Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Support Information

Butterfly-shaped asymmetric squaraine dimers for organic photovoltaics

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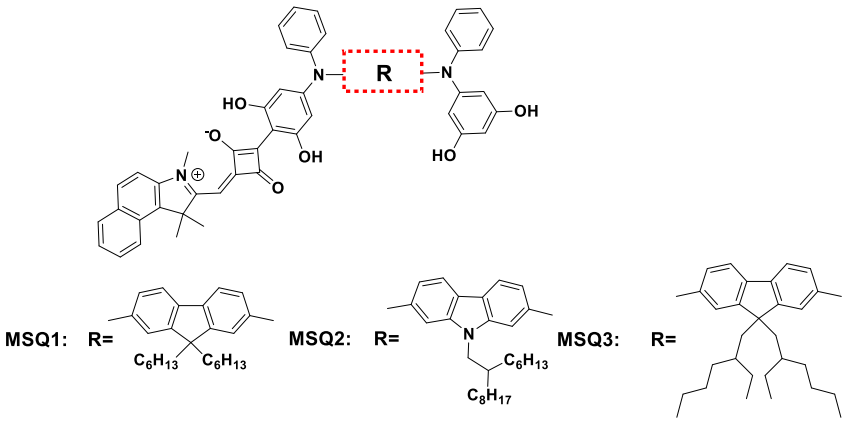
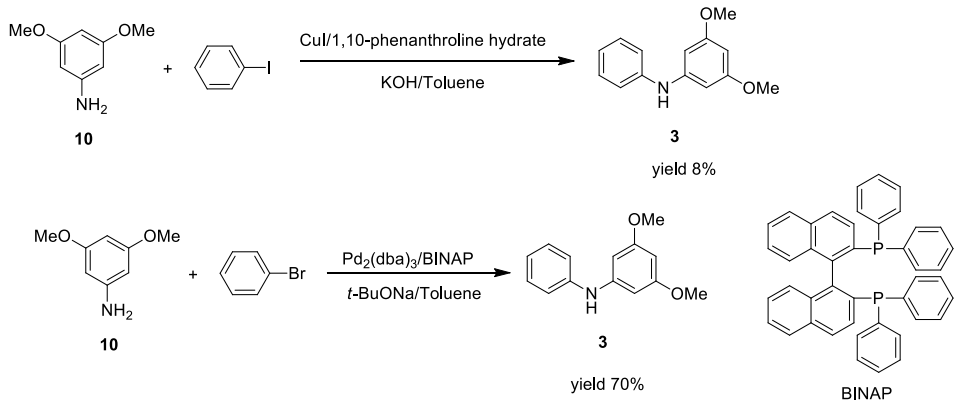
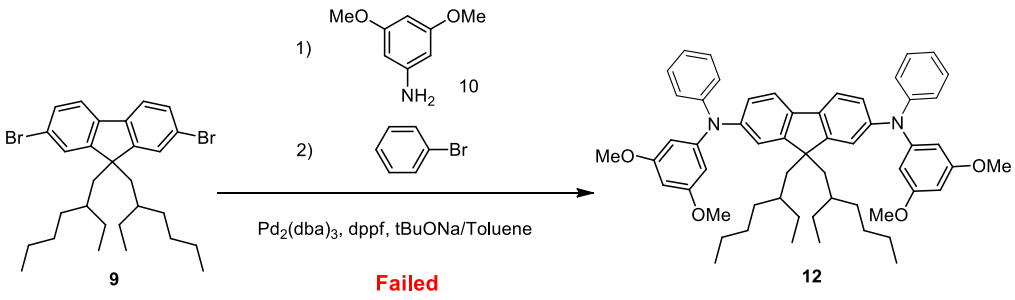


Chart S1. Structure of mono-substituted squaraines (**MSQ**).



Scheme S1. Two synthetic methods tried in this work for preparing compound **3**.



Scheme S2. Proposed one-pot approach of preparing compound **12**.

Table S1. Photovoltaic Performance of BHJ-OSCs[a] based on **DSQ1-3** with different D/A blend ratios.

Sample	Blending ratio (D:A)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	PCE (%)
DSQ1	1:3	0.70	4.00	0.36	1.00
	1:5	0.81	7.22	0.39	2.26
	1:7	0.81	6.61	0.38	2.01
DSQ2	1:3	0.81	9.77	0.43	3.44
	1:5	0.83	10.82	0.49	4.38
	1:7	0.83	10.29	0.47	4.02
DSQ3	1:3	0.83	8.83	0.45	3.27
	1:5	0.84	10.19	0.47	4.02
	1:7	0.85	9.82	0.46	3.80

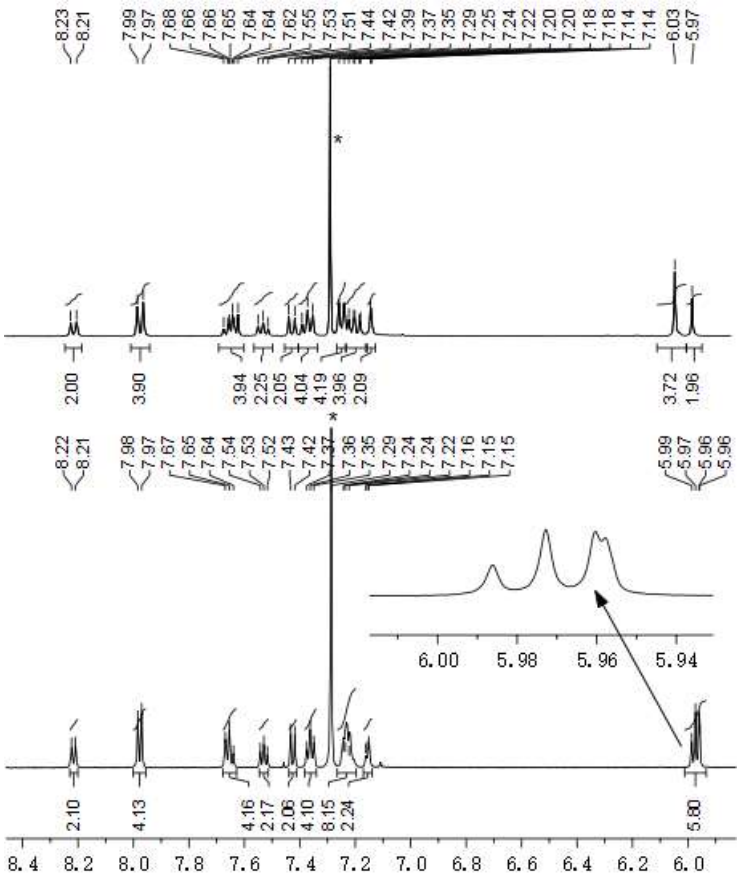


Fig. S1 ^{1}H NMR spectra of **DSQ1** and **DSQ3** conducted in $CDCl_3$(*).

