of VP4