Supporting Information

Synthesis and properties of a new second-order NLO chromophore containing the benzo[b]furan moiety for electro-optical materials

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Contents

1. Figure S1. The frontier HOMO and LUMO orbitals of the A (left) and B (right) at the B3LYP/6-311G* level.

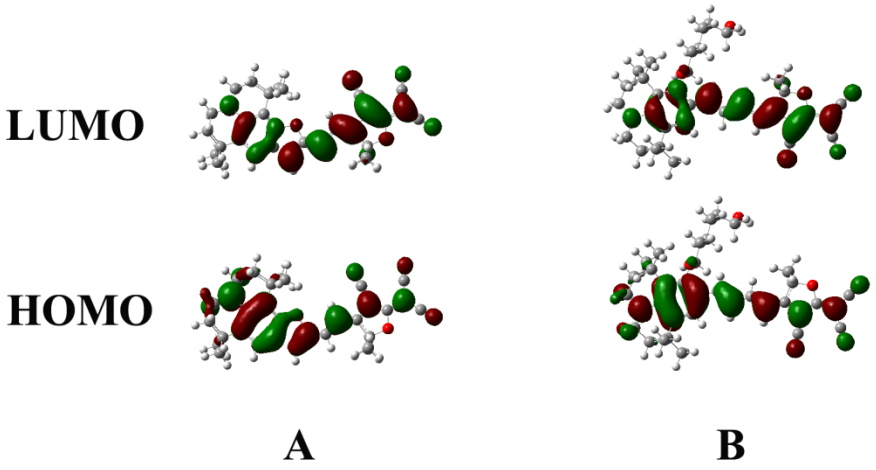
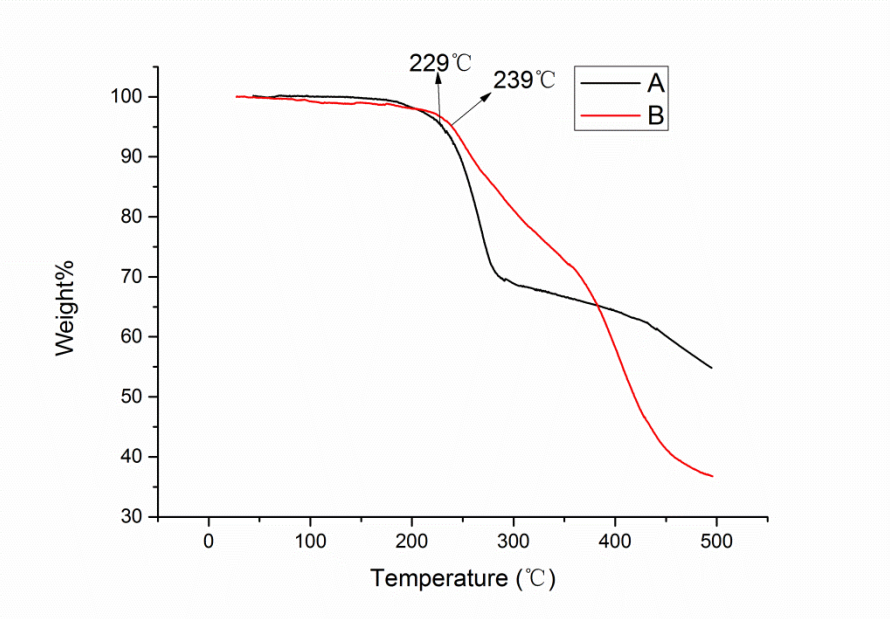


Table S1. TD-DFT Calculated properties of chromophores A and B.

	Excited state	Singlet-A	Excitation energies/eV	Maximum absorption/nm	Oscillator strengths
Chromophore A	Excited state 1		1.7959	690.39	0.3113
	127-128	0.66784			
	Excited state 2		2.7624	448.83	0.1513
	125-128	0.19078			
	126-128	0.65087			
	Excited state 3		3.2732	378.79	0.5964
	125-128	0.61038			
	126-128	-0.13912			
	127-129	0.13366			
Chromophore B	Excited state 1		2.3264	532.94	1.7208
	156-157	0.60283			
	Excited state 2		2.9845	415.43	0.1092
	153-157	-0.10531			
	155-157	0.63220			
	156-158	-0.19457			
	Excited state 3		3.3425	370.93	0.0056
	153-157	-0.14157			
	154-157	0.67331			

