

**Supplementary Material****Preparation and photophysical properties of all-*trans* acceptor- $\pi$ -donor (acceptor) compounds possessing obvious solvatochromic effects**

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**Table S1.** Calculated absorption spectrum properties, oscillator strengths, and major contribution for the target compounds (**BAQ**, **SFQ**, **BLQ**, and **XJQ**).

Compound	Transition	$\lambda^{\text{abs}}$ (nm)	Oscillator Strength, $f$	dominant transitions (percent contribution)
<b>BAQ</b>	S0→S1	387	1.3109	HOMO→LUMO (98%)
	S0→S4	321	0.4438	HOMO→LUMO+1 (82%)
<b>SFQ</b>	S0→S1	390	1.0698	HOMO→LUMO (99%)
	S0→S3	322	0.5544	HOMO→LUMO+1 (69%)

<b>BLQ</b>	S0→S1	417	0.6881	HOMO→LUMO (99%)
	S0→S3	327	0.9514	HOMO-1→LUMO (65%)
<b>XJQ</b>	S0→S5	368	0.9105	HOMO→LUMO+1 (87%)

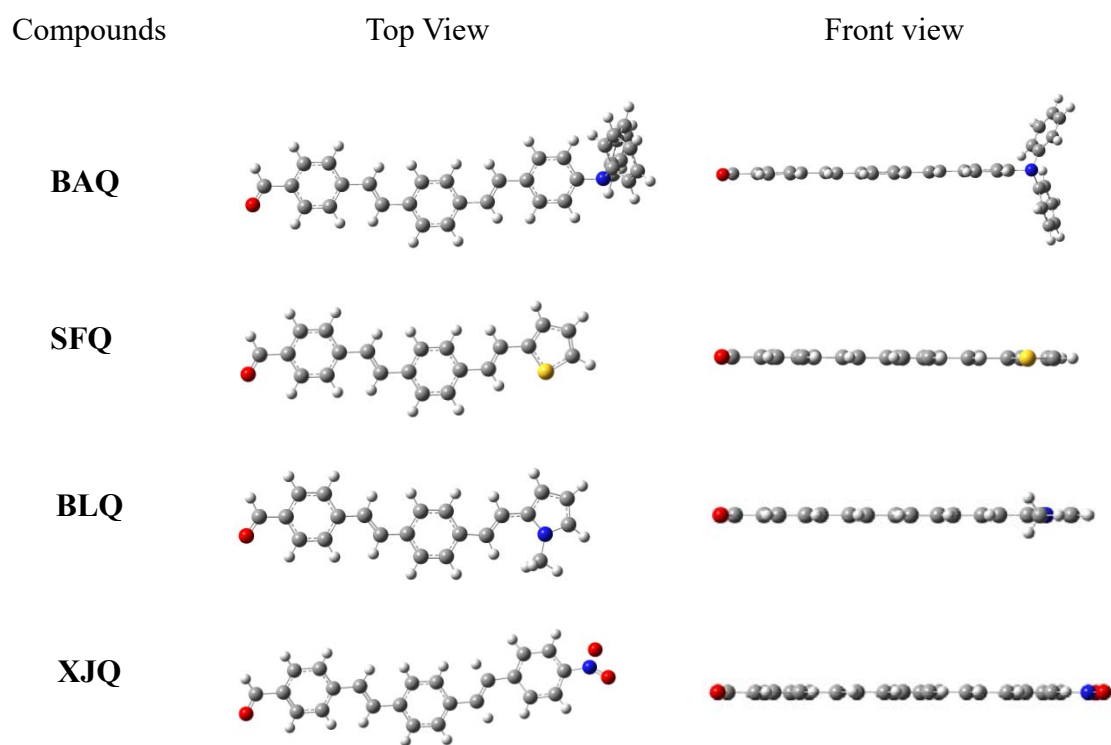


Figure S1 Optimized ground-state geometries of the target compounds (**BAQ**, **SFQ**, **BLQ**, and **XJQ**).