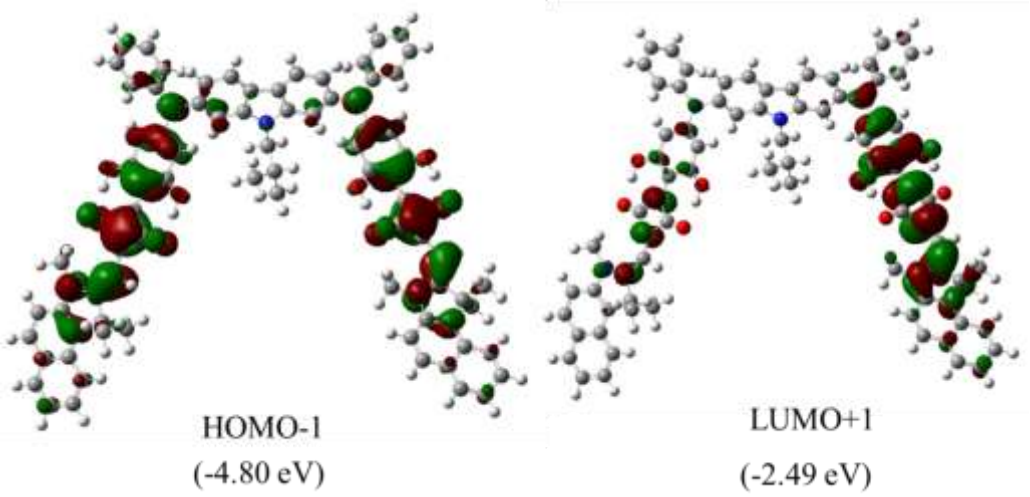


Fig. S2 The calculated HOMO-1 and LUMO+1 energies using Density function theory at the B3LYP/6-31G* level.

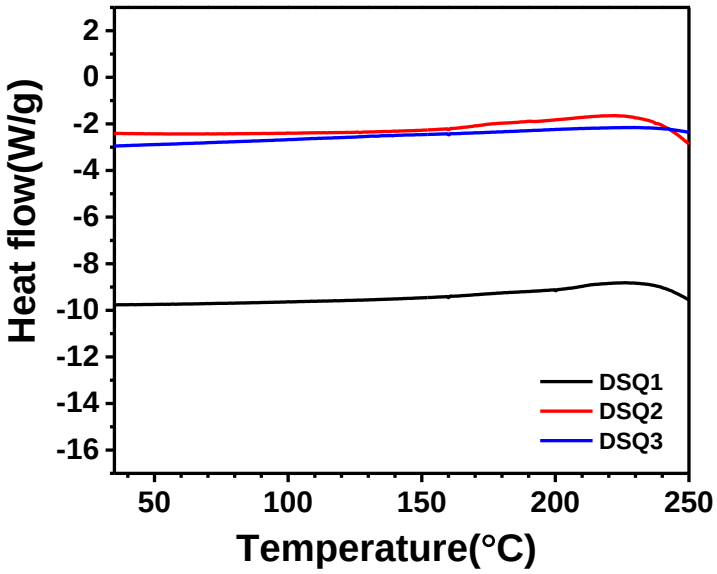


Fig. S3 Differential scanning calorimetry (DSC) curve of **DSQ1-3** between 35-250 ℃ under N_2 atmosphere with a heating rate of 10 ℃/min.

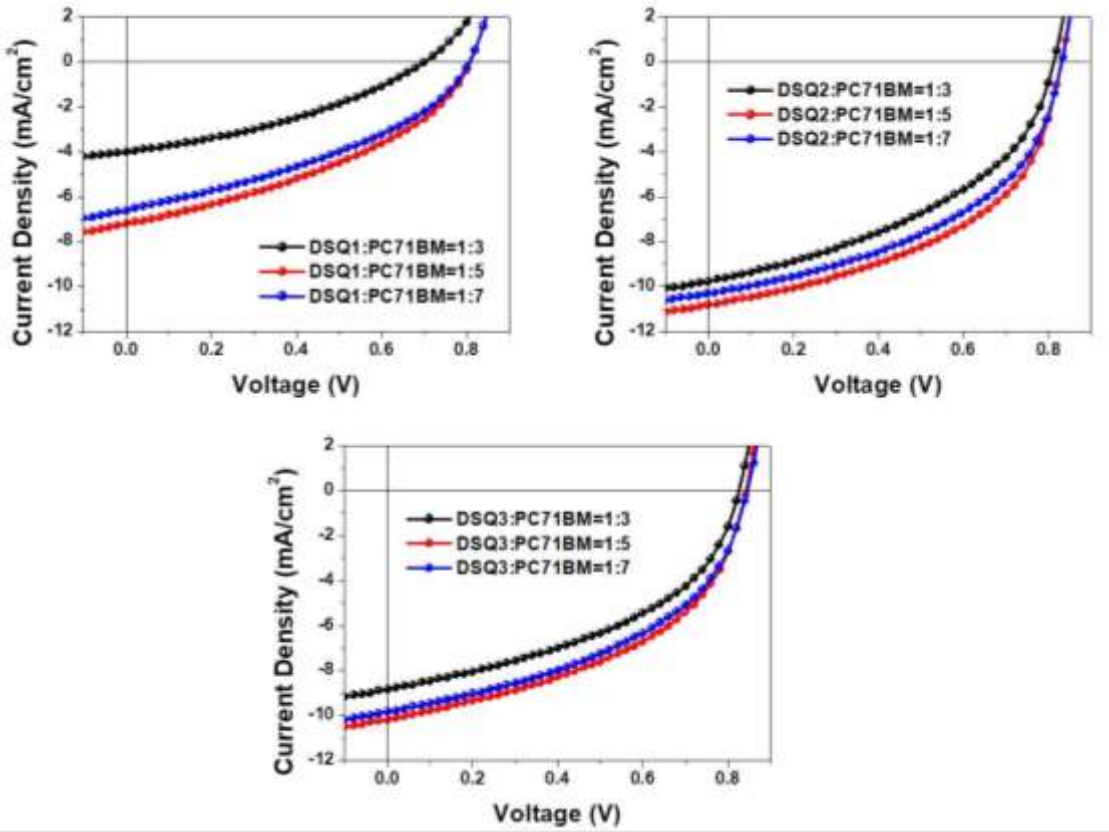


Fig. S4 Current density-voltage (*J*-*V*) curve of different D/A ratios based on a conventional single junction device structure of ITO/MoO_3 (8 nm)/**DSQ**:$PC_{71}BM$/BCP (4 nm)/Al (100 nm).