2. Figure S2. TGA curves of chromophores A and B.



3. Figures S3-S16. NMR spectra of resulted compounds.

Figure S3. ^{1}H NMR spectrum of compound 2

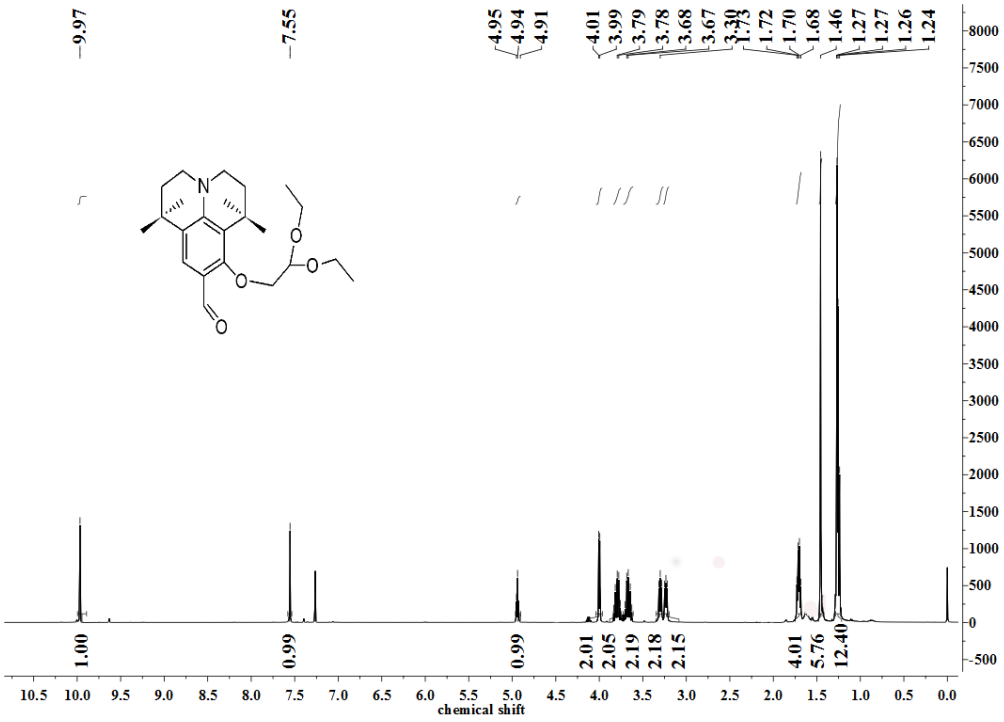