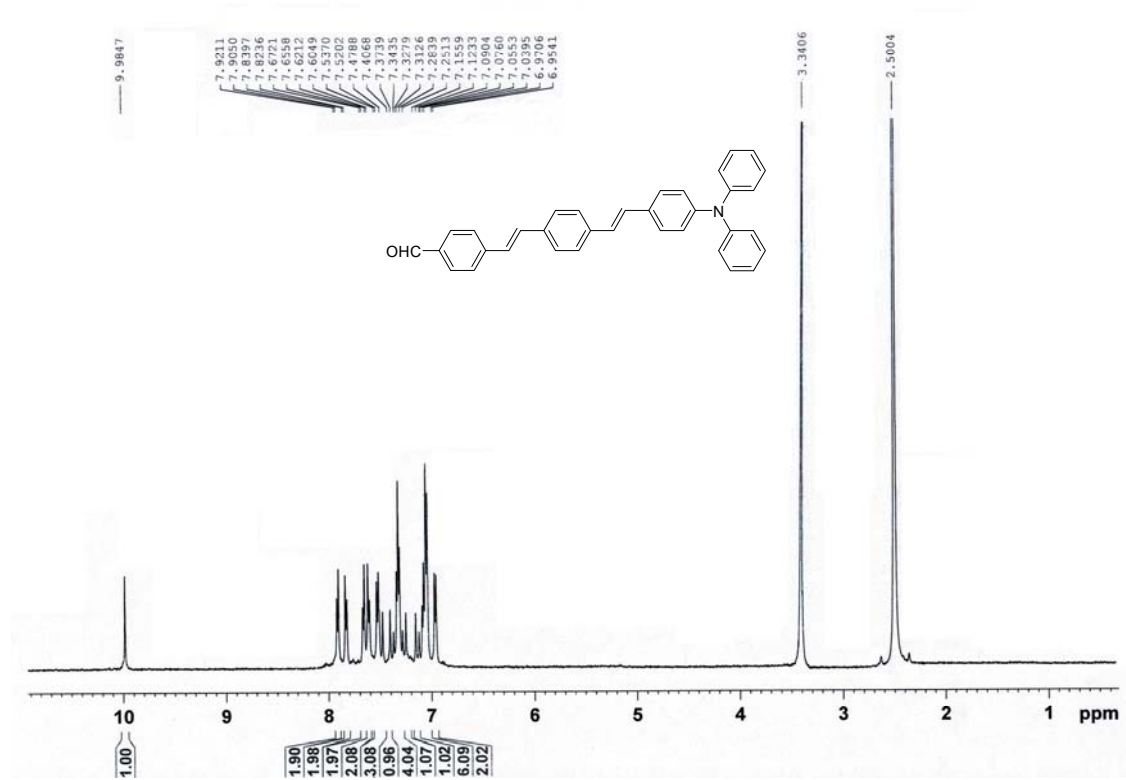


Figure S2 <sup>1</sup>H NMR spectrum of BAQ.