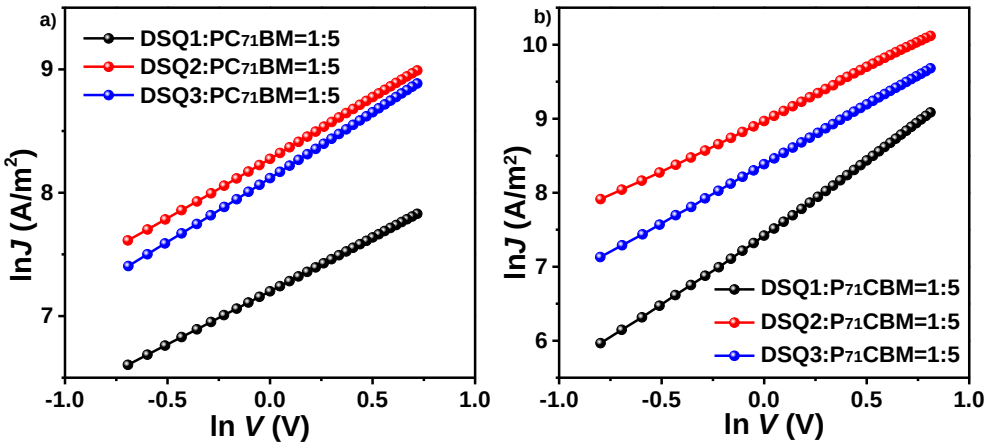


Fig. S5 (a) *J-V* characteristic of the single hole-carrier devices based on **DSQ1-3**: $PC_{71}BM$ (1:5) blend film; (b) *J-V* characteristic of the single electron-carrier devices based on **DSQ1-3**:$PC_{71}BM$ (1:5) blend film.

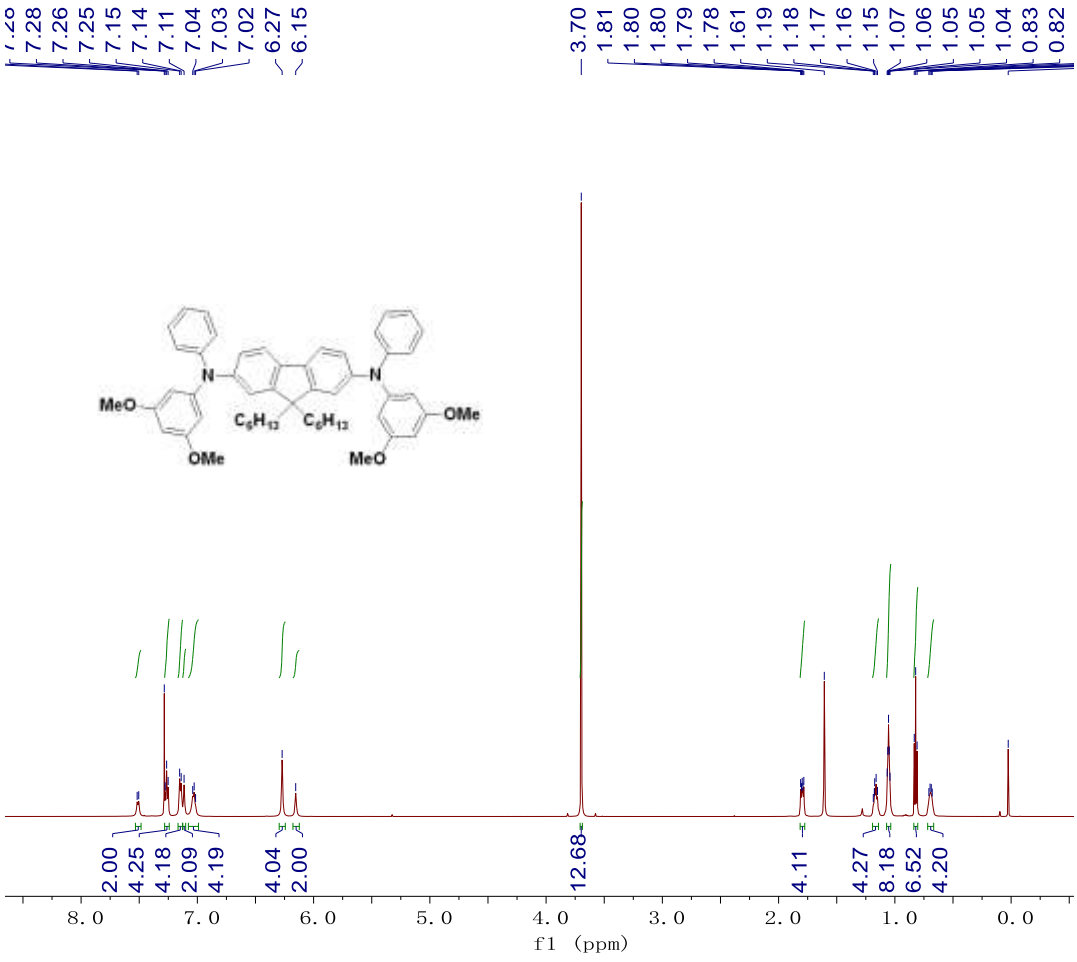


Fig. S6 ^{1}H NMR spectrum of **compound 4** in $CDCl_3$.

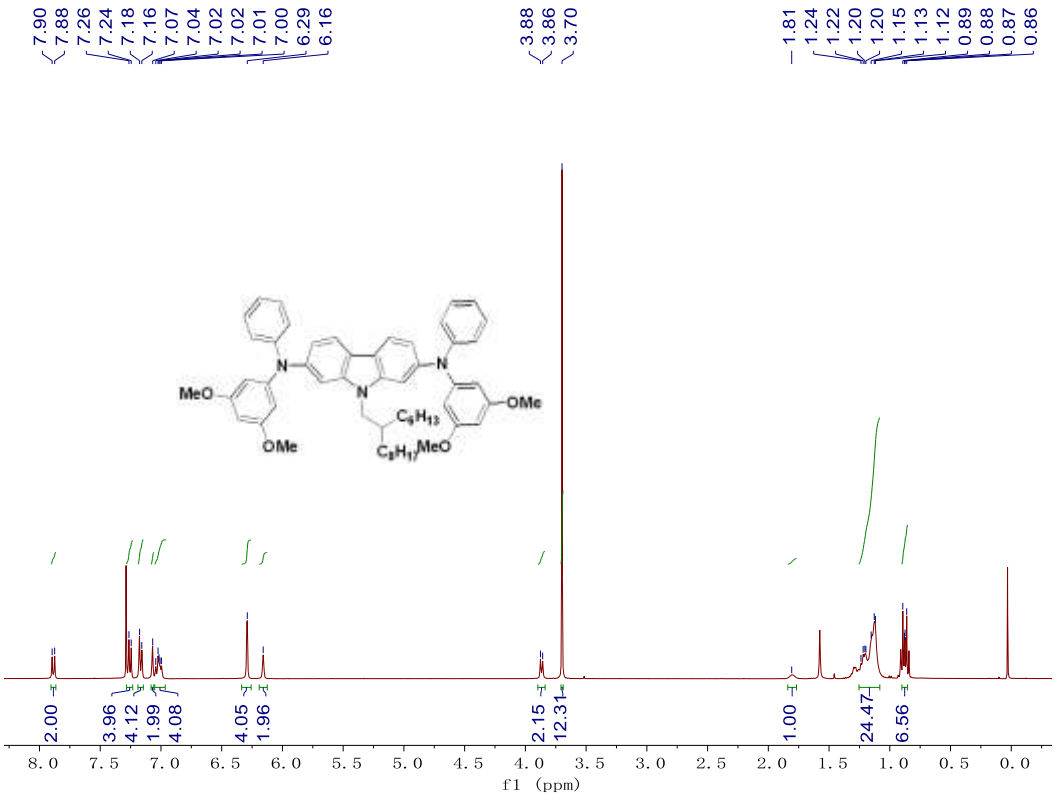


Fig. S7 ^{1}H NMR spectrum of **compound 5** in $CDCl_3$.