Figure S4. ^{13}C NMR spectrum of compound 2

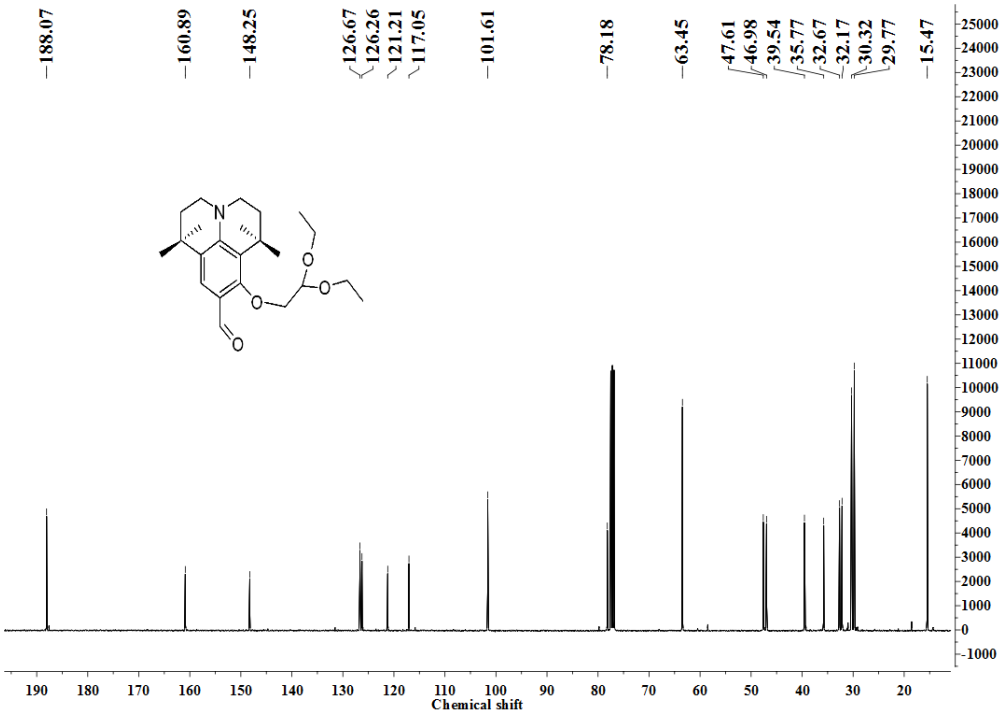


Figure S5. ^{1}H NMR spectrum of compound 3

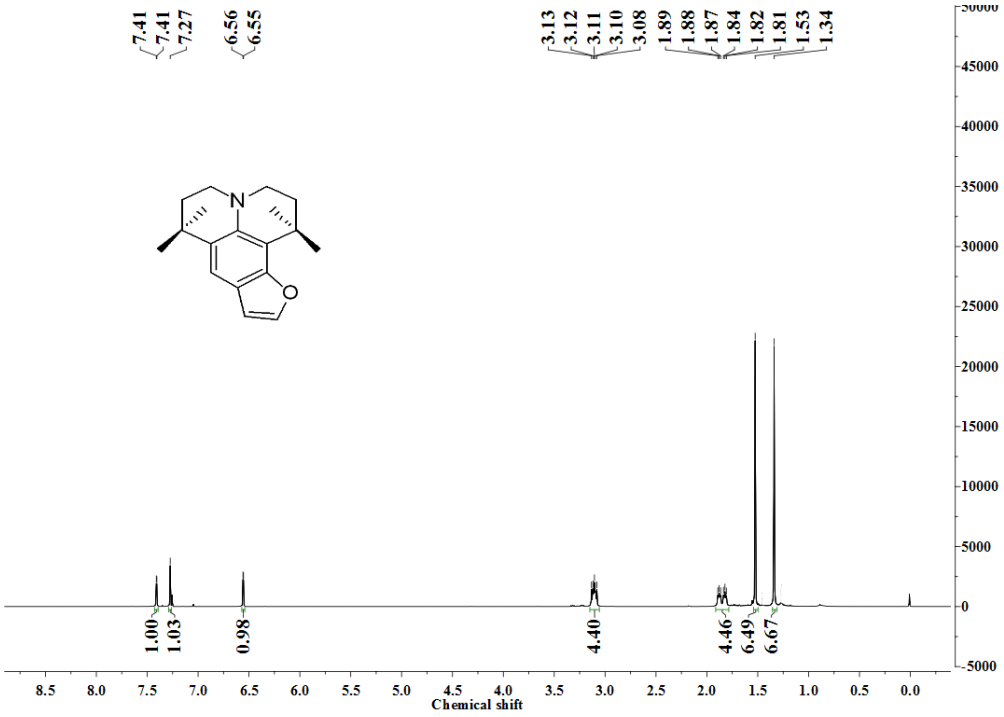