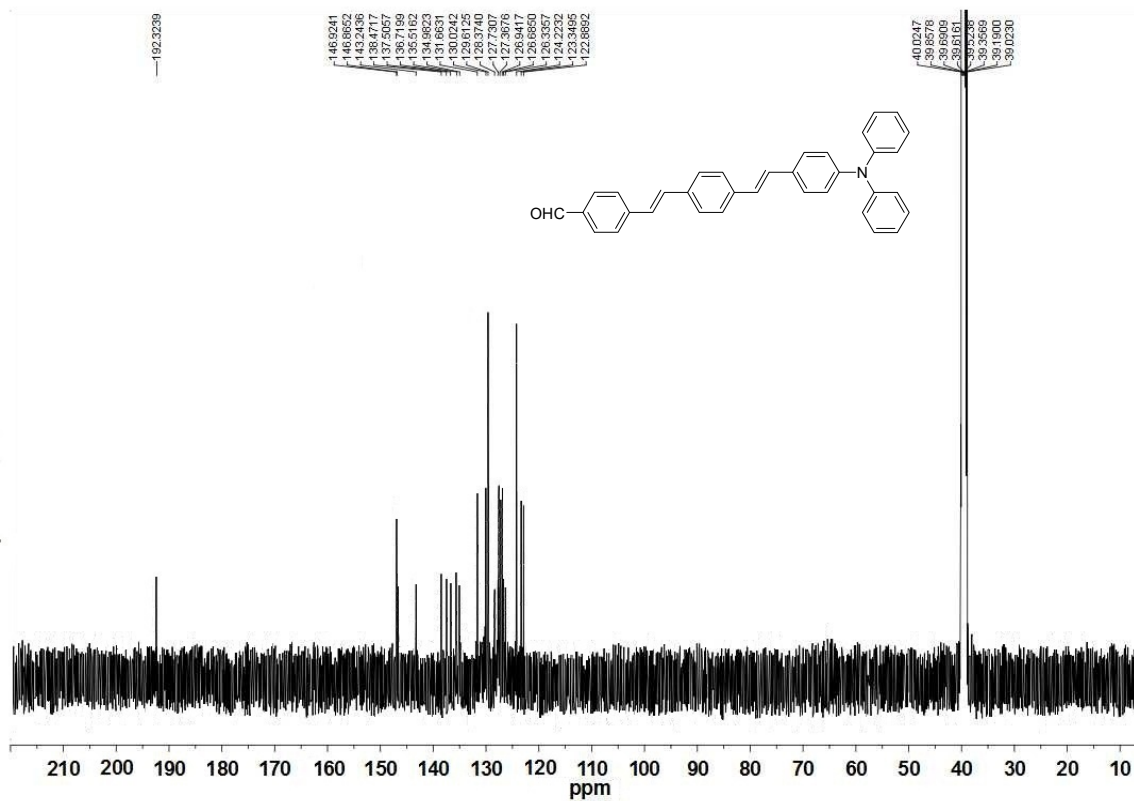


Figure S3 <sup>13</sup>C NMR spectrum of BAQ.

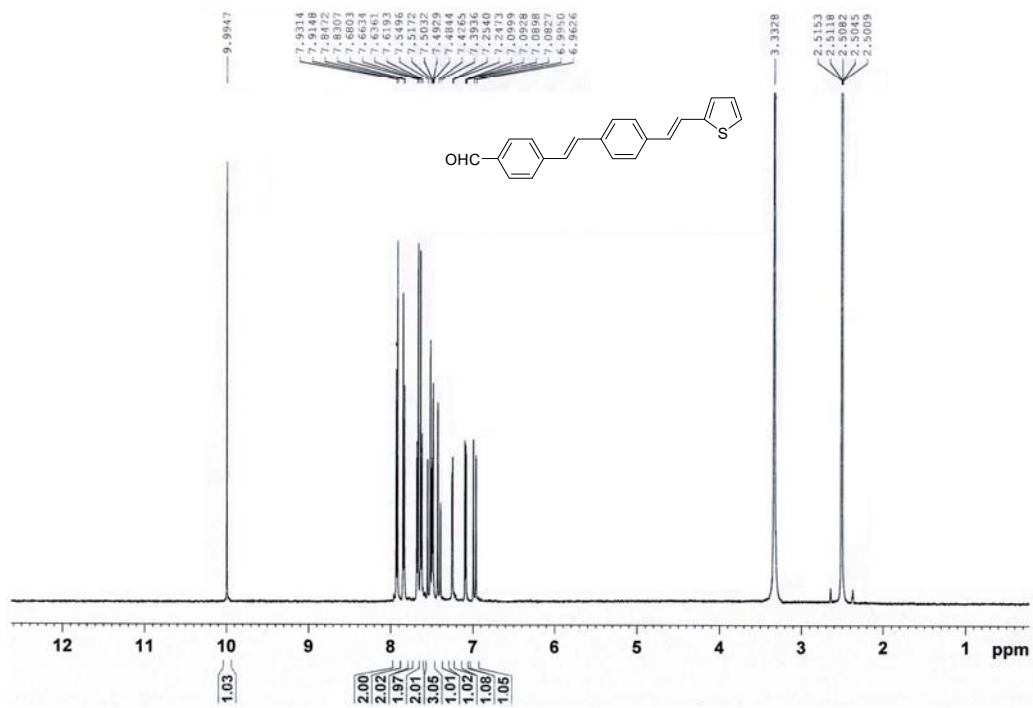


Figure S4 <sup>1</sup>H NMR spectrum of SFQ.