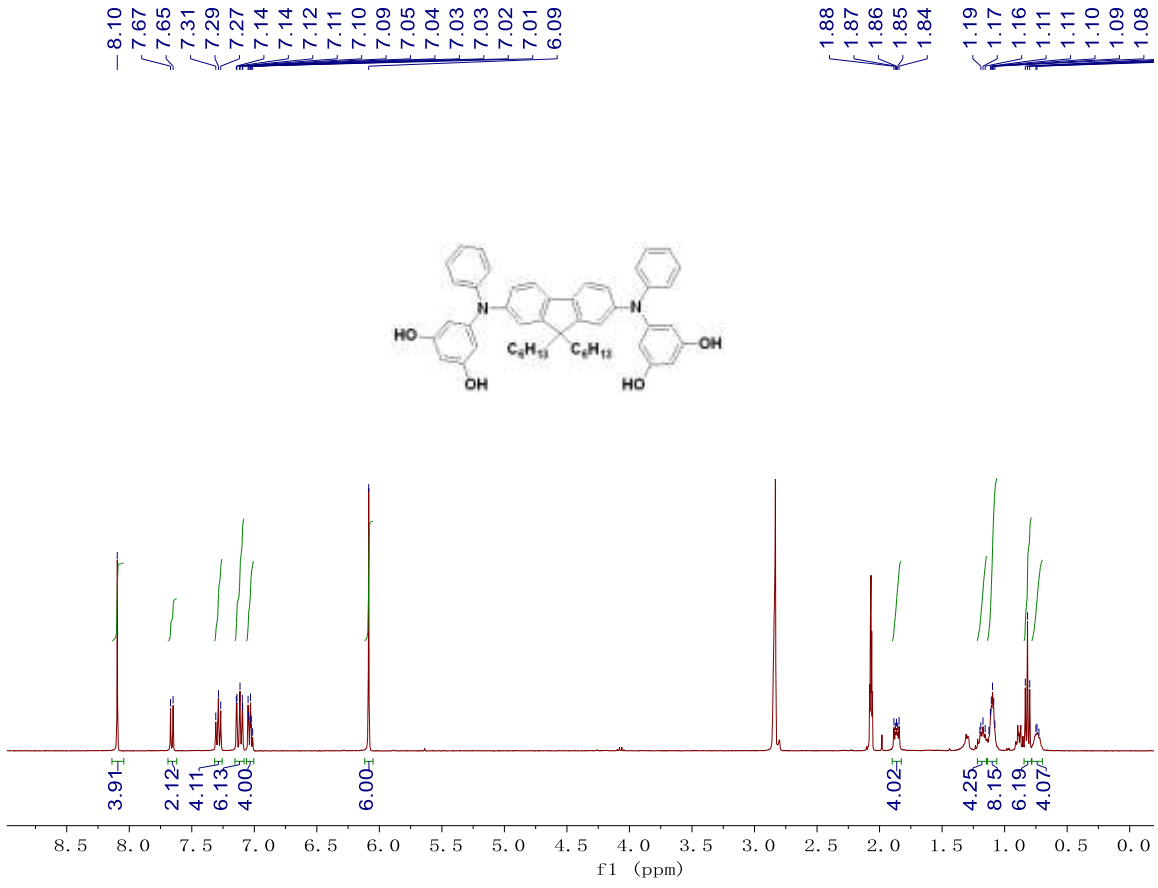


Fig. S8 ^{1}H NMR spectrum of **compound 6** in acetone-d_6.

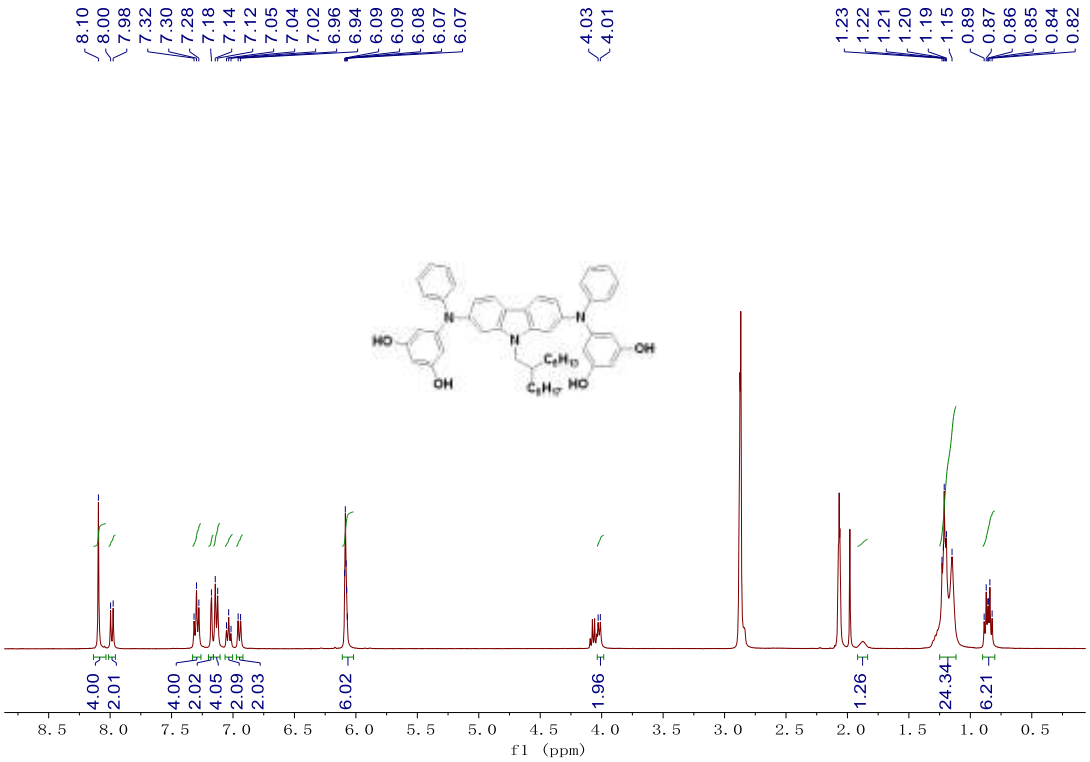


Fig. S9 ^{1}H NMR spectrum of **compound 7** in acetone-d_6.

