

Supplementary Material**Preparation and photophysical properties of all-*trans* acceptor- π -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	λ^{abs} (nm)	Oscillator Strength, f	dominant transitions (percent contribution)
BAQ	S0→S1	387	1.3109	HOMO→LUMO (98%)
	S0→S4	321	0.4438	HOMO→LUMO+1 (82%)
SFQ	S0→S1	390	1.0698	HOMO→LUMO (99%)
	S0→S3	322	0.5544	HOMO→LUMO+1 (69%)

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

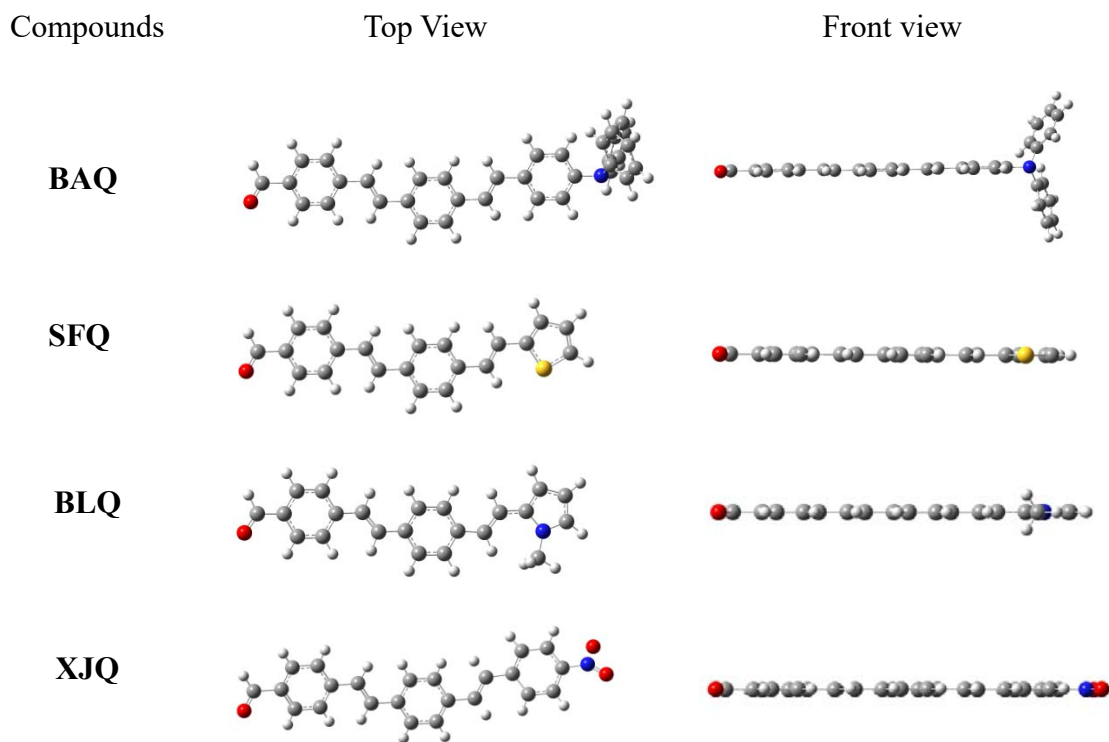


Figure S1 Optimized ground-state geometries of the target compounds (**BAQ**, **SFQ**, **BLQ**, and **XJQ**).