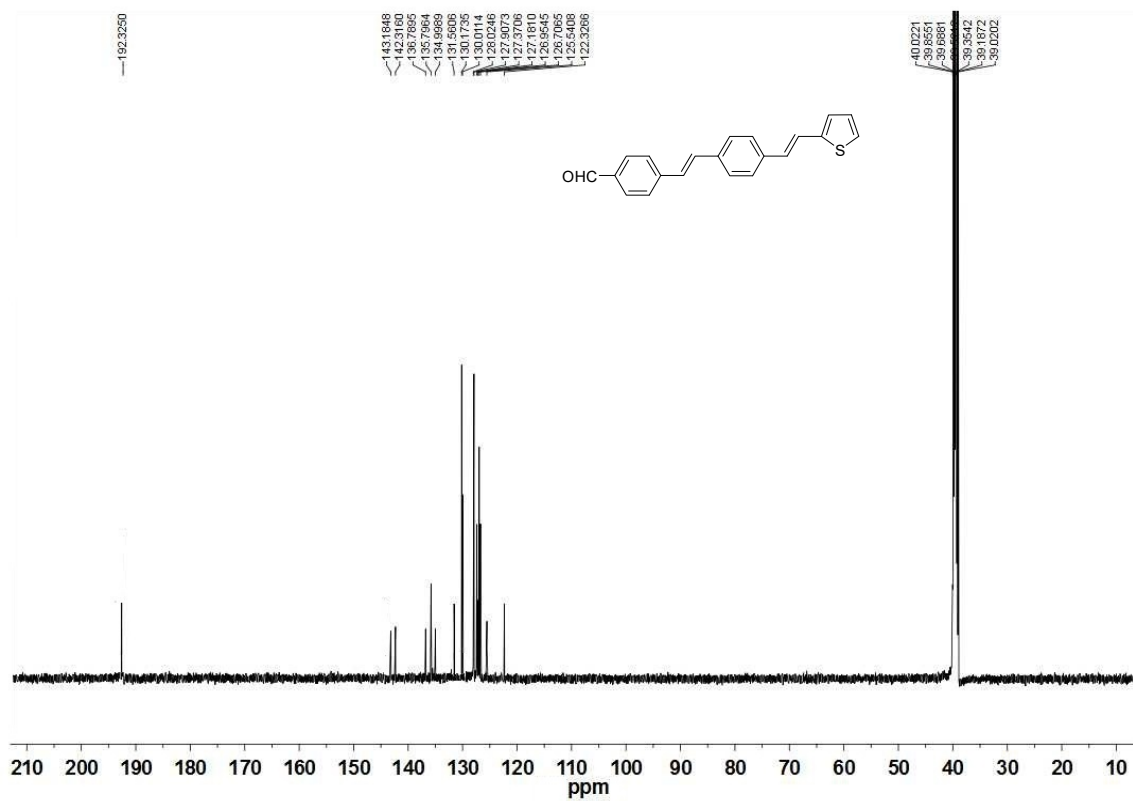


Figure S5  $^{13}\text{C}$  NMR spectrum of SFQ.

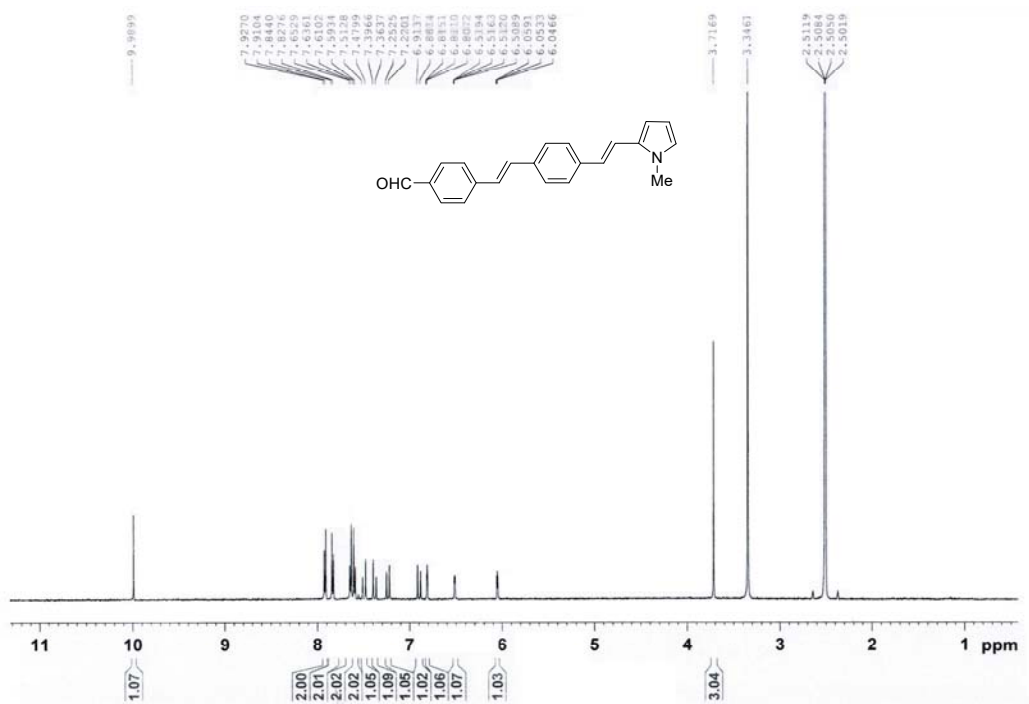


Figure S6 <sup>1</sup>H NMR spectrum of **BLQ**.

