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PAPER

High birefringence liquid crystals with wide temperature range and low melting point for augmented reality displays

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Electronic supplementary information

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1. Synthesis process

The final products ***n*TFV**, **4TV**, **4FTV** and **4FTFV** were synthesized by four-step reactions in turn, as shown in **Scheme 1.** Herein, as an example, synthesis procedure of **2TFV** is shown below.

1.1 Synthesis of 4-(4-(2-(*trans*-4-ethylcyclohexyl)ethyl)phenyl)-2-methylbut-3-yn-2-ol (**20T)**

Under nitrogen protection, 2-methyl-3-butyn-2-ol (0.56 g, 6.7 mmol), 4-(2-(*trans*-4-ethylcyclohexyl)ethyl)iodobenzene (2 g, 5.60 mmol), CuI (0.02 g, 0.11 mmol) and PPh_3 (0.07 g, 0.28 mmol), triethylamine (50 mL) were added to a three-necked flask. After stirring at 60 °C for 30 min, $Pd(PPh_3)_4$ (0.13 g, 0.11 mmol) was added into the mixture. Then, the solution was heated at 80 °C and stirred for 8 h. The mixture was then cooled and filtered, and DCM was added and the organic layer was washed with saturated ammonium chloride solution, dried over anhydrous $MgSO_4$ and the solvents were evaporated. The crude product was purified through recrystallization from PE to give a pale yellow solid, yield 65% with HPLC purity of 98%. ^{1}H NMR ($CDCl_3$, 300 MHz, TMS) δ (ppm): 7.31 (d, *J*= 8.1 Hz, 2H), 7.08 (d, *J*= 8.0 Hz, 2H), 2.63-2.51 (m, 2H), 1.80-1.70 (m, 4H), 1.60 (s, 6H), 1.50-1.43 (m, 2H), 1.27-1.11 (m, 4H), 0.93-0.81 (m, 7H). ^{13}C NMR ($CDCl_3$, 75 MHz, TMS) δ (ppm): 143.62, 131.59, 128.29, 119.87, 93.22, 82.31, 65.61, 39.61, 39.04, 37.47, 33.28, 32.82, 31.57, 30.02, 11.52. IR (KBr, pellet, cm^{-1}): 3315, 2983, 2920, 2857, 2231, 1914, 1615, 1520, 1457, 1378, 1283, 1164, 967, 822. EI-MS m/z (rel. int.): 298(M^+, 9), 283(100), 155(28), 115(11), 55(8).

1.2 Synthesis of 2-(4-((4-(2-(*trans*-4-ethylcyclohexyl)ethyl)phenyl)ethynyl)-3-fluorophenethyl)-1,3-dioxolane (**201T)**

Under nitrogen protection, a mixture of **20T** (1.91 g, 6.40 mmol), KOH (2.91 g, 52 mmol) and TBAB (0.19 g, 0.60 mmol) in 50 mL of PhMe/H_2O at a ratio of 4:1 (V/V) was stirred at 60 °C for 30 min. Then the aryl halide **1SQ** (1.60 g, 5.80 mmol) and $Pd(PPh_3)_4$ (0.23 g, 0.20 mmol) were added and the stirred mixture was heated at 80 °C for 8 h. After the mixture was cooled to room temperature, the solution was filtered over a pad of silica gel. Then the mixture was diluted with water and extracted with ethyl acetate for three times. The combined organic phase was dried over $MgSO_4$. After removal of the solvent in *vacuo*, the residue was first purified *via* column chromatography on silica gel using PE/EA (20/1) as eluent, then it was purified through recrystallization from PE/EA (5/1) to give a white crystal, yield 48% with HPLC purity of 99%. ^{1}H NMR ($CDCl_3$, 300 MHz, TMS) δ (ppm): 7.33 (dd, *J* = 17.7, 7.8 Hz, 3H), 7.05 (d, *J* = 7.9 Hz, 2H), 6.86 (d, *J* = 8.0 Hz, 2H), 4.86-4.71 (m, 1H), 3.99-3.62 (m, 4H), 2.78-2.42 (m, 4H), 1.99-1.80 (m, 2H), 1.77-1.53 (m, 4H), 1.48-1.29 (m, 2H), 1.21-0.95 (m, 4H), 0.89-0.67 (m, 7H). ^{13}C NMR ($CDCl_3$, 75 MHz, TMS) δ (ppm): 164.44, 160.52, 144.54, 143.96, 133.21, 131.60, 128.41, 124.06, 120.16, 115.56, 109.66, 103.50, 94.36, 82.18, 65.01, 39.61, 39.07, 37.49, 34.95, 33.36, 33.23, 32.83, 30.04, 29.86, 11.55. EI-MS *m/z* (rel. int.): 434(M^+, 26), 372(15), 309(18), 207(100), 100(73), 73(78). IR (KBr, pellet, cm^{-1}): 2955, 2912, 2848, 2205, 1907, 1605, 1515, 1438, 1217, 1130, 1038, 886, 812.

1.3 Synthesis of 3-(4-((4-(2-(*trans*-4-ethylcyclohexyl)ethyl)phenyl)ethynyl)-3-fluorophenyl)propanal (**201TQ)**

Under nitrogen protection, the coupled products **201T** (0.86 g, 2 mmol) , formic acid (18.4 g, 0.40 mol) and THF (50 mL) were mixed and stirred at 55 °C for 5 h. After cooling the mixture to room temperature, the mixture was diluted with water and extracted three times with ethyl acetate. The combined organic layers were dried over $MgSO_4$. After removal of the solvent in *vacuo*, the residue was purified through recrystallization from EA to give a pale yellow solid, yield 80% with HPLC purity of 98%. ^{1}H NMR ($CDCl_3$, 400 MHz, TMS) δ (ppm): 9.81 (s, 1H), 7.45-7.39 (m, 3H), 7.17-7.14 (m, 2H), 6.96-6.92 (m, 2H), 2.96-2.93 (t, *J* = 7.8 Hz, 2H), 2.81-2.77 (t, *J* = 7.8 Hz, 2H), 2.64-2.59 (m, 2H), 1.80-1.72 (m, 4H), 1.50-1.47 (m, 2H), 1.20-1.17 (m, 4H), 0.90-0.84 (m, 7H). ^{13}C NMR ($CDCl_3$, 100 MHz, TMS) δ (ppm): 200.83, 163.86, 144.18, 143.16, 133.49, 131.68, 128.52, 128.50, 124.09, 120.04, 115.60, 115.39, 110.18, 94.48, 91.98, 44.81, 39.66, 39.16, 37.52, 33.44, 33.28, 32.88, 32.88, 30.11, 30.11, 27.81, 11.66. EI-MS *m/z* (rel. int.): 390 (M^+, 50), 265 (100), 244 (30), 222 (54), 111 (6). IR (KBr, pellet, cm^{-1}): 3088, 2915, 2848, 2725, 2238, 1725, 1448, 1120, 829.