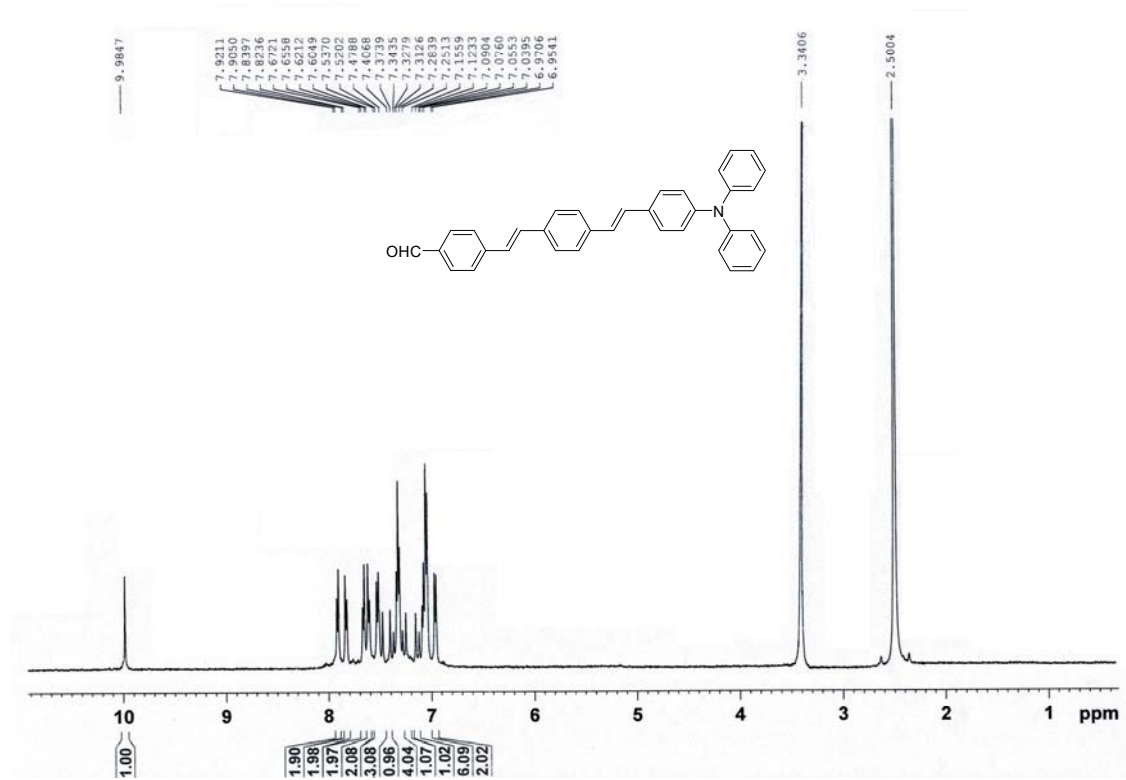


Figure S2 ¹H NMR spectrum of BAQ.

