Supporting Information

Systematic study on optimization of bis(N,N-diethyl)aniline based NLO chromophore via stronger electron acceptor, extended π-conjugation and isolation groups

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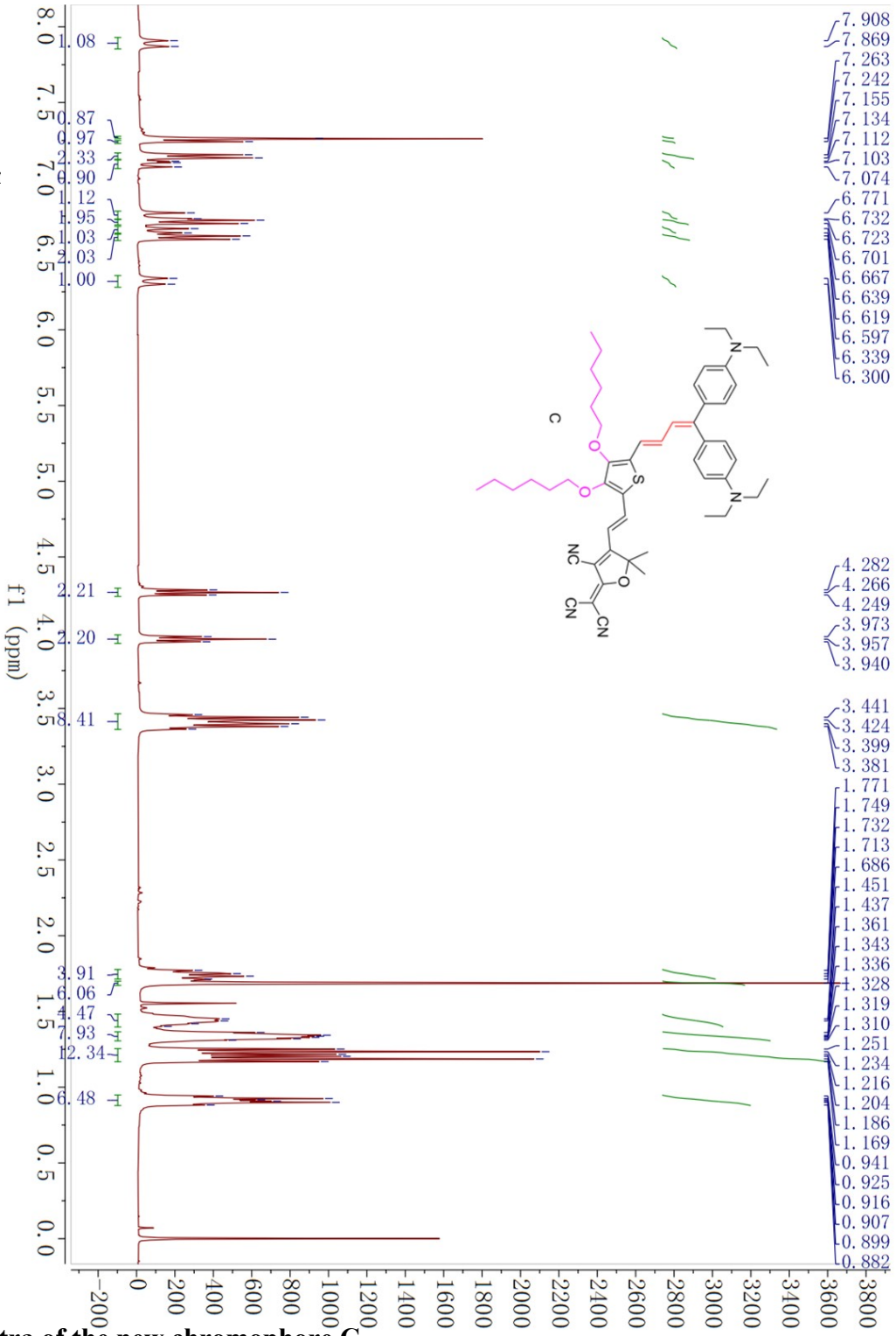
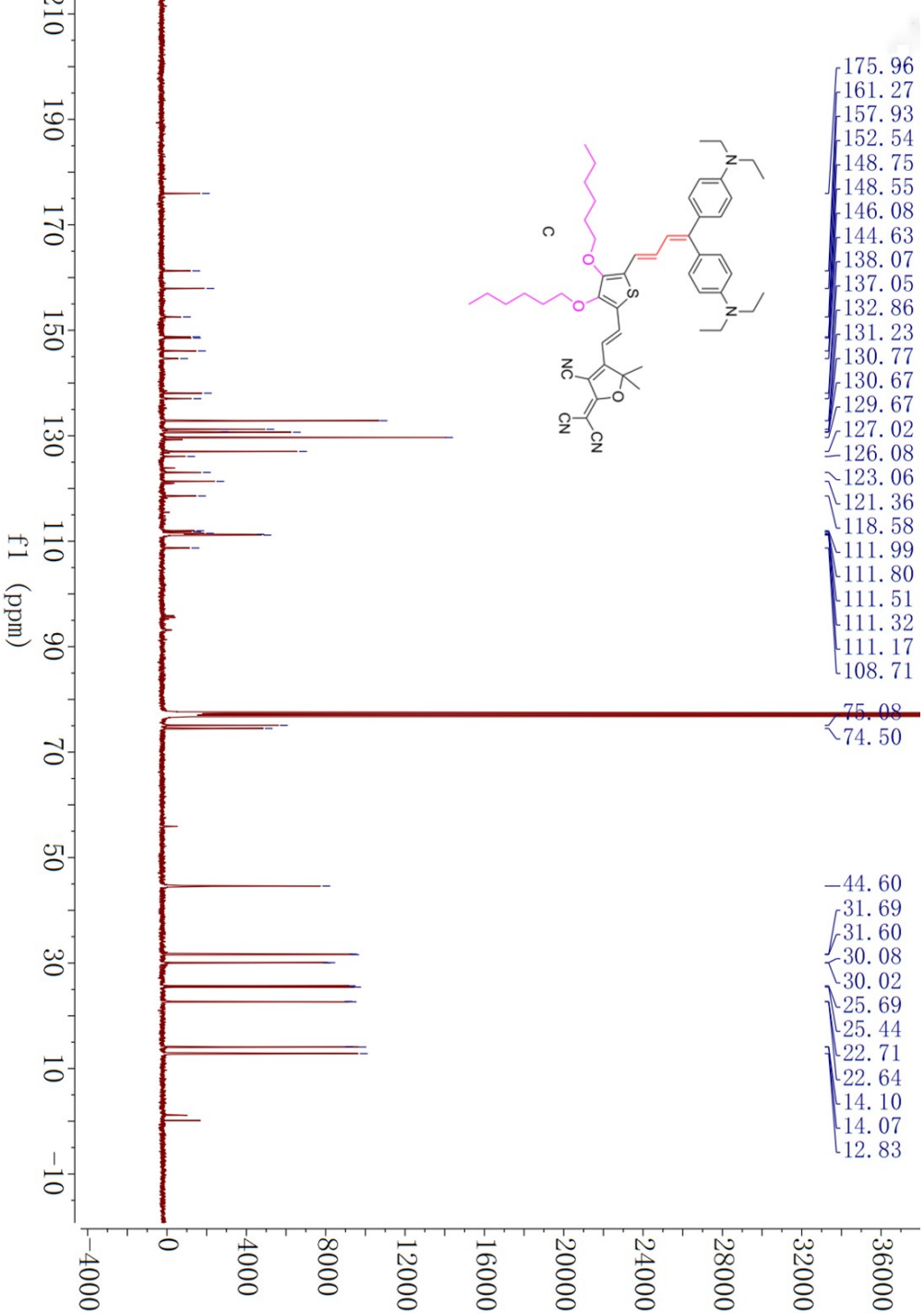
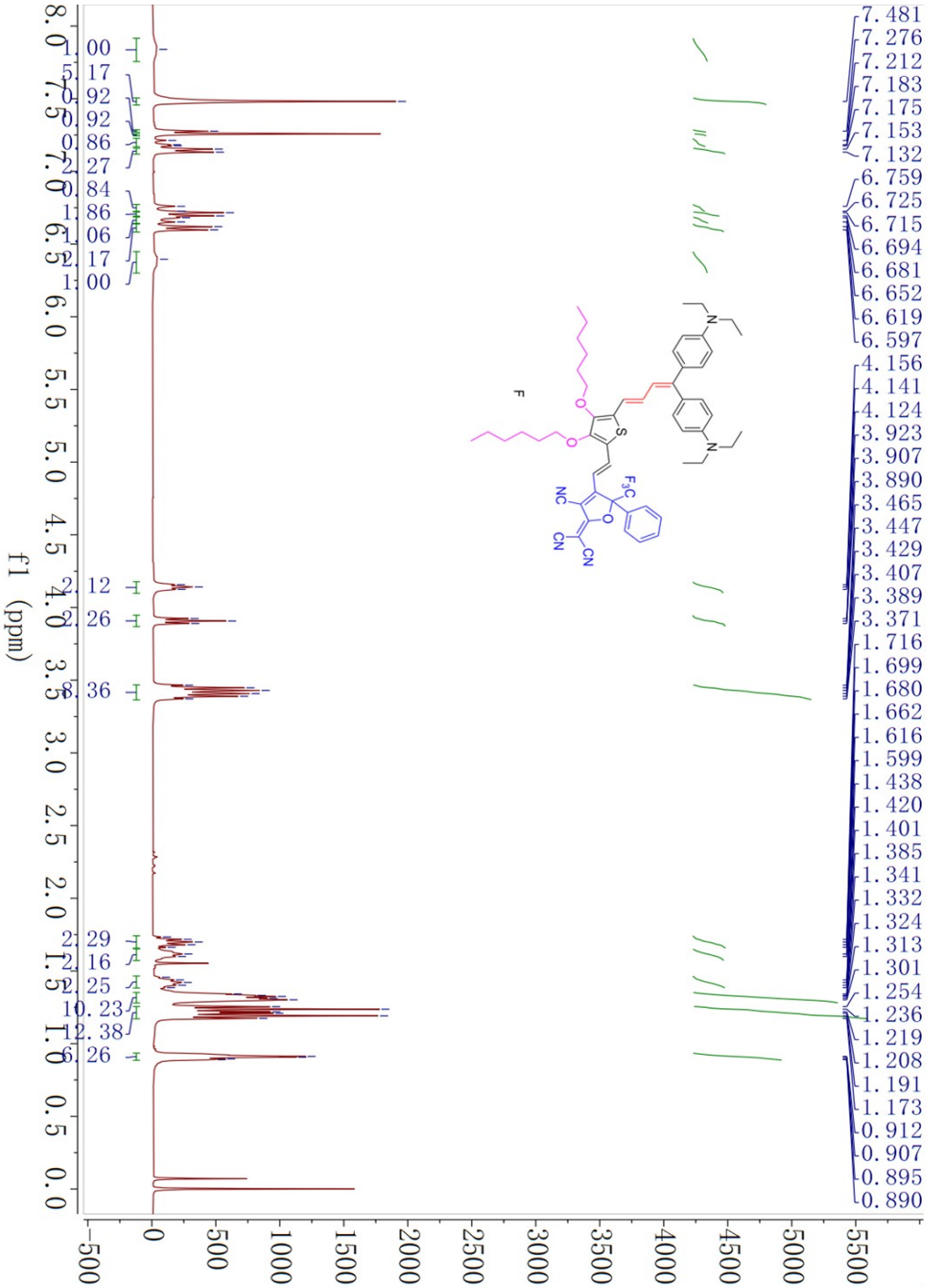
1. ^{1}H NMR spectra