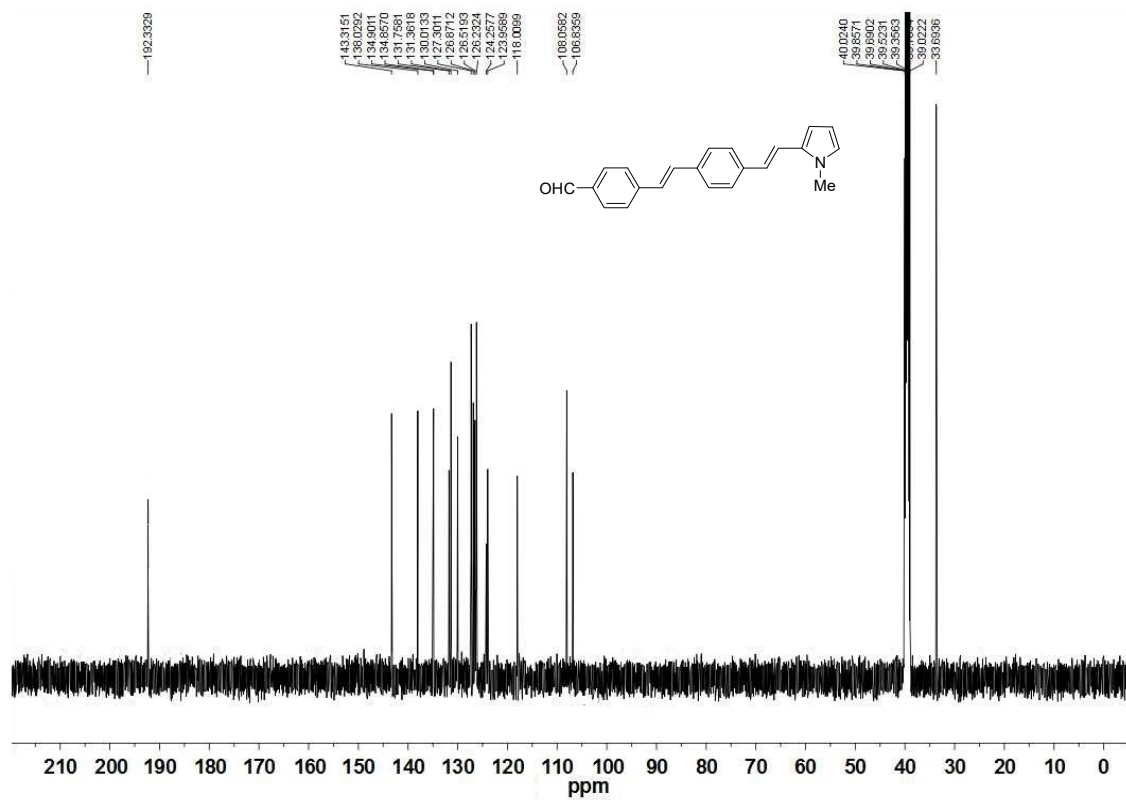


Figure S7  $^{13}\text{C}$  NMR spectrum of BLQ.