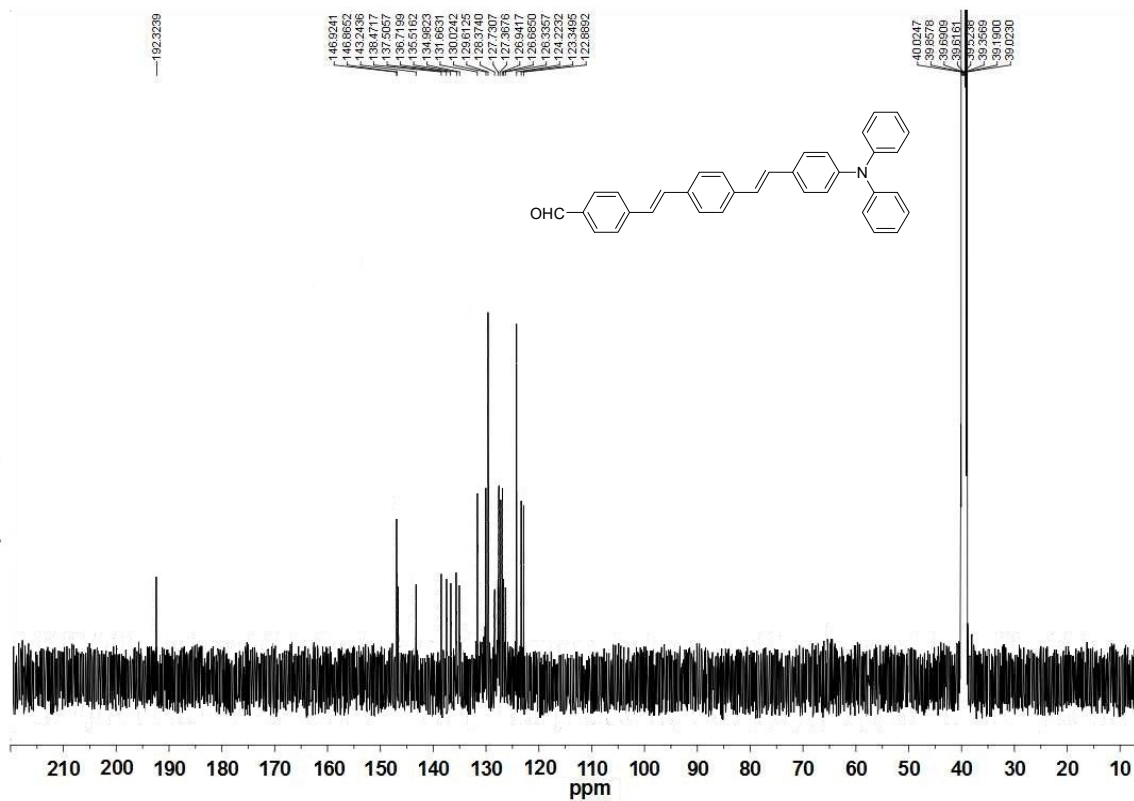


Figure S3 ¹³C NMR spectrum of BAQ.

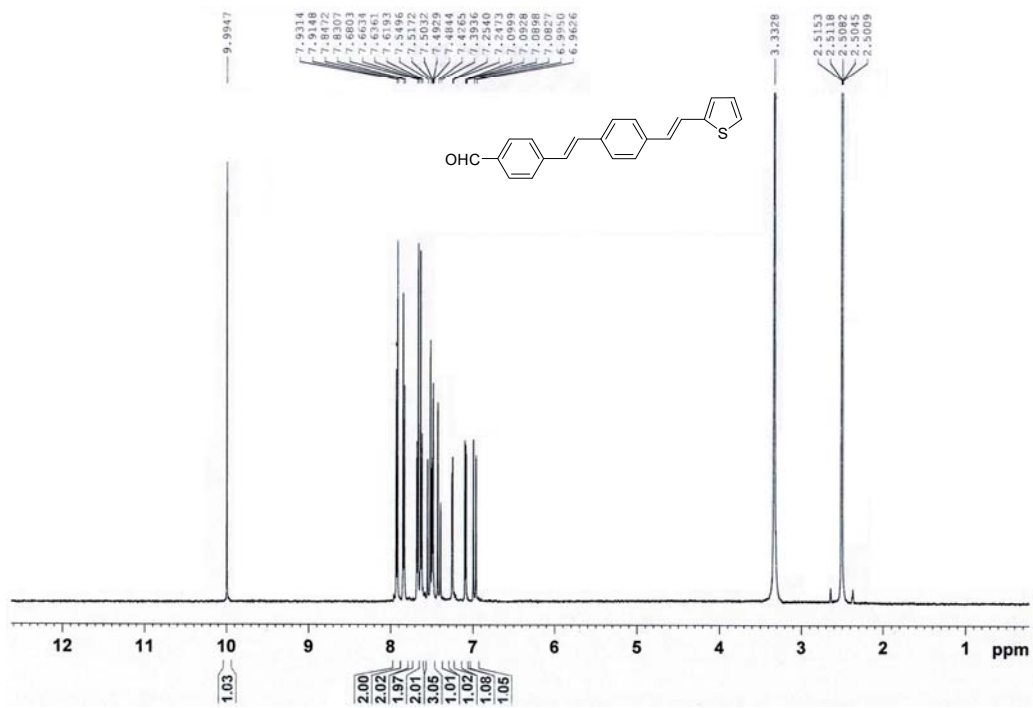


Figure S4 ¹H NMR spectrum of SFQ.