1.4 Synthesis of 4-(3-butylene)-1-((4-(2-(*trans*-4-ethylcyclohexyl)ethyl)phenyl)ethynyl)-2-fluorobenzene (**2TFV)**

Under nitrogen protection, a mixture of methyltriphenylphosphonium bromide (0.50 g, 1.40 mmol) and *t*-BuOK (0.17 g, 1.50 mmol) in THF (50 mL) was cooled to -15 °C and stirred for 30 min. To the mixture, **201TQ** (0.50 g, 1.20 mmol) in THF (5 mL) was added. The resulting solution was stirred for 2 h and allowed to warm to room temperature naturally. The mixture was diluted with water and extracted three times with PE. The combined organic layers were dried over $MgSO_4$. After removal of the solvent *in vacuo*, the residue was first purified *via* column chromatography on silica gel using PE as eluent, then it was purified through recrystallization from ethanol to give purity above 99% for HPLC measurement. (Yield: 58%). ^{1}H NMR ($CDCl_3$, 400 MHz, TMS) δ (ppm): 7.47-7.44 (m, 3H), 7.19-7.14 (m, 4H), 5.86-5.58 (m, 1H), 5.05-4.97 (m, 2H), 2.72-2.68 (t, *J* = 7.60 Hz, 2H), 2.64-2.59 (t, *J* = 7.60 Hz, 2H), 2.38-2.35 (m, 2H), 1.95-1.73 (m, 4H), 1.63-1.47 (m, 2H), 1.24-1.15 (m, 4H), 0.96-0.82 (m, 7H). ^{13}C NMR ($CDCl_3$, 100 MHz, TMS) δ (ppm): 163.82, 161.33, 144.70, 144.06, 137.41, 133.17, 131.67, 128.50, 124.24, 124.21, 120.18, 115.61, 115.43, 109.54, 94.18, 82.25, 39.66, 39.18, 37.52, 35.18, 35.04, 33.44, 33.88, 32.88, 32.28, 32.28, 30.12, 11.67. EI-MS *m/z* (rel. int.): 388 (M^+, 45), 347 (100), 263 (25), 222 (97), 111 (14), 55 (58). IR (KBr, pellet, cm^{-1}): 3088, 2915, 2848, 2238, 1635, 1516, 1448, 1120, 943, 829.

The other target compounds were prepared by using above similar procedures, their structure data are listed below.

3TFV: ^{1}H NMR ($CDCl_3$, 400 MHz, TMS) δ (ppm): 7.51-7.39 (m, 3H), 7.17-7.11 (m, 2H), 6.95-6.92 (m, 2H), 5.86-5.78 (m, 1H), 5.05-4.99 (m, 2H), 2.75-2.69 (t, *J* = 7.60 Hz, 2H), 2.65-2.61 (t, *J* = 7.40 Hz, 2H), 2.40-2.33 (m, 2H), 1.80-1.73 (m, 4H), 1.51-1.47 (m, 2H), 1.35-1.27 (m, 2H), 1.21-1.12 (m, 4H), 0.95-0.82 (m, 7H). ^{13}C NMR ($CDCl_3$, 100 MHz, TMS) δ (ppm): 163.85, 161.35, 144.70, 144.04, 137.40, 133.17, 131.68, 128.49, 124.23, 124.20, 120.24, 115.64, 115.61, 109.61, 94.19, 82.29, 39.89, 39.19, 37.63, 37.56, 35.19, 35.02, 33.45, 33.32, 33.32, 33.30,

33.30, 20.16, 14.55. EI-MS m/z (rel. int.): 402 (M^+, 35), 361 (100), 263 (27), 222 (92), 111 (8), 55 (41). IR (KBr, pellet, cm^{-1}): 3087, 2913, 2849, 2235, 1638, 1516, 1448, 1121, 949, 829.

4TFV: ^{1}H NMR ($CDCl_3$, 400 MHz, TMS) δ (ppm): 7.46-7.38 (m, 3H), 7.20-7.12 (m, 2H), 6.98-6.91 (m, 2H), 5.87-5.77 (m, 1H), 5.06-4.98 (m, 2H), 2.73-2.69 (t, *J* = 7.60 Hz, 2H), 2.64-2.60 (t, *J* = 7.40 Hz, 2H), 2.39-2.34 (m, 2H), 1.76-1.72 (m, 4H), 1.54-1.46 (m, 2H), 1.27-1.16 (m, 8H), 0.97-0.81 (m, 7H). ^{13}C NMR ($CDCl_3$, 100 MHz, TMS) δ (ppm): 163.84, 161.34, 144.76, 144.03, 137.40, 133.17, 131.67, 128.49, 124.19, 120.21, 115.63, 115.60, 115.42, 109.59, 94.16, 82.27, 39.18, 37.89, 37.55, 37.27, 35.20, 35.18, 35.02, 33.44, 33.34, 33.33, 33.33, 29.36, 23.15, 14.28. EI-MS m/z (rel. int.): 416 (M^+, 40), 375 (100), 263 (15), 222 (25), 55 (3). IR (KBr, pellet, cm^{-1}): 3090, 2923, 2839, 2225, 1635, 1513, 1418, 1111, 949, 810.