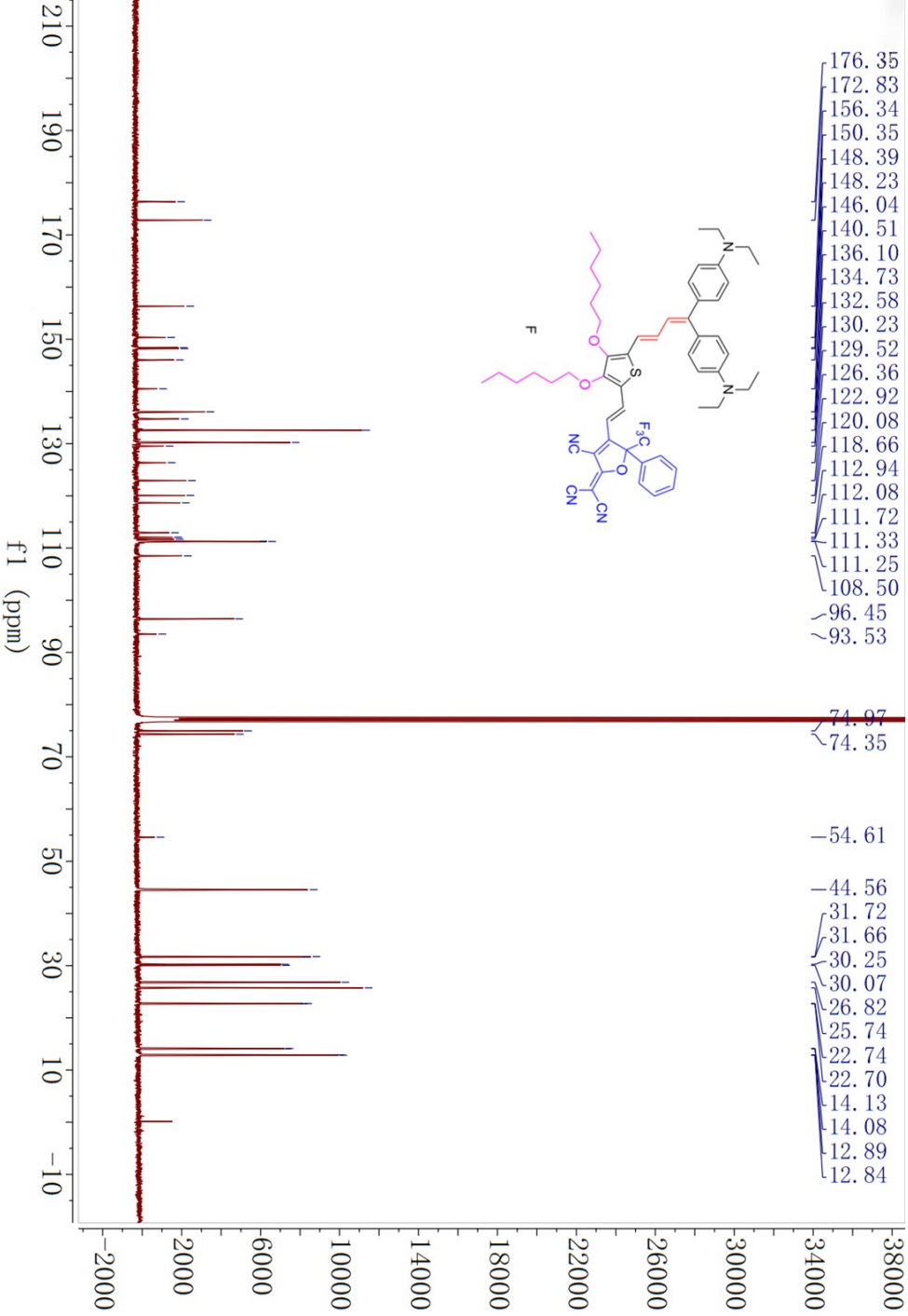
2. ^{13}C NMR spectra of the new chromophore C.