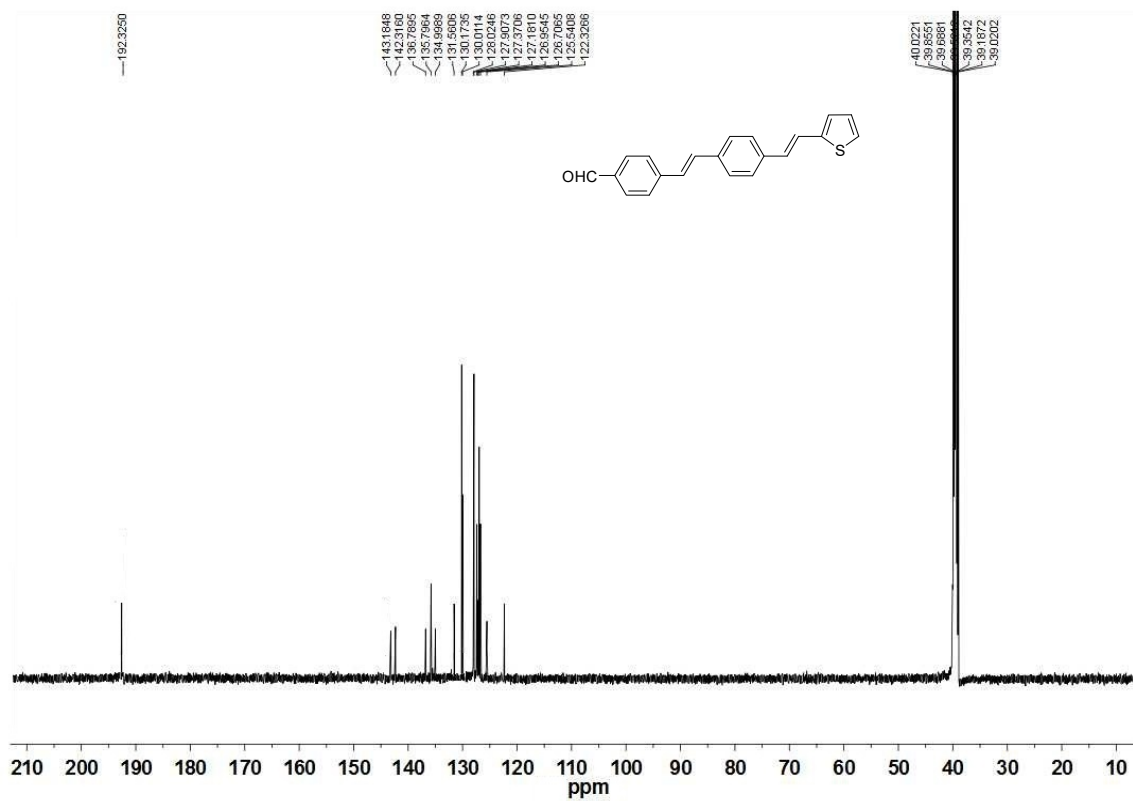


Figure S5 ^{13}C NMR spectrum of SFQ.

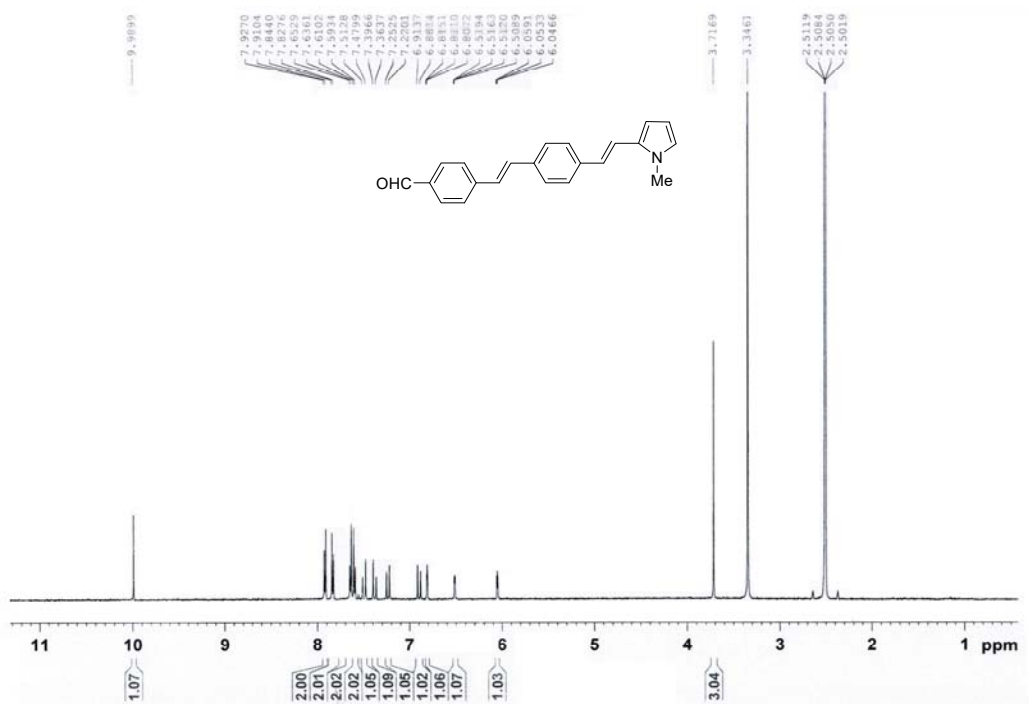


Figure S6 ^1H NMR spectrum of **BLQ**.