Figure S6. ^{13}C NMR spectrum of compound 3

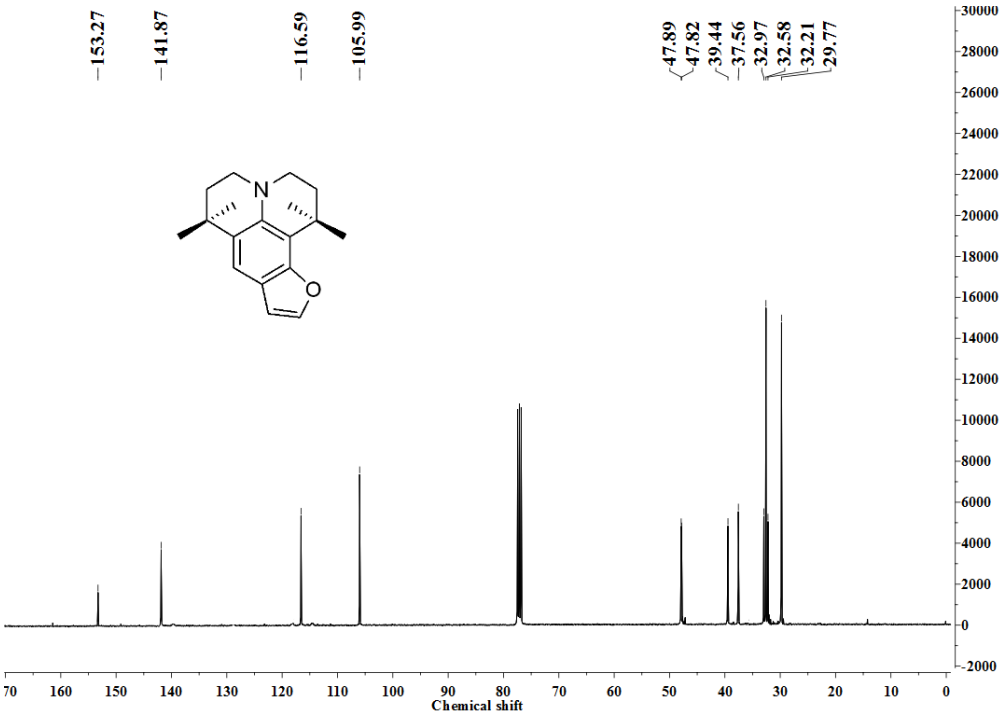


Figure S7. ^{1}H NMR spectrum of compound 4

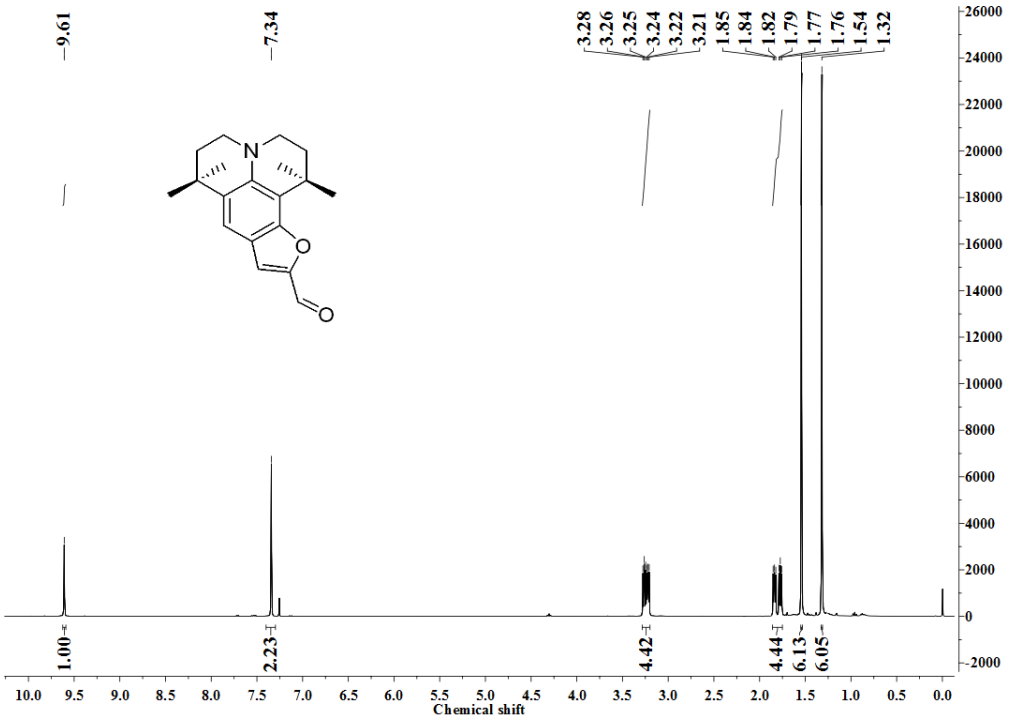