5TFV: ^{1}H NMR ($CDCl_3$, 400 MHz, TMS) δ (ppm): 7.49-7.39 (m, 3H), 7.19-7.14 (m, 2H), 6.94-6.90 (m, 2H), 5.85-5.78 (m, 1H), 5.05-4.97 (m, 2H), 2.72-2.68 (t, *J* = 7.60 Hz, 2H), 2.68-2.59 (t, *J* = 7.40 Hz, 2H), 2.39-2.33 (m, 2H), 1.78-1.71 (m, 4H), 1.51-1.45 (m, 2H), 1.28-1.14 (m, 10H), 0.96-0.85 (m, 7H). ^{13}C NMR ($CDCl_3$, 100 MHz, TMS) δ (ppm): 163.82, 161.32, 144.76, 144.05, 137.40, 133.45, 131.69, 128.53, 124.22, 120.18, 115.63, 115.60, 115.42, 109.55, 94.10, 82.24, 39.17, 37.89, 37.52, 35.18, 35.17, 35.03, 33.43,33.43, 33.43, 33.34, 33.33, 33.33, 33.32, 26.76, 22.82, 14.24. EI-MS m/z (rel. int.): 430 (M^+, 40), 391 (100), 263 (15), 222 (25), 55 (3). IR (KBr, pellet, cm^{-1}): 3080, 2933, 2839, 2235, 1645, 1503, 1408, 1101, 940, 815.

4FTV: ^{1}H NMR ($CDCl_3$, 400 MHz, TMS) δ (ppm): 7.48-7.37 (m, 3H), 7.21-7.16 (m, 2H), 6.93-6.90 (m, 2H), 5.87-5.81 (m, 1H), 5.06-4.94 (m, 2H), 2.74-2.60 (t, *J* = 7.60 Hz, 2H), 2.63-2.59 (t, *J* = 7.40 Hz, 2H), 2.40-2.34 (m, 2H), 1.79-1.73 (m, 4H), 1.52-1.46 (m, 2H), 1.27-1.16 (m, 8H), 0.97-0.84 (m, 7H). ^{13}C NMR ($CDCl_3$, 100 MHz, TMS) δ (ppm): 163.89, 161.39, 146.28, 142.52, 137.82, 133.12, 131.69, 128.59, 124.13, 124.10, 120.63, 115.49, 115.30, 109.17, 93.79, 82.54, 38.84, 37.87, 37.49, 37.25, 35.41, 35.41, 35.36, 33.29, 33.29, 33.29, 33.29, 29.36, 23.15, 14.29. EI-MS m/z (rel. int.): 416 (M^+, 28), 375 (100), 263 (5), 222 (20), 55 (3). IR (KBr, pellet, cm^{-1}): 3079, 2919, 2829, 2245, 1645, 1570, 1410, 1110, 949, 829.

4FTFV: ^{1}H NMR ($CDCl_3$, 400 MHz, TMS) δ (ppm): 7.44-7.39 (m, 7H), 6.95-6.90 (m, 4H), 5.86-5.76 (m, 1H), 5.06-4.98 (m, 2H), 2.73-2.69 (t, *J* = 7.60 Hz, 2H), 2.64-2.60 (t, *J* = 7.40 Hz, 2H), 2.39-2.35 (m, 2H), 1.78-1.72 (m, 4H), 1.49-1.47 (m, 2H), 1.28-1.15 (m, 8H), 0.94-0.87 (m, 7H). ^{13}C NMR ($CDCl_3$, 100 MHz, TMS) δ (ppm): 163.84, 161.39, 146.79, 145.20, 137.35, 133.26, 133.17, 124.29, 124.13, 115.66, 115.51, 115.30, 109.25, 108.66, 87.50, 87.46, 38.81, 37.86, 37.48, 37.25, 35.21, 35.20, 35.00, 33.70, 33.29, 33.28, 32.93, 29.35, 23.14, 14.28. EI-MS m/z (rel. int.): 434 (M^+, 55), 393 (100), 280 (10), 242 (15), 55 (3). IR (KBr, pellet, cm^{-1}): 3089, 2929, 2826, 2226, 1635, 1570, 1410, 1110, 949, 829.

4TV: ^{1}H NMR ($CDCl_3$, 400 MHz, TMS) δ (ppm): 7.49-7.44 (m, 4H), 7.19-7.15 (m, 4H), 5.91-5.85 (m, 1H), 5.10-4.99 (m, 2H), 2.74-2.70 (t, *J* = 7.60 Hz, 2H), 2.64-2.60 (t, *J* = 7.60 Hz, 2H), 2.38-2.36 (m, 2H), 1.80-1.75 (m, 4H), 1.5-1.48 (m, 2H), 1.29-1.15 (m, 8H), 0.91-0.83 (m, 7H). ^{13}C NMR ($CDCl_3$, 100 MHz, TMS) δ (ppm): 143.68, 142.16, 137.87, 131.60, 131.60, 131.57, 131.57, 128.58, 128.58, 128.48, 128.48, 120.98, 120.56, 115.28, 89.91, 88.18, 39.20, 39.20, 37.90, 37.55, 37.28, 35.39, 35.38, 33.37, 33.37, 33.35, 33.35, 29.37, 23.15, 14.30. EI-MS m/z

(rel. int.): 398 (M^+, 25), 357 (100), 245 (5), 204 (30). IR (KBr, pellet, cm^{-1}): 3089, 2914, 2849, 2228, 1630, 1516, 1448, 911, 829.