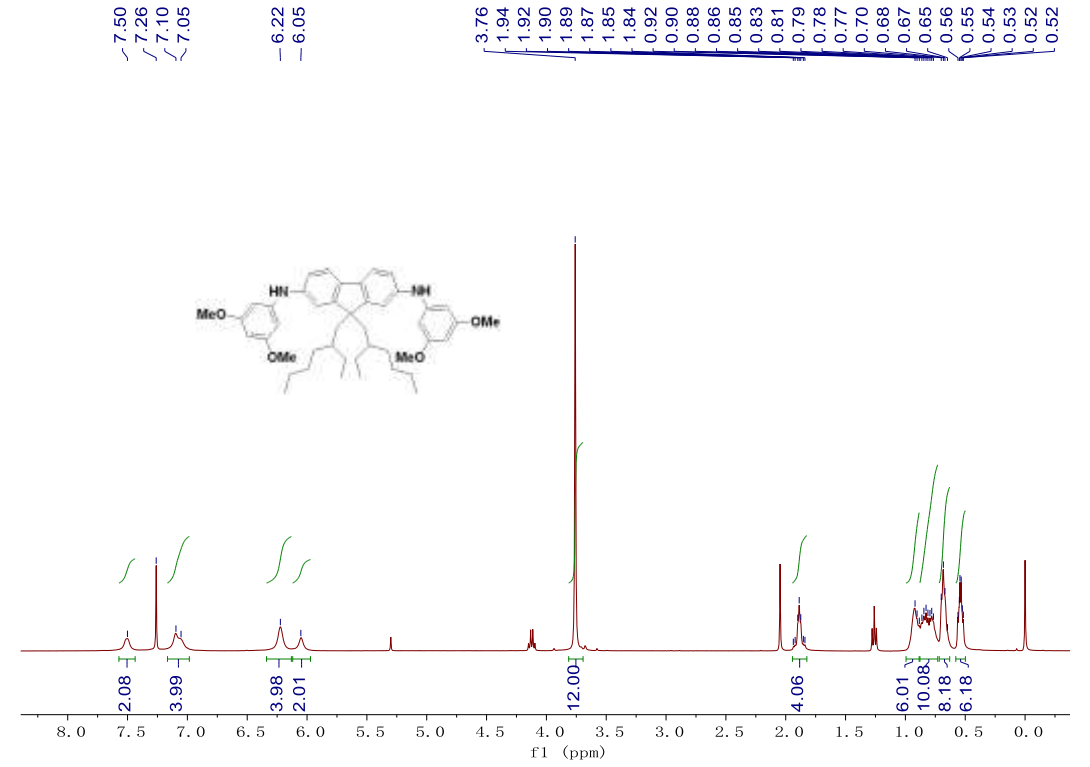


Fig. S10 ^{1}H NMR spectrum of **compound 11** in $CDCl_3$.

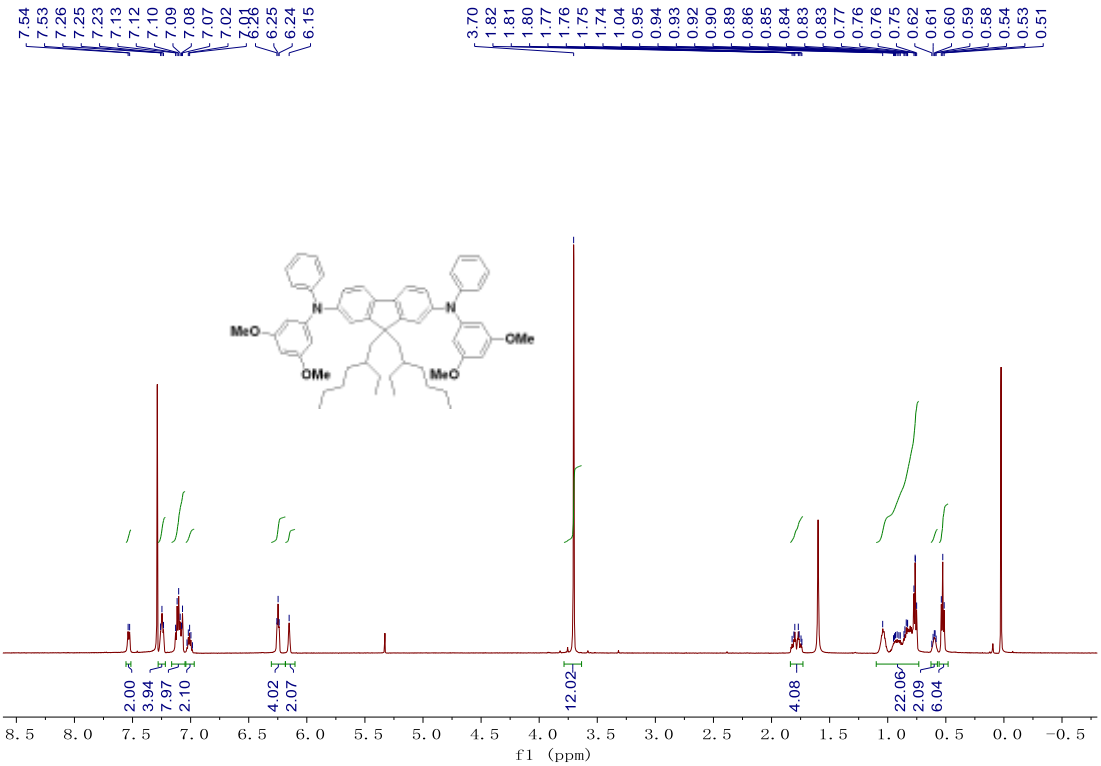


Fig. S11 ^{1}H NMR spectrum of **compound 12** in $CDCl_3$.

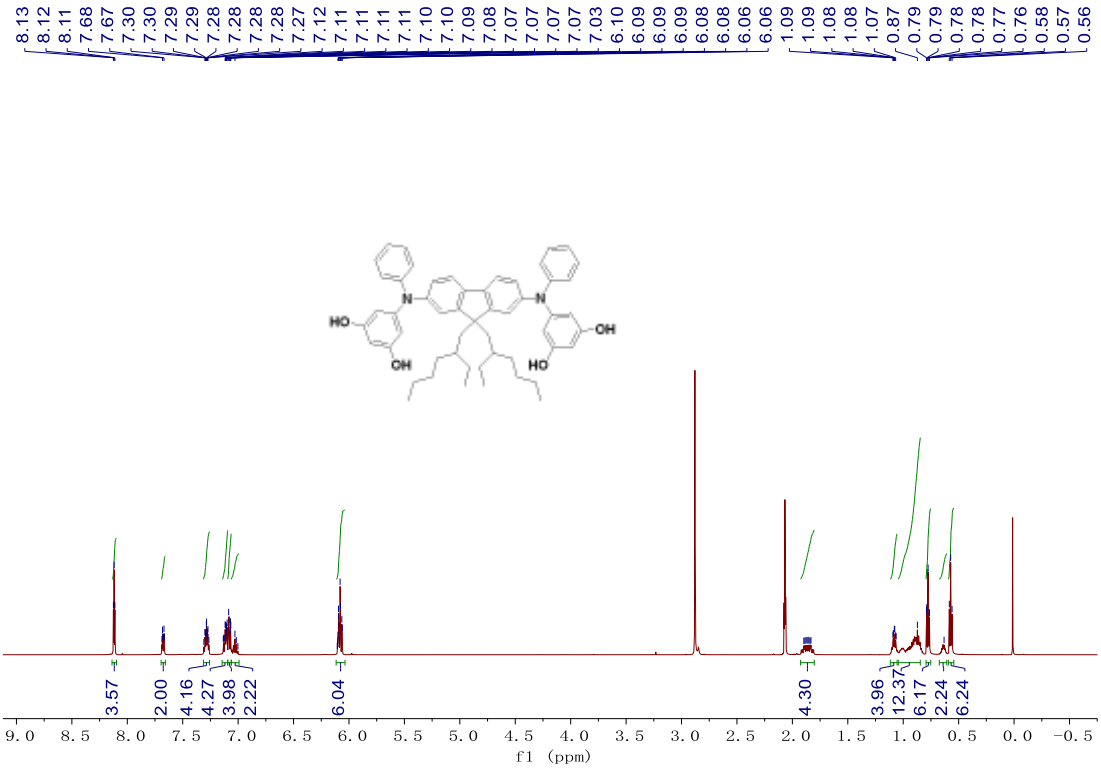


Fig. S12 ^{1}H NMR spectrum of **compound 13** in acetone-d_6.