3. ^{1}H NMR spectra of the new chromophore F.



4. ^{13}C NMR spectra of the new chromophore F.



5. The solvatochromic shifts in eV and the extinction coefficients in UV-Vis spectra.

Table S1. The solvatochromic shifts in eV and values of the extinction coefficients.

Compound	Properties	dioxane	THF	$CHCl_3$	acetone	acetonitrile	DMF
A	ΔE/eV	1.89	1.85	1.74	1.85	1.86	1.82
	ε/$10^4$$M^{-1}$$cm^{-1}$	4.19	3.71	4.41	3.72	3.81	3.22
B	ΔE/eV	1.83	1.77	1.69	1.78	1.77	1.72
	ε/$10^4$$M^{-1}$$cm^{-1}$	5.48	5.05	6.09	5.47	5.15	4.42
C	ΔE/eV	1.77	1.72	1.61	1.73	1.73	1.69
	ε/$10^4$$M^{-1}$$cm^{-1}$	5.01	5.45	5.63	5.46	5.45	4.99
D	ΔE/eV	1.66	1.58	1.51	1.55	----	----

	$\varepsilon/10^4 M^{-1}cm^{-1}$	6.01	5.85	7.67	5.63	----	----
E	ΔE/eV	1.61	1.53	1.49	1.48	----	----
	$\varepsilon/10^4 M^{-1}cm^{-1}$	6.59	6.95	8.01	7.17	----	----
F	ΔE/eV	1.56	1.47	1.39	1.45	1.46	1.34
	$\varepsilon/10^4 M^{-1}cm^{-1}$	5.49	5.63	5.87	5.22	5.09	0.52

6. The data of β_i and β_{tot} for the chromophores.

Table S2. The data of β_i and β_{tot} for the chromophores.