2. Characterization spectra of target compounds

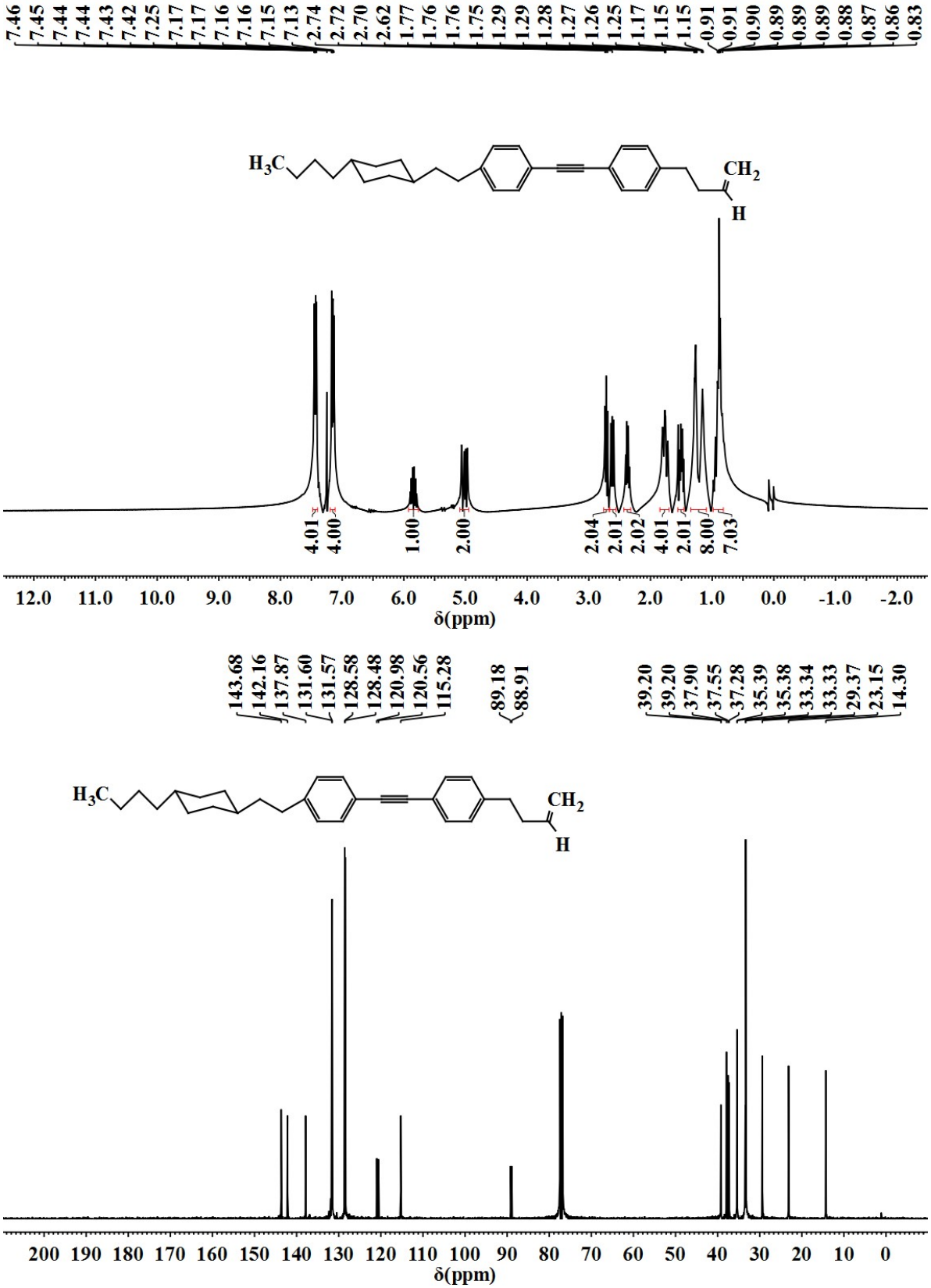


Fig. S1 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **4TV** recorded in $CDCl_3$.

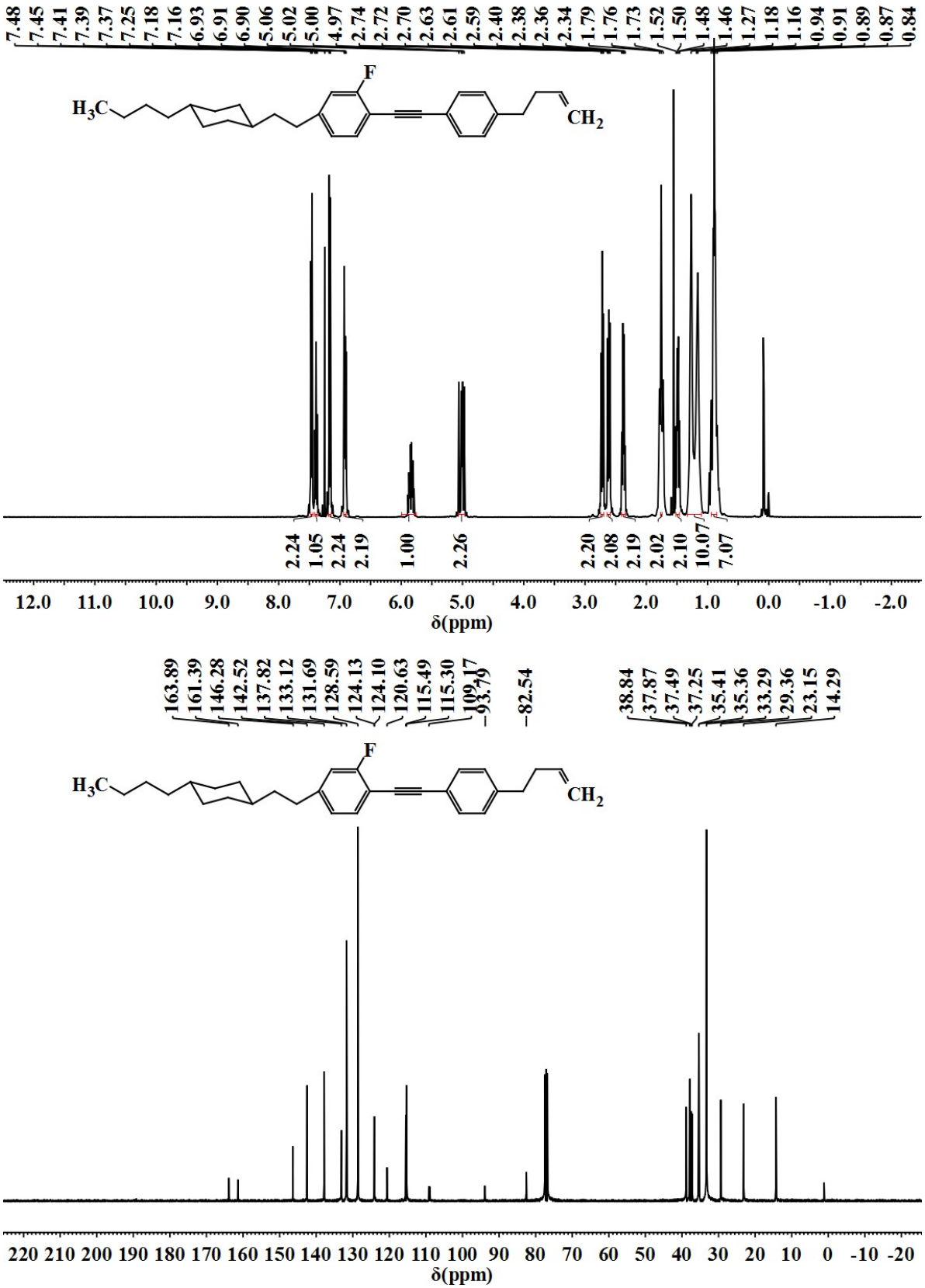


Fig. S2 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **4FTV** recorded in $CDCl_3$.