Figure S8. ^{13}C NMR spectrum of compound 4

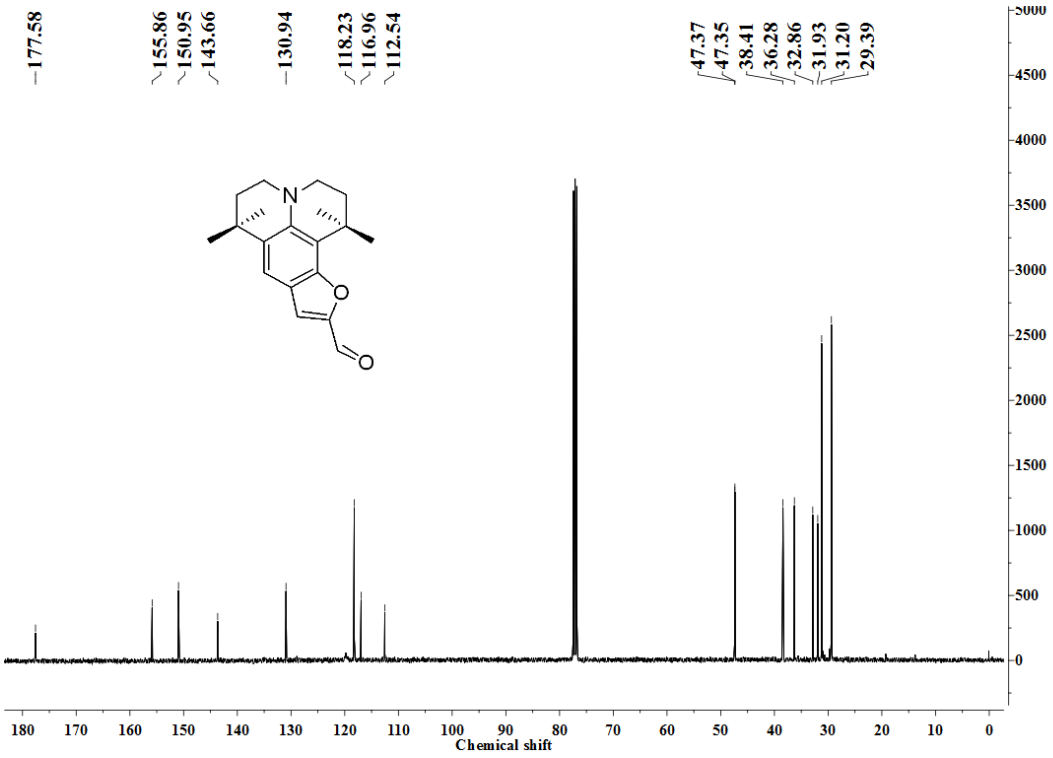


Figure S9. ^{1}H NMR spectrum of compound A

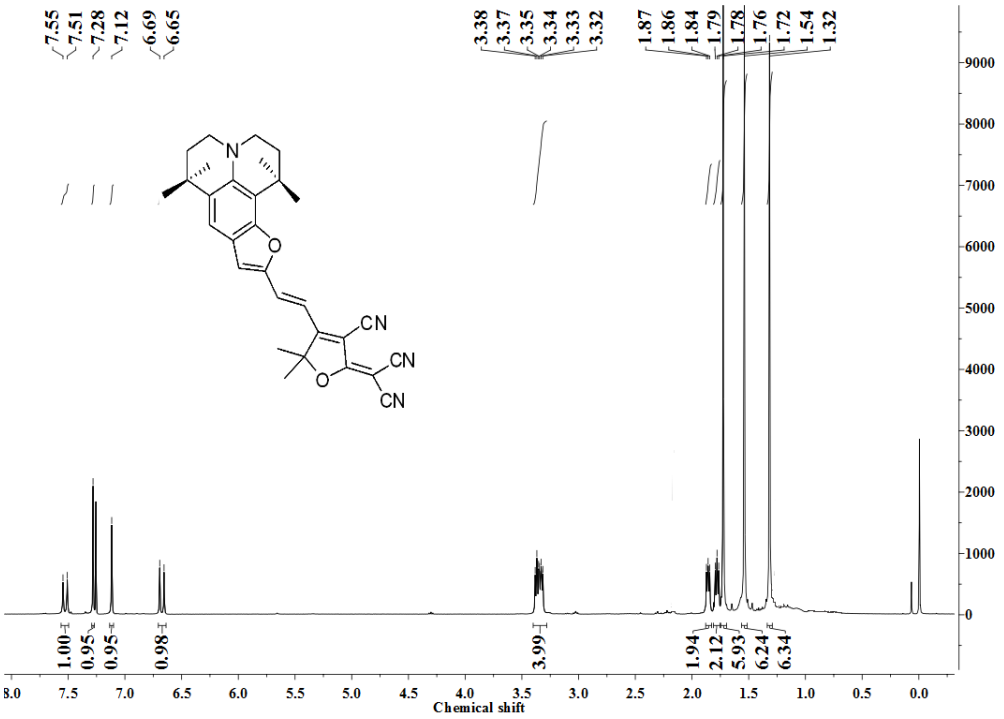