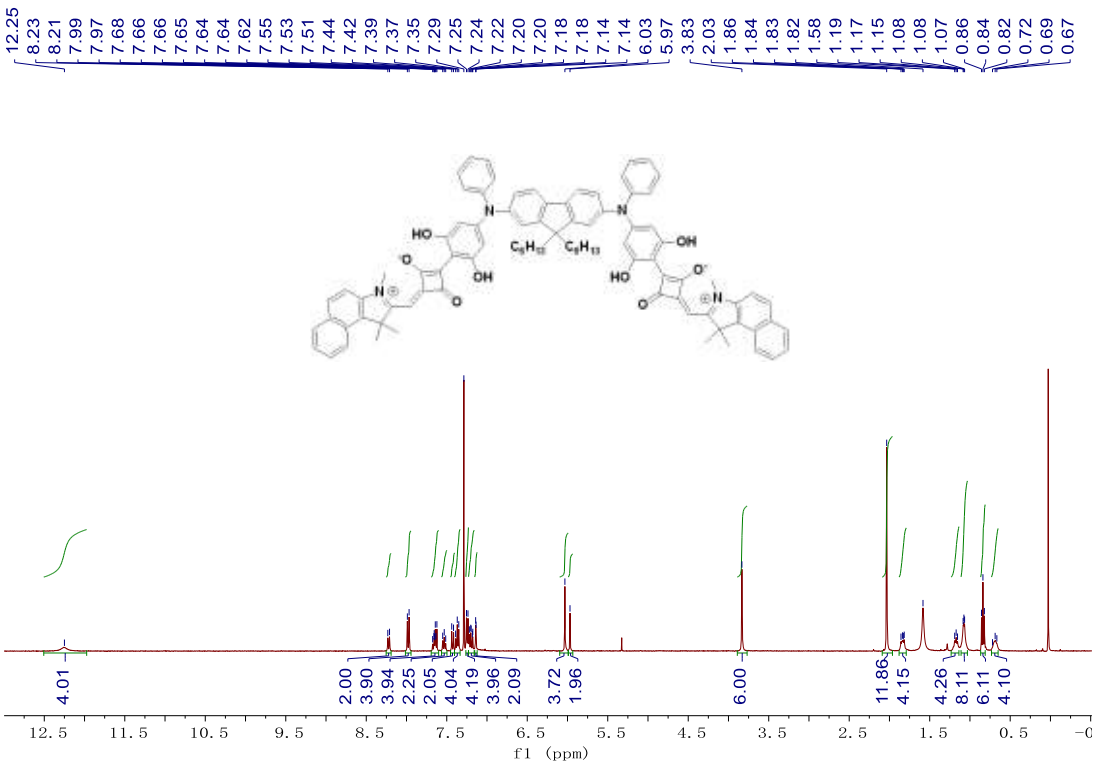


Fig. S13 ^{1}H NMR spectrum of **DSQ1** in $CDCl_3$.

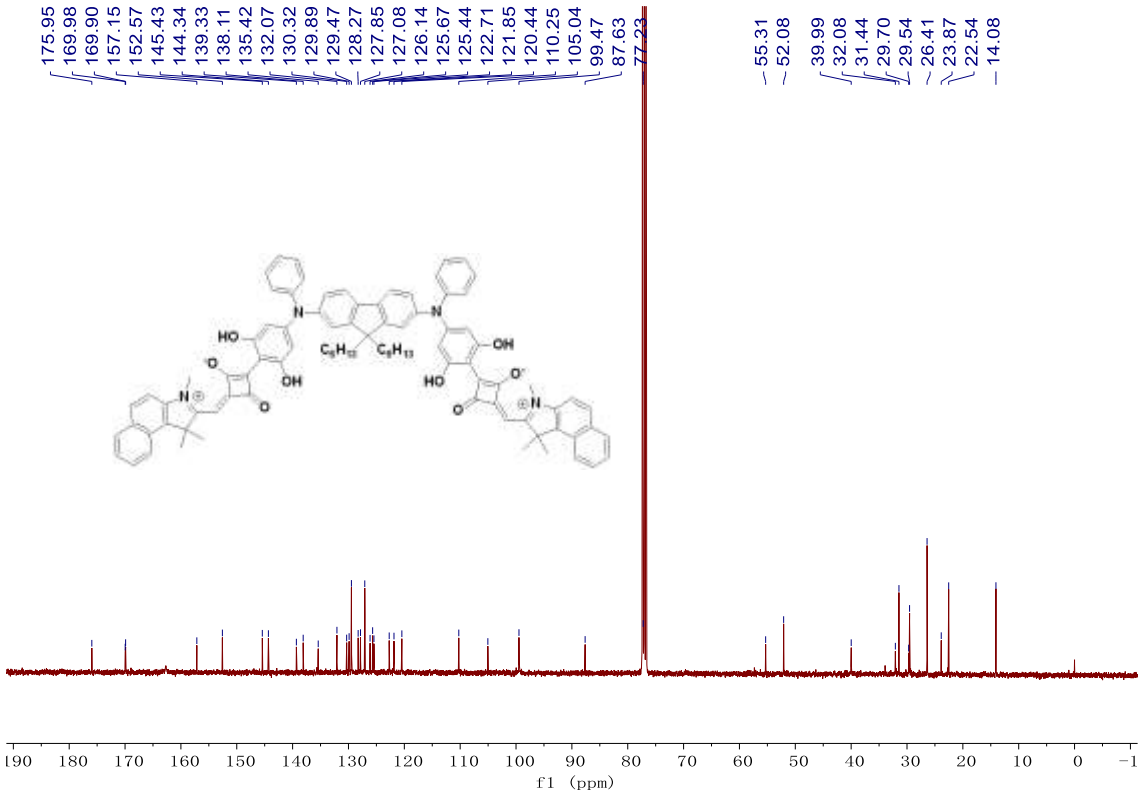


Fig. S14 ^{13}C NMR spectrum of **DSQ1** in $CDCl_3$.