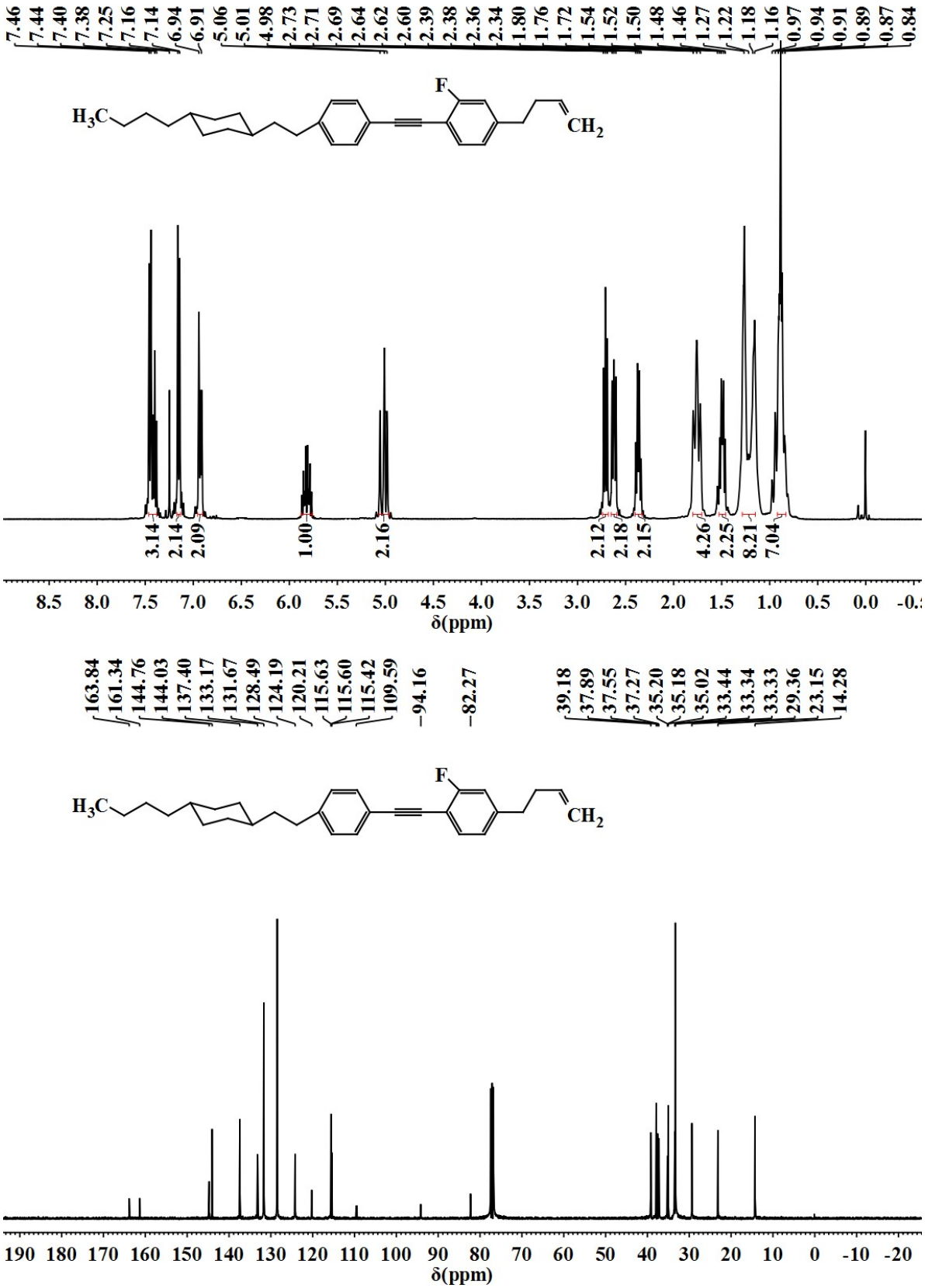


Fig. S3 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **4TFV** recorded in $CDCl_3$.