Figure S10. ^{13}C NMR spectrum of compound A

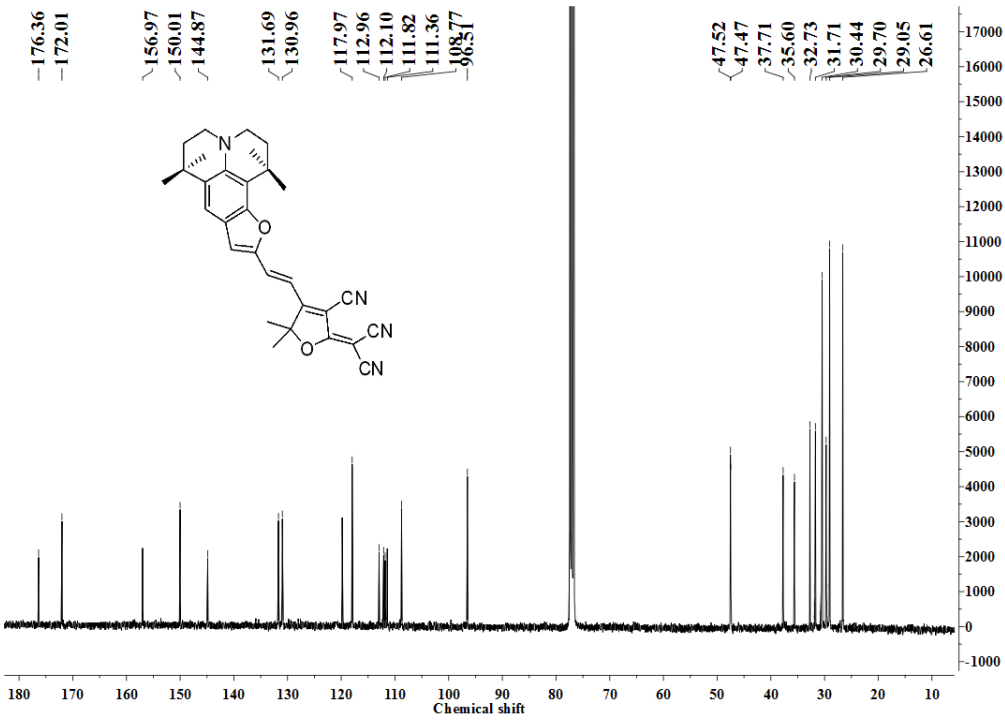


Figure S11. ^{1}H NMR spectrum of compound 5

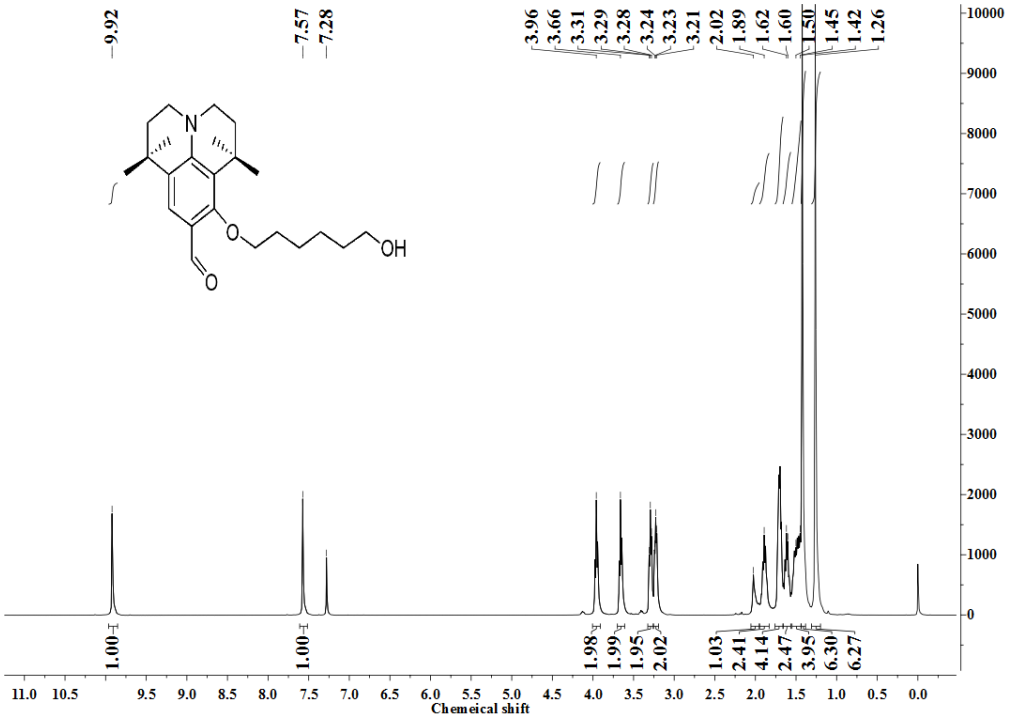


Figure S12. ^{13}C NMR spectrum of compound 5