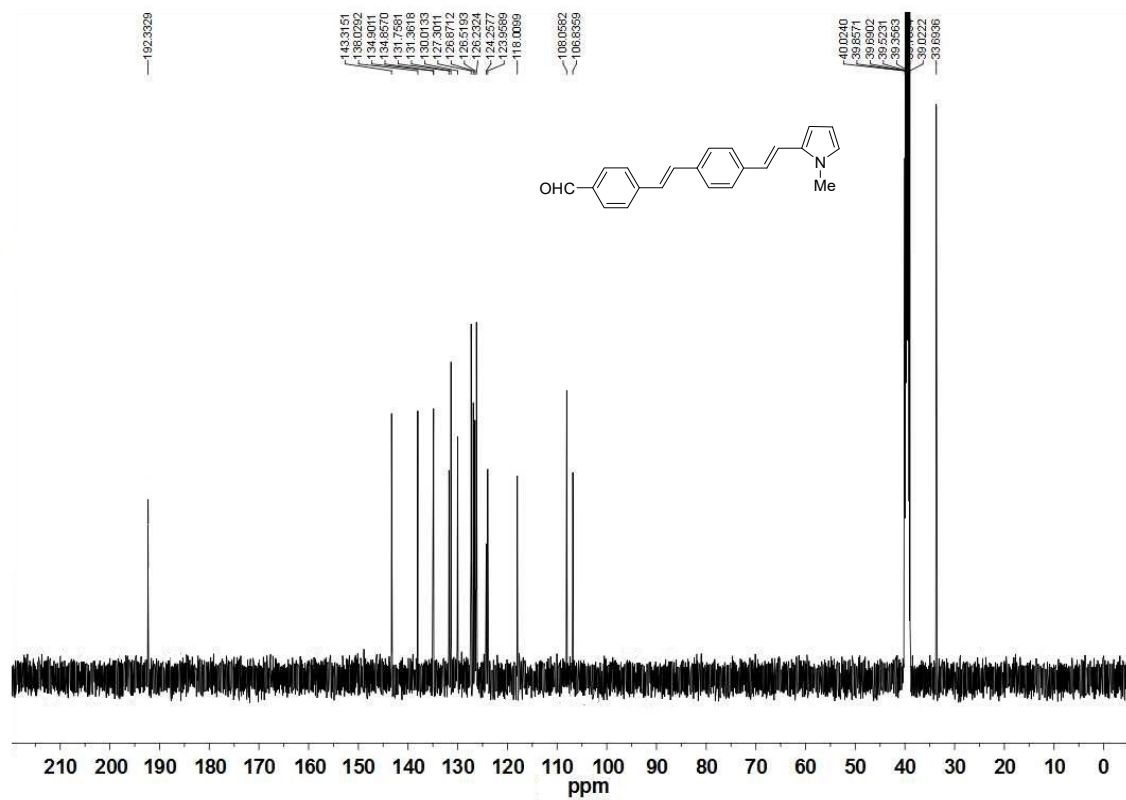


Figure S7 ^{13}C NMR spectrum of BLQ.