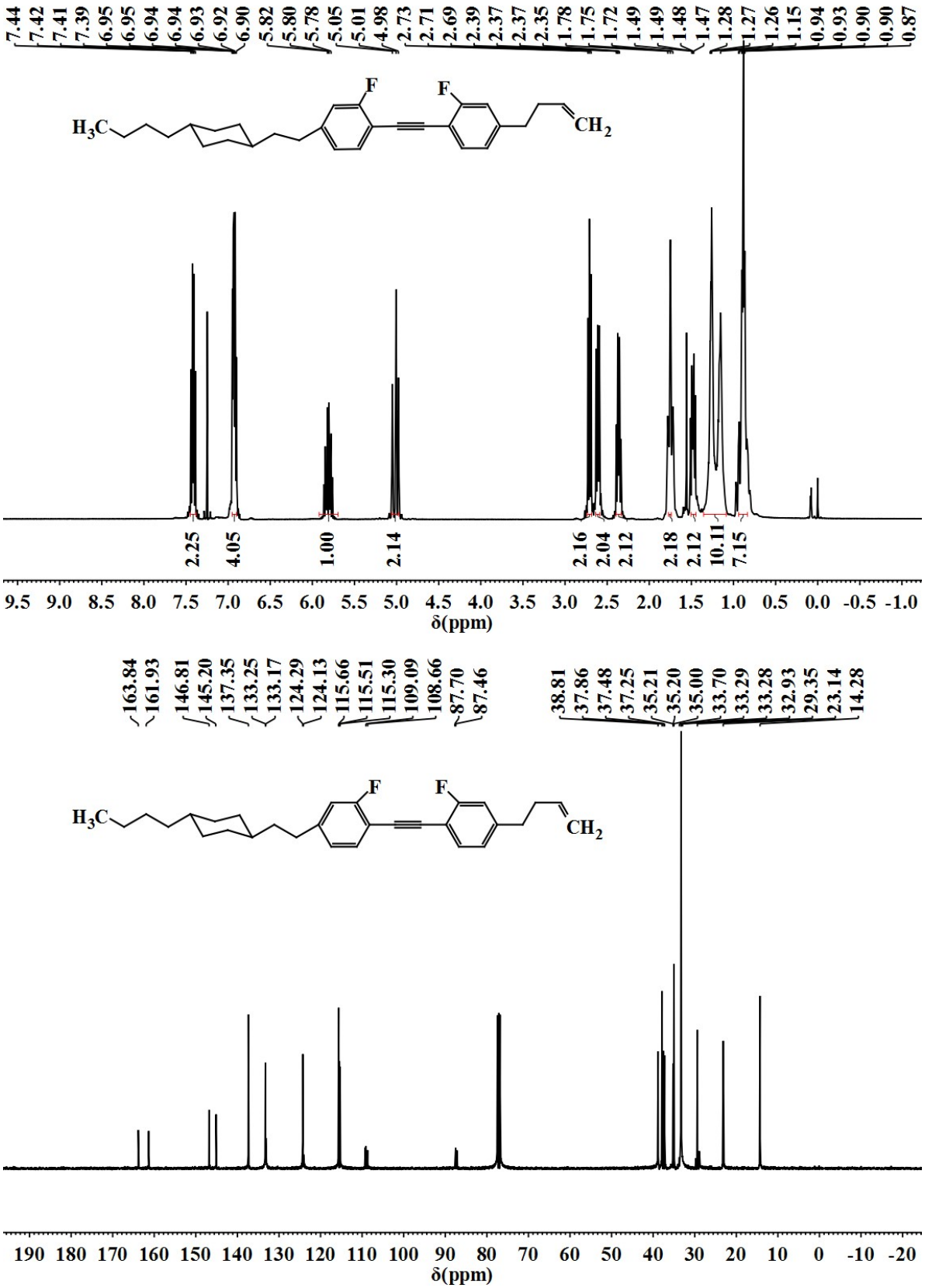


Fig. S4 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **4FTFV** recorded in $CDCl_3$.

3. Tables S1-S4, Figures S5 and S6

Table S1. Phase transitions temperatures and corresponding enthalpies for the compounds ***n*TFV**, **4TV**, **4FTV** and **4FTFV**.[a]

Compd.	Phase transition (°C)	$\Delta H_{C\text{-}N}$ (kJ/mol)	$\Delta H_{N\text{-}I}$ (kJ/mol)	Nematic range (°C)
2TFV	Cr 33.9 N 127.4 I	12.4	1.0	93.5
3TFV	Cr 51.0 N 151.1 I	5.4	0.6	100.1
4TFV	Cr 42.0 N 149.5 I	12.0	0.9	107.5
5TFV	Cr 50.5 N 141.4 I	5.3	0.6	90.9
4FTV	Cr 45.4 N 137.1 I	21.1	0.6	91.7
4FTFV	Cr 30.5 N 140.7 I	13.4	0.8	110.2
4TV	Cr 100.2 N 161.1 I	4.6	1.8	60.9
4FT4	Cr 50.4 Sm 71.8 N 147.1 I	15.0	-	75.3
4FBV	Cr 41.8 SmA 71.5 N 115.1 I	3.2	2.1	43.6
4BFV	Cr 23.8 N 109.5 I	3.9	2.2	85.7
2BFV	Cr 15.8 N 88.0 I	19.5	1.0	72.2
3BFV	Cr 30.3 N 115.1 I	13.2	1.3	84.8
5BFV	Cr 38.9 N 118.9 I	2.9	2.3	80.0

[a] Cr: crystal; N: nematic mesophase phase; I: isotropic liquid.

Table S2. The effect of compound **2TFV** on the properties of LC mixture **P02-F**.

LC mixture	Phase transition (°C)	Nematic range (°C)	Δn	γ_1 (mPa·s)
P02-F	Cr -18.2 N 123.3 I	141.5	0.2908	221.1
F	Cr -34.1 N 123.3 I	157.4	0.2825	185.5

Table S3. Selected nine phase levels between 0 and 2π, and the corresponding operation voltage of **SNUP04**.

Phase level	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
Voltage (V)	0	1.52	1.76	1.97	2.22	2.58	3.02	3.63	5
Phase change (π)	0	0.2595	0.5190	0.7785	1.0380	1.2975	1.5570	1.8165	2.0760

Table S4. Measured PTP response time of **SNUP04** in a transmissive cell with d=3.12 μm. For a 1.56 μm reflective LCoS panel, the response time should be 4x faster than the data shown here.

		Rise time (ms)								
Decay time (ms)		**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
	1	*	51.08	36.29	23.92	18.18	12.05	8.72	5.45	2.53
	2	14.37	*	24.54	20.11	14.35	9.83	7.33	4.69	2.14
	3	13.79	29.84	*	17.35	12.59	8.89	6.65	4.26	1.95
	4	12.85	21.18	18.75	*	11.62	8.31	6.19	3.96	1.83
	5	12.45	19.44	17.37	15.03	*	7.40	4.72	3.71	1.67
	6	12.31	18.37	16.94	14.43	10.39	*	3.86	3.35	1.55
	7	12.24	17.47	16.35	13.77	9.87	6.12	*	3.32	1.52
	8	11.96	16.35	15.39	12.80	8.97	6.06	4.58	*	1.48
	9	11.84	15.25	14.83	12.22	8.62	5.85	4.55	3.28	*