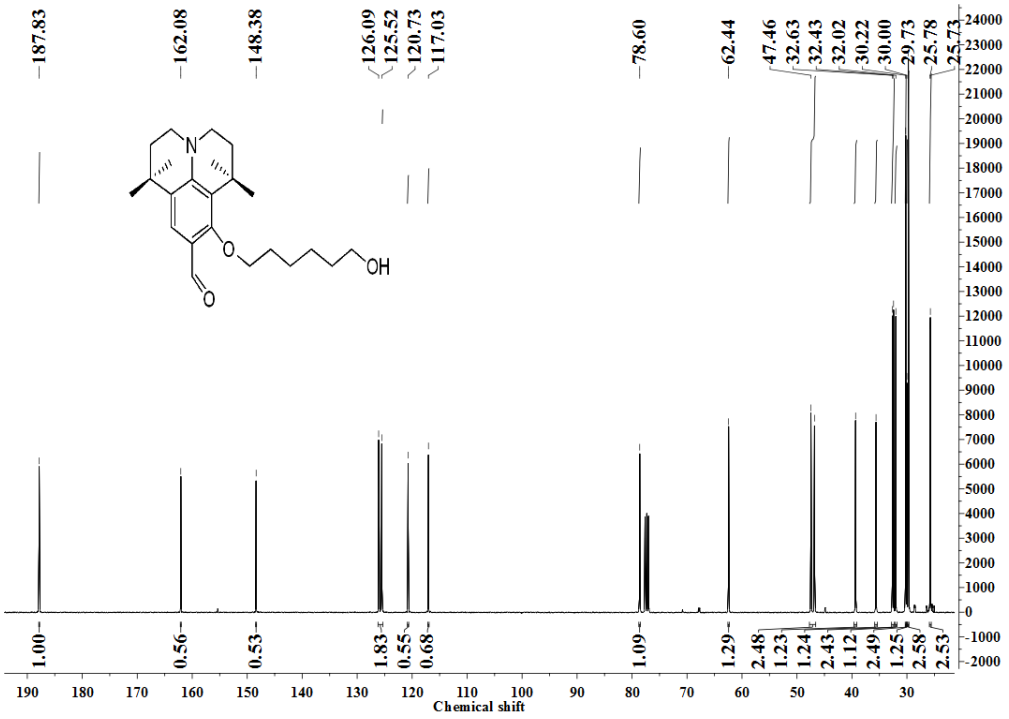


Figure S13. ^{1}H NMR spectrum of compound 6

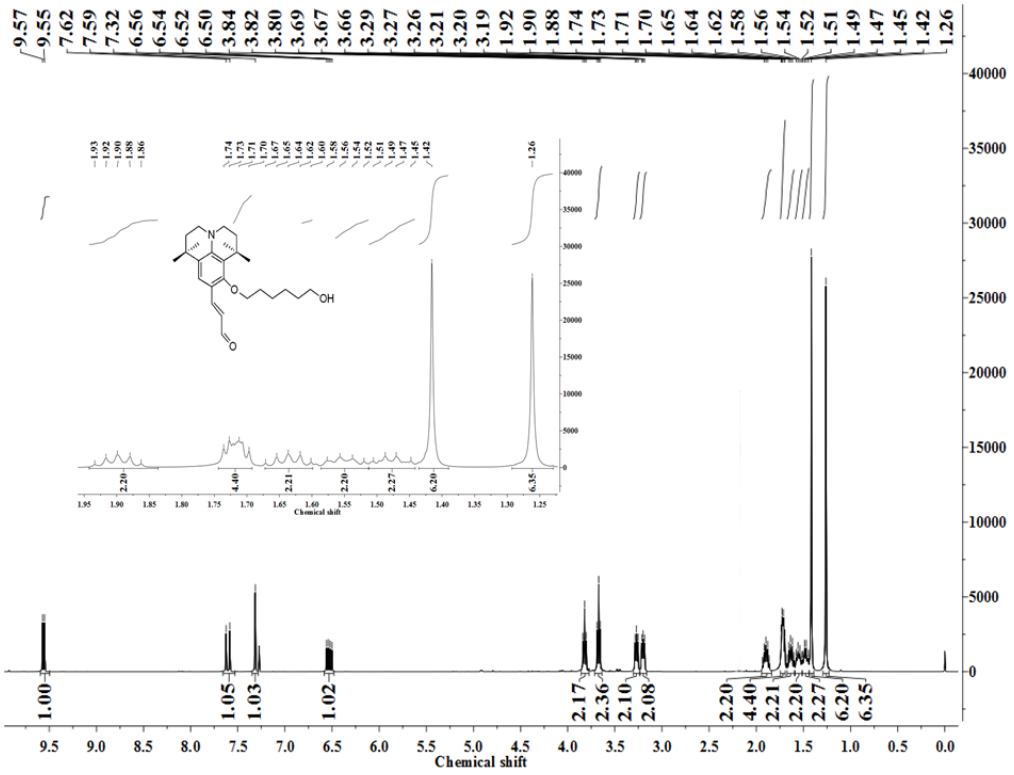


Figure S14. ^{13}C NMR spectrum of compound 6