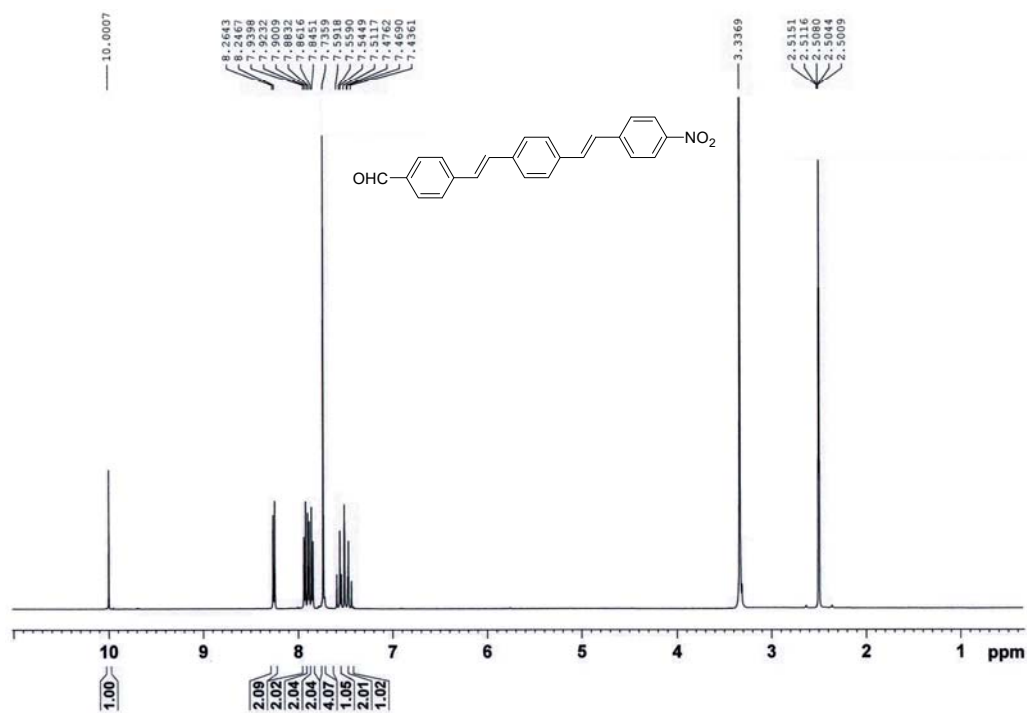


Figure S8 ¹H NMR spectrum of XJQ.

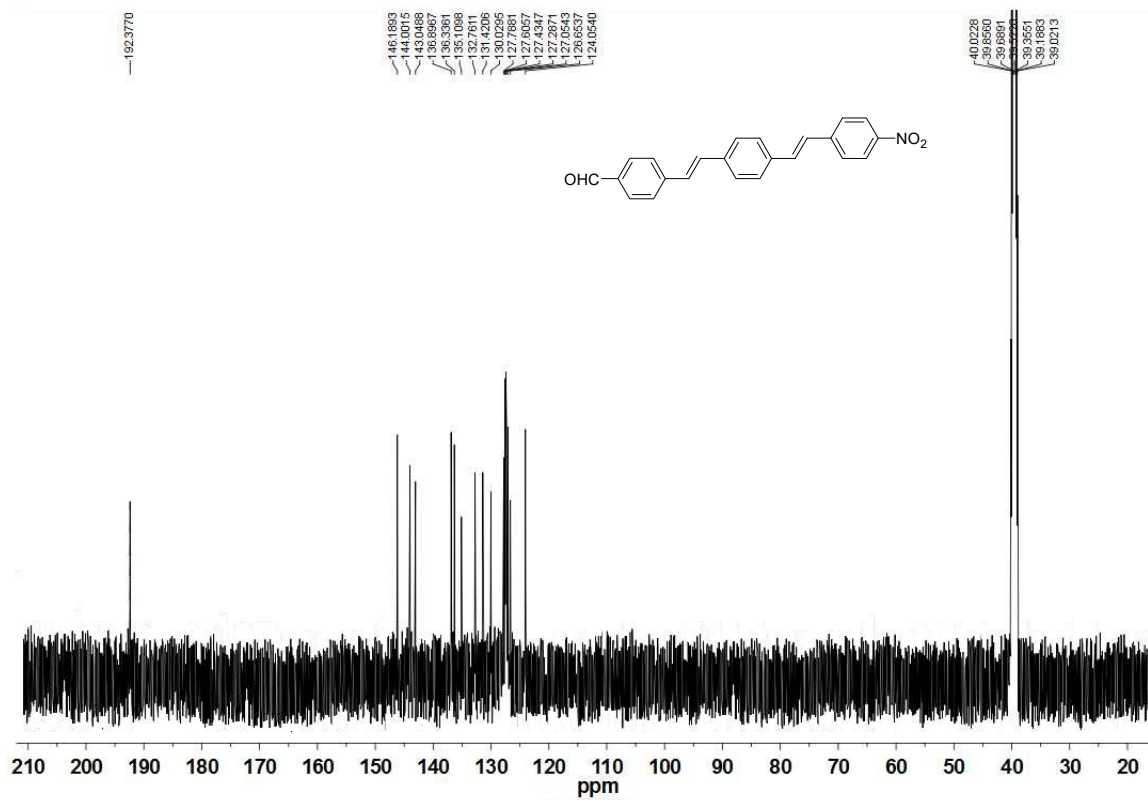


Figure S9 ^{13}C NMR spectrum of XJQ.