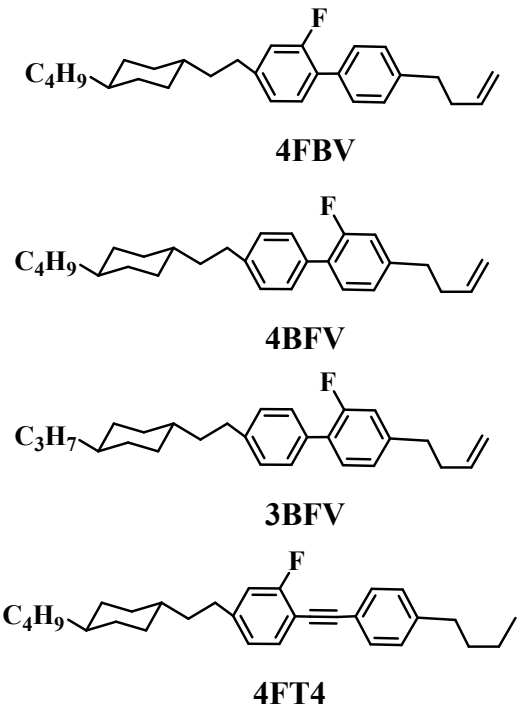


Fig. S5 The molecular structures of reference compounds **4FBV**, **4BFV**, **3BFV** and **4FT4**.

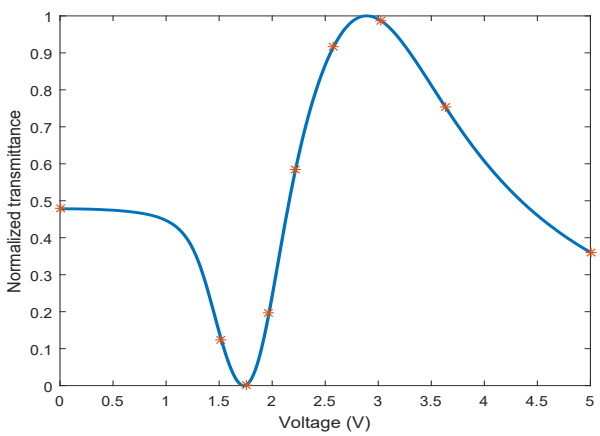


Fig. S6 Measured voltage-dependent transmittance change curve for **SNUP04** at 40°C, λ = 633 nm and 1 kHz.

4. Compositions of mixtures SNUP03 and SNUP04

Table S4. Chemical structures and compositions of LC mixture **SNUP03**.

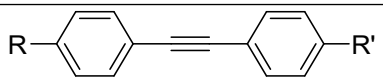
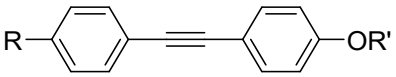
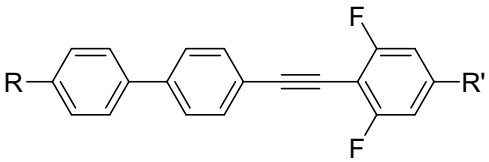
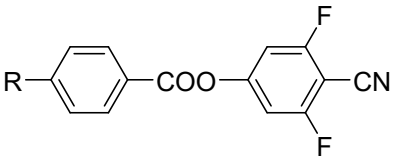
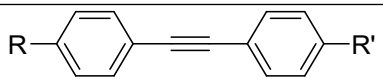
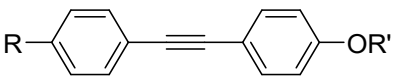
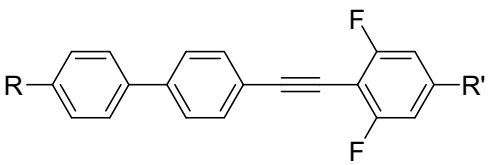
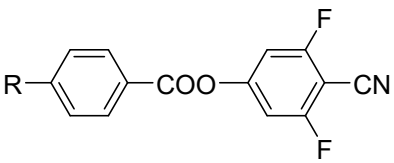
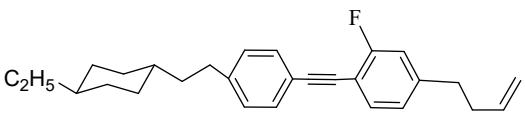
Code	Compound structures	wt%
1		20
2		10
3		55
4		15

Table S5. Chemical structures and compositions of LC mixture **SNUP04**.

Code	Compound structures	wt%
1		
2		
3		90
4		
2TFV		10

5. Geometric data

Optimized geometry for molecular **3BFV**

C	-4.39565200	-1.31160500	-0.21310500
C	-5.75423800	-1.27088000	-0.50312000
C	-6.41135600	-0.05280200	-0.70387900
C	-5.65733300	1.11869600	-0.60570000
C	-4.30440400	1.05429800	-0.31721800
C	-3.61912800	-0.14673000	-0.11013400
H	-3.91616500	-2.26837400	-0.04209700
H	-6.31285300	-2.19848400	-0.57052500
H	-6.10428900	2.09357700	-0.76498300
C	-2.16586400	-0.21046700	0.18322800
C	-1.54677600	0.68838400	1.06362300
C	-1.37045200	-1.20916400	-0.39595100
C	-0.19162500	0.58211300	1.35435200
C	-0.01527300	-1.30924100	-0.10094300
C	0.60194600	-0.41647100	0.78045700
C	-7.89664700	0.00234800	-0.97469700
C	-8.73901000	0.11080600	0.32023000
H	-8.20602700	-0.89355600	-1.52110000
H	-8.12191600	0.85792200	-1.61999200
H	-8.53177500	-0.75081900	0.96237800
H	-8.41083900	1.00074800	0.87178000
C	-10.21279200	0.20445500	0.04438500
C	-11.12649400	-0.67206300	0.45051200
H	-10.53196700	1.06350600	-0.54503800
H	-12.17786900	-0.54999700	0.21535200
H	-10.85554700	-1.54347000	1.03953500
C	2.08261200	-0.50311700	1.07251100
C	2.93683900	0.32263100	0.08912500
H	2.39595200	-1.55099400	1.04219900
H	2.27361600	-0.14825000	2.09169800
H	2.76573200	-0.04421000	-0.93101200
H	2.58001000	1.35895000	0.10412300
C	4.44357300	0.30539700	0.38909100