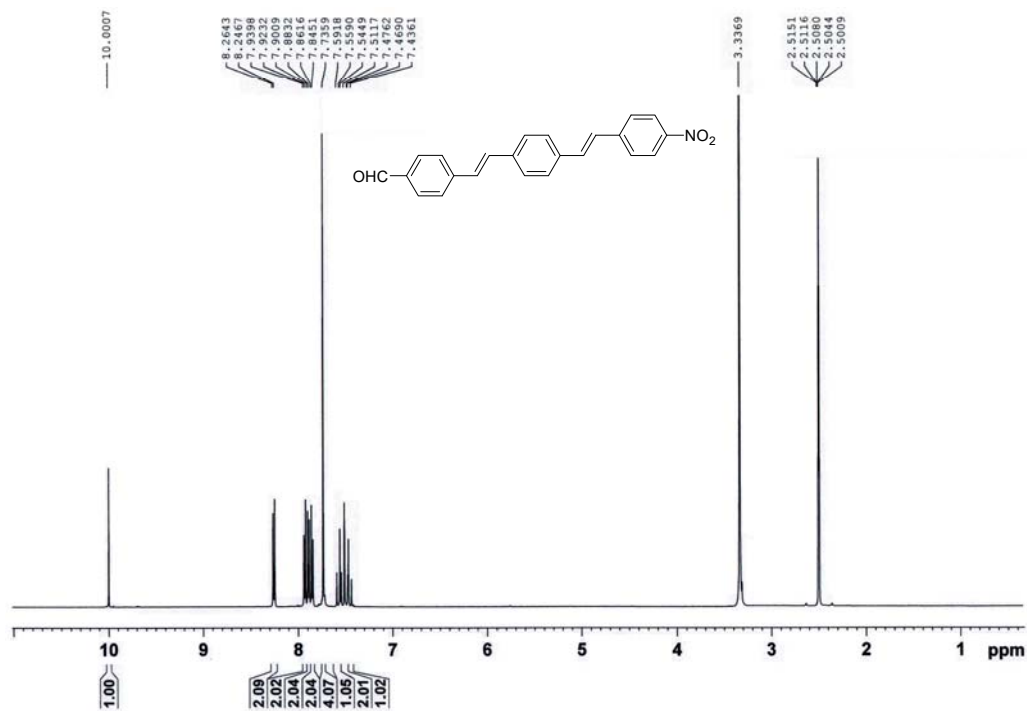


Figure S8 <sup>1</sup>H NMR spectrum of XJQ.

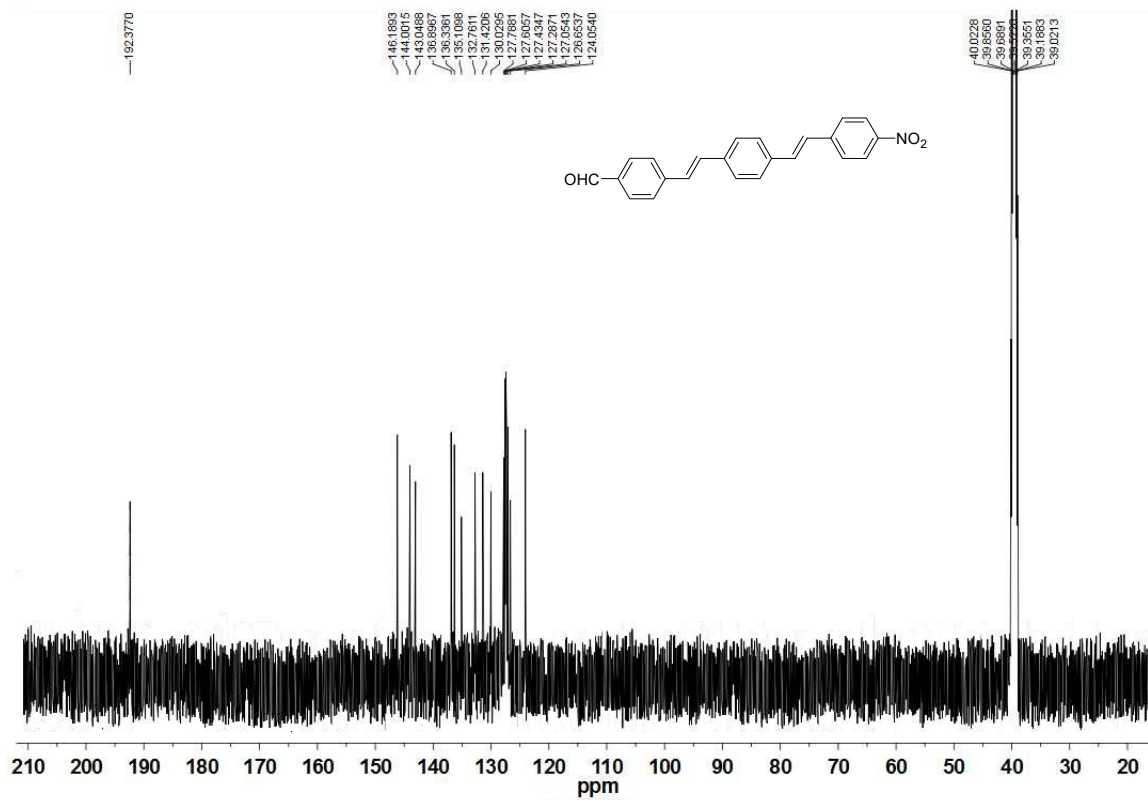


Figure S9  $^{13}\text{C}$  NMR spectrum of XJQ.