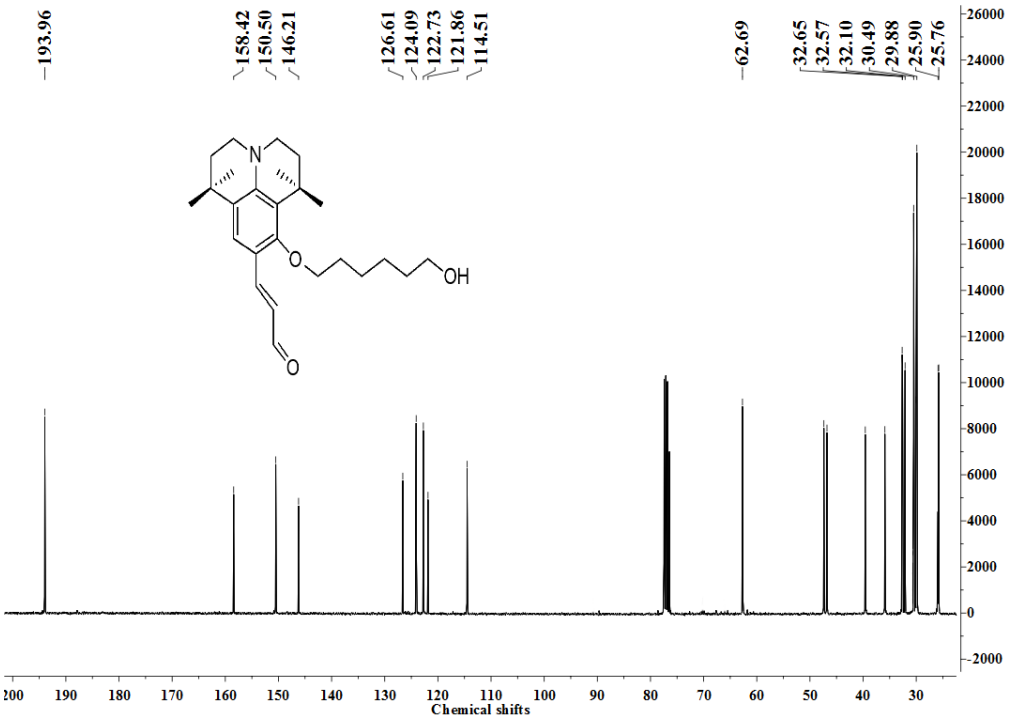


Figure S15. ^{1}H NMR spectrum of compound B

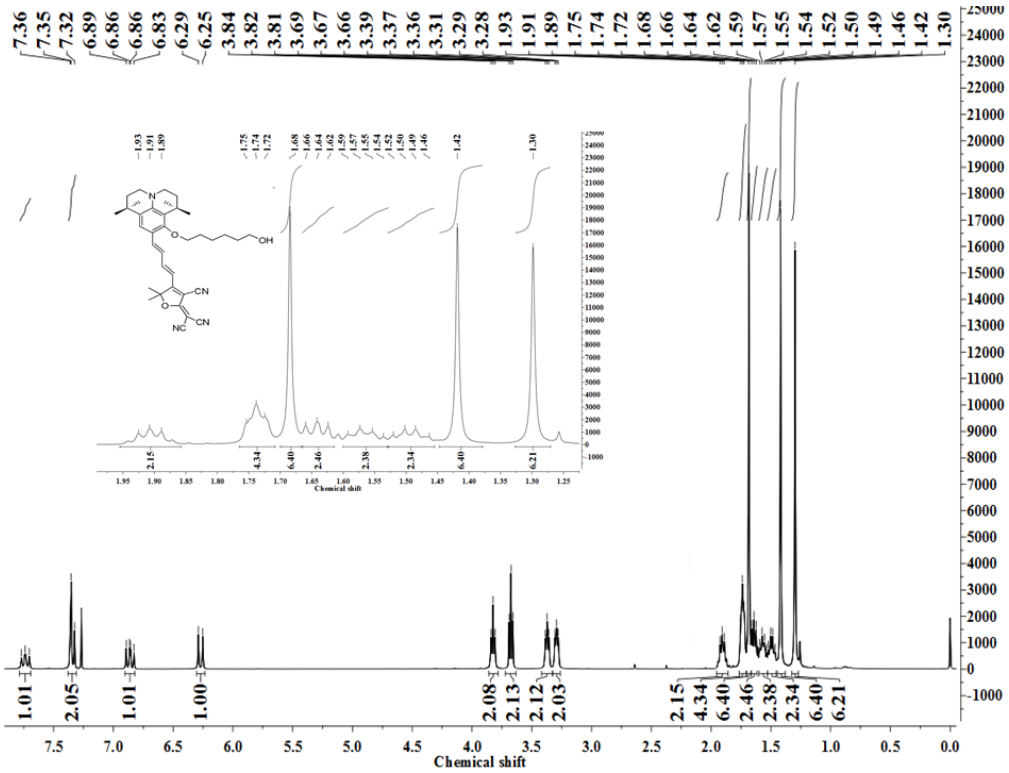


Figure S16. ^{13}C NMR spectrum of compound B