Comp	β_{xxx}	β_{xyy}	β_{xzz}	β_{yyy}	β_{yzz}	β_{yxx}	β_{zzz}	β_{zxx}	β_{zyy}	β_x	β_y	β_z	β_{tot}
							$\times 10^{-30}$esu						
A	-36911.64	792.9	110.3	-1132	34.47	-690.0	-125.1	-523.1	19.28	311.1	15.44	5.434	311.5
B	28428.406	-410.7	9.907	44.042	8.270	1963.2	-90.54	742.5	-254.0	242.1	17.41	3.438	242.8
C	38351.344	4658	-130.6	-1104	-9.21	-12943	-119.6	-1121	-111.4	370.4	121.4	11.68	390.0
D	42411.556	-322.3	-68.09	-1490	12.25	3696.2	194.1	1570	-131.9	363.0	19.17	14.10	363.8
E	-41794.03	636.8	-57.78	551.99	12.41	-2428	178.9	-769.4	286.8	356.1	16.10	2.623	356.4
F	58006.952	4026	29.67	206.45	-21.3	-14432	-62.84	-3137	-352.5	536.2	123.1	25.51	551.0

7. The values of glass transition temperature of the chromophore doped APC.

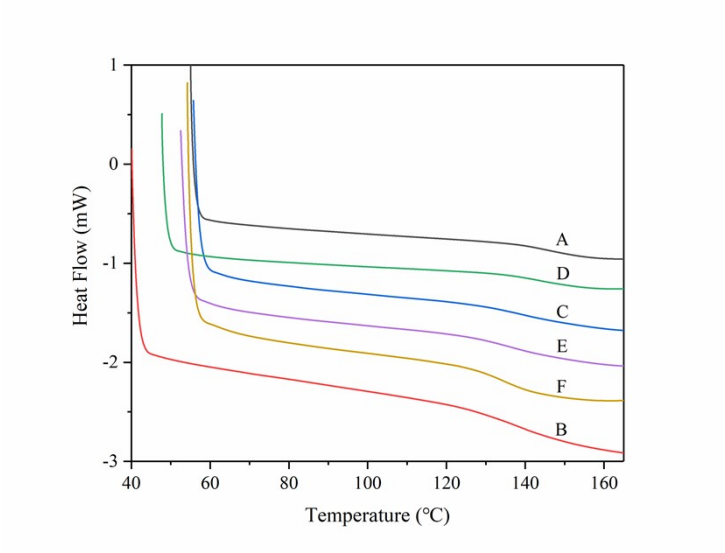


Figure S1. The DSC curves of the 25wt% chromophore doped APC

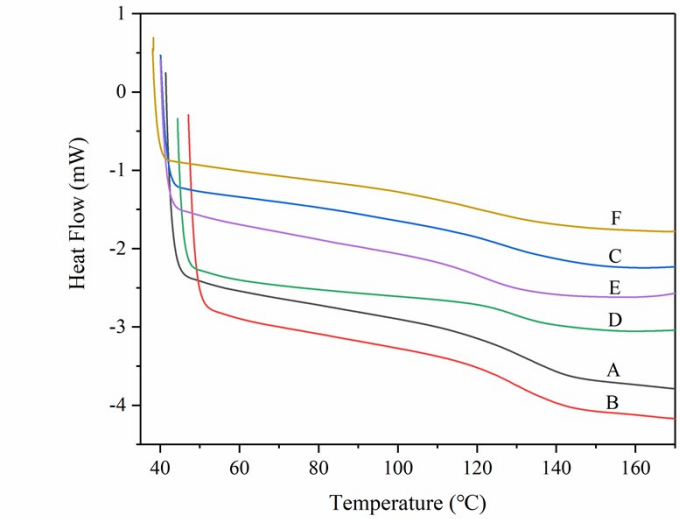


Figure S2. The DSC curves of the 35wt% chromophore doped APC

Table S3. The values of glass transition temperature (T_g) of the chromophore doped APC

Chromophore	A	B	C	D	E	F
T_g (25wt%)	145.9	139.5	138.8	143.3	136.9	134.3
T_g (35wt%)	134.3	128.6	127.3	129.2	121.9	118.5