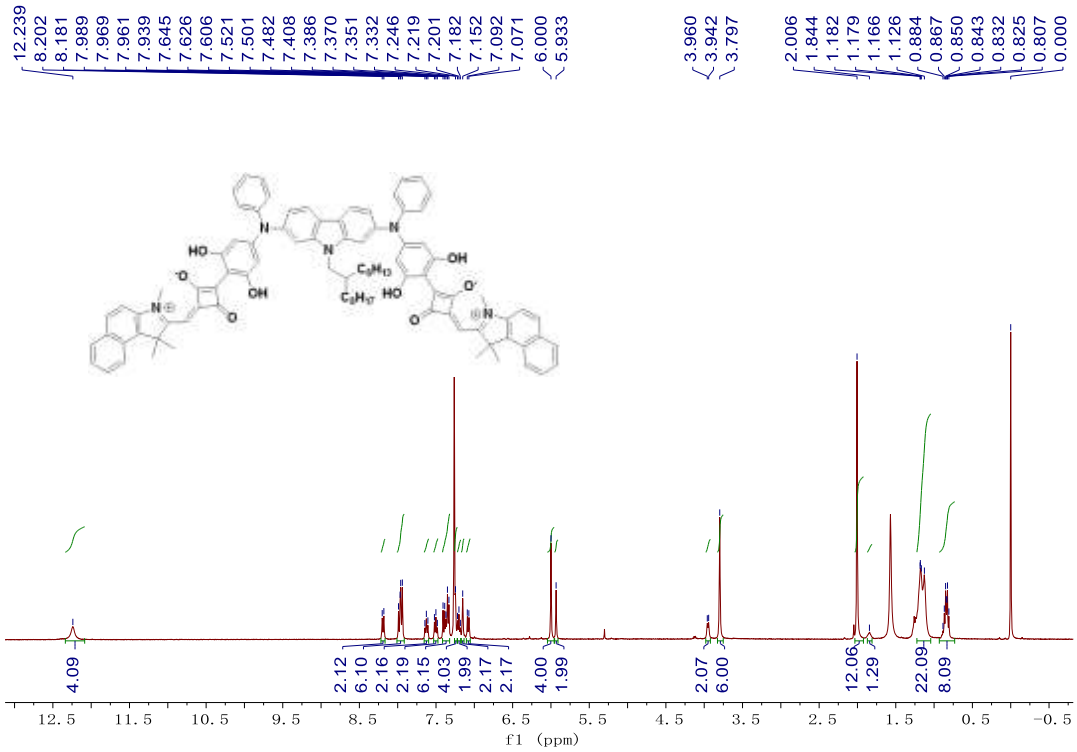


Fig. S15 ^{1}H NMR spectrum of **DSQ2** in $CDCl_3$.

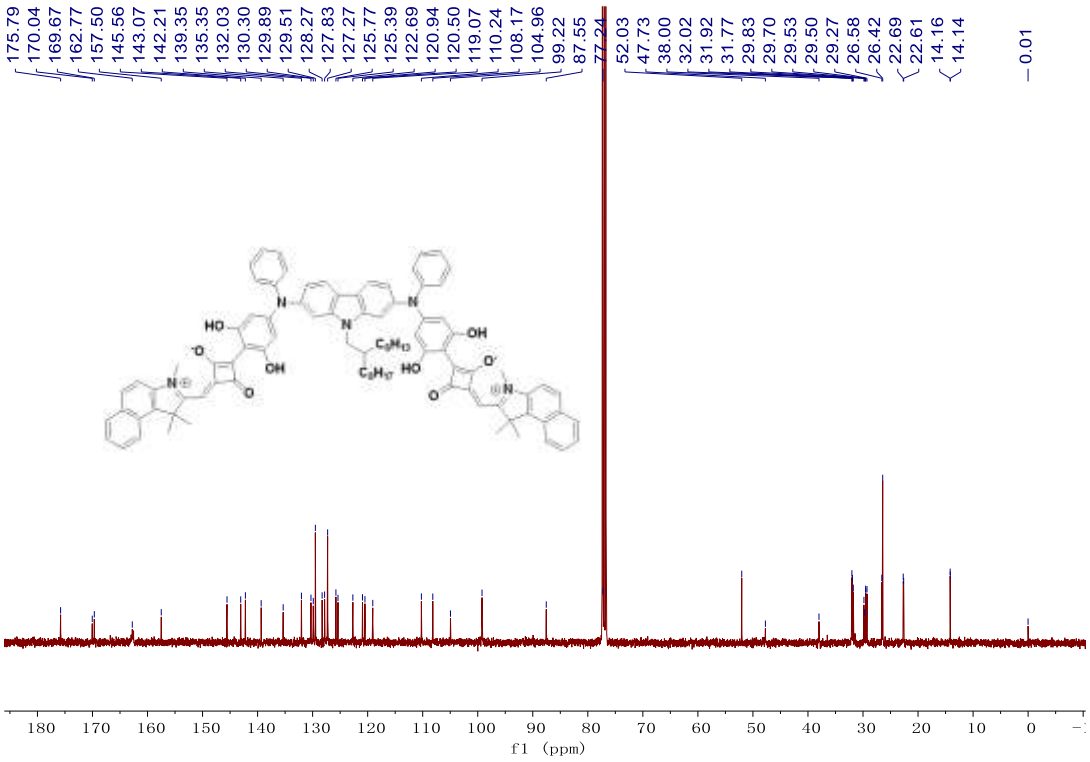


Fig. S16 ^{13}C NMR spectrum of **DSQ2** in $CDCl_3$.

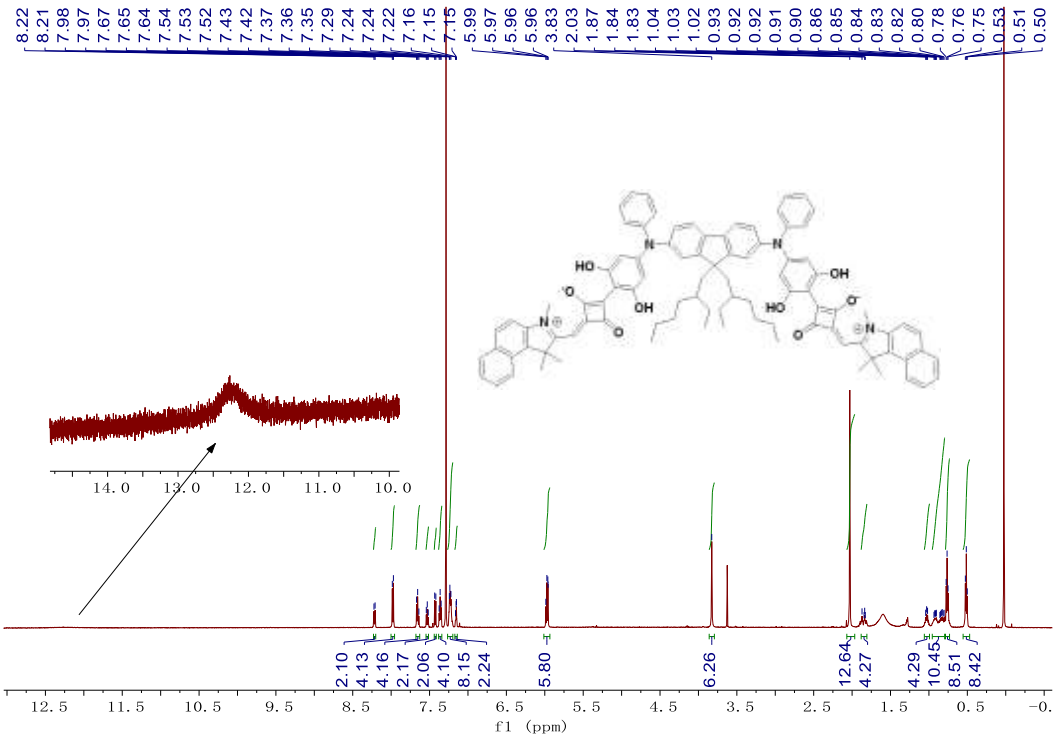


Fig. S17 ^{1}H NMR spectrum of **DSQ3** in $CDCl_3$.

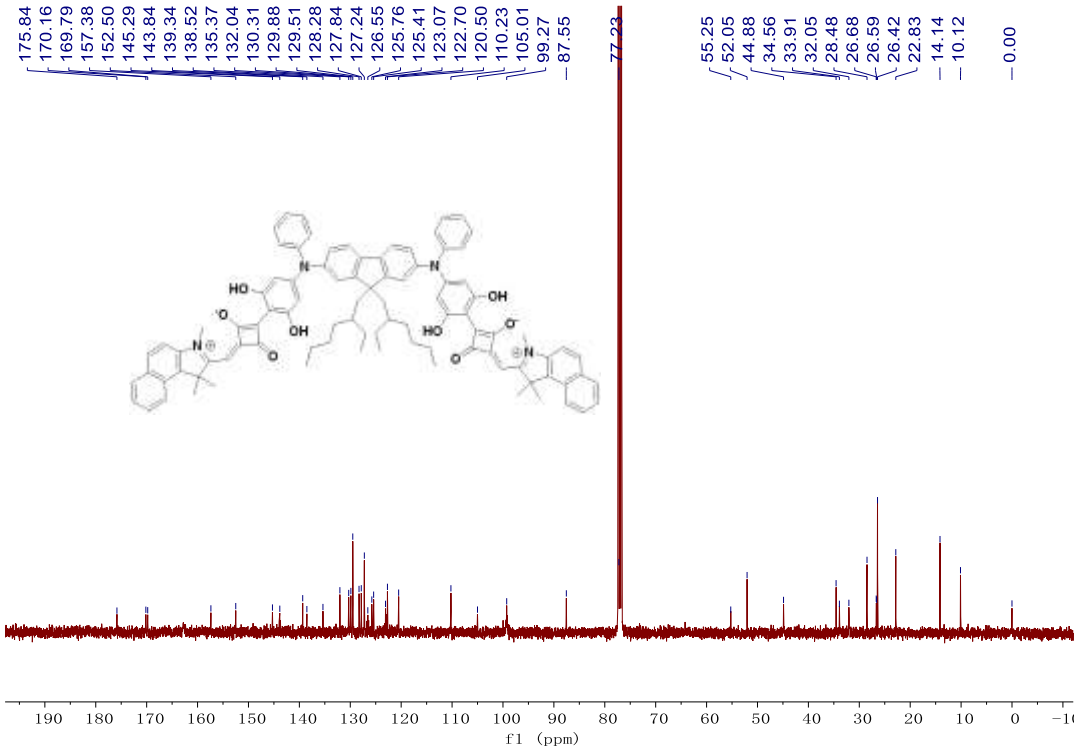


Fig. S18 ^{13}C NMR spectrum of **DSQ3** in $CDCl_3$.

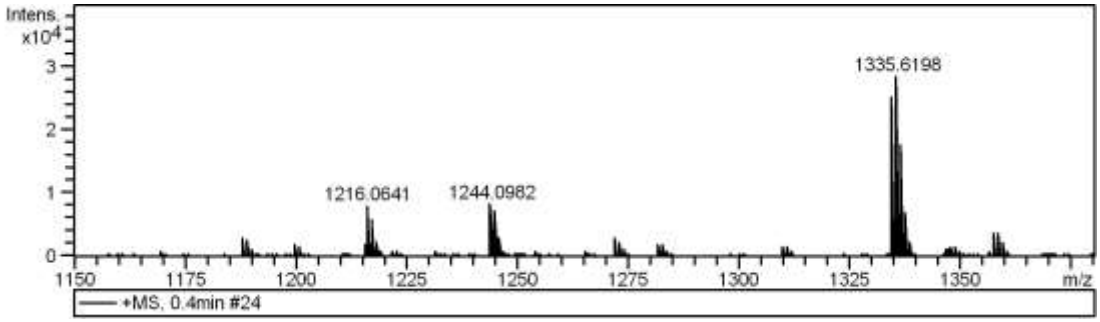


Fig. S19 HRMS spectrum of **DSQ1**.

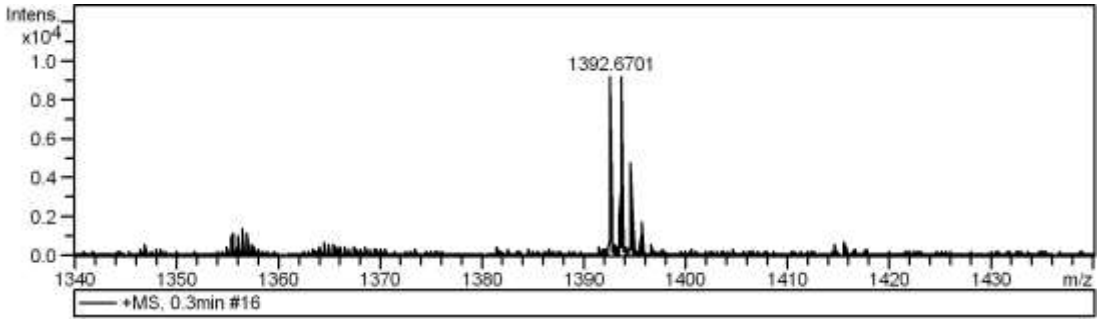


Fig. S20 HRMS spectrum of **DSQ2**.

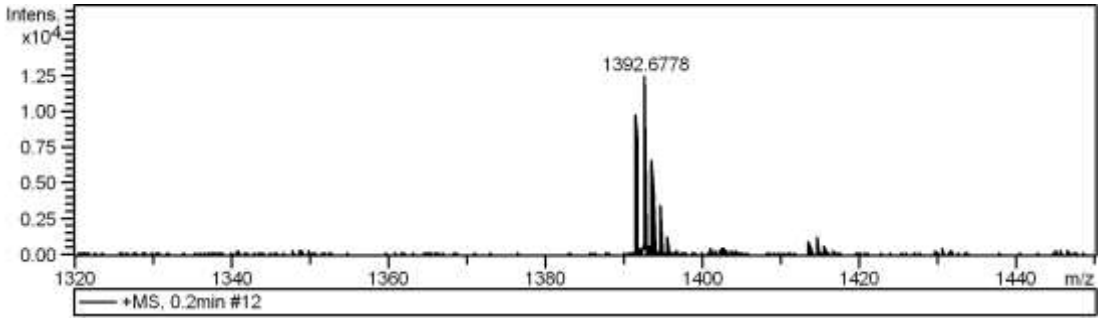


Fig. S21 HRMS spectrum of **DSQ3**.