C	5.22015600	1.24785500	-0.54371900
C	5.05132200	-1.12103100	0.31432100
C	6.69507900	1.39790800	-0.11061900
H	4.73946900	2.23076900	-0.57581100
C	6.55287700	-1.12269500	-0.05289600
H	4.91070400	-1.62786100	1.27440900
C	7.26972900	0.10659200	0.52716100
H	6.78817500	2.21795100	0.60981900
H	6.66569200	-1.12789700	-1.14247200
C	8.80790400	0.03065500	0.44980200
C	9.41432800	-0.20656300	-0.94040700
H	9.14966400	-0.77133200	1.11681800
H	9.22149600	0.96037500	0.86294100
C	10.94648800	-0.20282100	-0.92030900
H	9.06349000	-1.16525400	-1.33703500
H	9.06402500	0.55937300	-1.64095200
H	11.33569200	0.75885800	-0.57146500
H	11.33540400	-0.97736300	-0.25170800
H	0.25714500	1.28477900	2.04983500
H	0.57354700	-2.09389200	-0.56615900
H	-1.81515100	-1.90573000	-1.09793300
H	7.29312100	1.68802800	-0.98034200
H	5.16826600	0.85147300	-1.56520300
H	4.50075200	-1.71195100	-0.42753800
H	7.02188700	-2.04476600	0.30653700
H	4.57567600	0.68083600	1.41374900
H	7.02441000	0.13500400	1.59723300
H	-2.13238100	1.46874200	1.53189900
F	-3.62683100	2.22789600	-0.25550000
H	11.35946900	-0.38668100	-1.91603400

Optimized geometry for molecular **4TV**

C	6.33089100	-1.07189500	0.59898900
C	7.69037000	-1.04093700	0.87942700
C	8.41808900	0.15334500	0.82432600
C	7.73214800	1.32392300	0.47941800

C	6.37332500	1.30760500	0.19597400
C	5.64548700	0.10524900	0.24938000
H	5.78398200	-2.00571900	0.65079200
H	8.19718900	-1.96132100	1.15218800
H	8.27100900	2.26552000	0.43846600
H	5.85901000	2.22490300	-0.06449500
C	1.67285800	0.04523800	-0.56614900
C	1.00519400	1.20991400	-0.98571300
C	0.92634600	-1.13960500	-0.43841200
C	-0.35515300	1.18358300	-1.26094200
C	-0.43383200	-1.15087800	-0.71678900
C	-1.10261700	0.00696700	-1.13071200
C	9.90488200	0.17143400	1.09126000
C	10.74811000	-0.02269300	-0.19349000
H	10.16482100	-0.61721100	1.80373700
H	10.18330700	1.12181500	1.55918700
H	10.48805100	-0.97850800	-0.65892600
H	10.47088800	0.76141300	-0.90911400
C	12.22568700	0.03560100	0.07133200
C	13.08473500	-0.95507300	-0.14939700
H	12.59665000	0.97190100	0.48744800
H	14.14200700	-0.85205800	0.06786500
H	12.76120000	-1.90643700	-0.56168000
C	-2.59160700	-0.00266900	-1.38858400
C	-3.41412100	0.36882400	-0.13735600
H	-2.89018000	-0.99277100	-1.74538500
H	-2.82870500	0.70494300	-2.19115600
H	-3.18862900	-0.34512400	0.66505500
H	-3.07642700	1.34773300	0.22240100
C	-4.93290200	0.41252200	-0.36558300
C	-5.67746600	0.92804700	0.87627300
C	-5.51196700	-0.96421200	-0.78861700
C	-7.17691800	1.16748600	0.59276000
H	-5.21553000	1.85206800	1.23838500
C	-6.98986000	-1.15490500	-0.38005300
H	-5.41578300	-1.08225200	-1.87271100
C	-7.76230800	0.17203300	-0.44181600

H	-7.32579400	2.18795600	0.22319800
H	-7.04136100	-1.55830900	0.63699100
C	-9.29301900	0.01669200	-0.32970400
C	-9.81510500	-0.72847900	0.90788500
H	-9.65256500	-0.50973800	-1.22353100
H	-9.73811100	1.01780800	-0.37114000
C	-11.34868600	-0.83088200	0.97358700
H	-9.40107700	-1.74221100	0.91818100
H	-9.45579700	-0.24364700	1.82372500
H	-11.71973800	-1.28010100	0.04399700
H	-0.84804500	2.09388600	-1.58798300
H	-0.98874900	-2.07831900	-0.61491100
H	1.42638200	-2.04727100	-0.12219000
H	-7.73069500	1.10153400	1.53443200
H	-5.56102000	0.19509200	1.68419300
H	-4.91095700	-1.76374800	-0.33904800
H	-7.45991300	-1.90214900	-1.02821700
H	-5.12089400	1.12838400	-1.17830600
H	-7.57885400	0.59400800	-1.43908800
H	1.56698500	2.12980000	-1.09578800
C	3.06659200	0.06478300	-0.28213300
C	4.25235600	0.08251300	-0.03701000
H	-11.61699000	-1.52928400	1.77413000
C	-12.06758800	0.50046100	1.22062300
H	-11.89781600	1.21552800	0.41151100
H	-13.14793900	0.35342200	1.30452300
H	-11.72342500	0.96451600	2.15061500

Optimized geometry for molecular **4TFV**

C	6.11108600	-1.41129700	0.25180400
C	7.47486700	-1.49631500	0.49454900
C	8.23563900	-0.35199400	0.76327500
C	7.58422400	0.88541900	0.78409600
C	6.22530700	0.95763100	0.54069900
C	5.44256900	-0.17324000	0.26642200
H	5.53446400	-2.30529100	0.04852000
H	7.95846300	-2.46710100	0.48038100

H	8.12143500	1.80322400	0.99461300
C	1.47014800	0.15200100	-0.45216700
C	0.85256500	1.41550700	-0.44795600
C	0.67845800	-0.97728300	-0.72579900
C	-0.50540800	1.53629400	-0.70916200
C	-0.67837300	-0.84059100	-0.98568200
C	-1.29764700	0.41496700	-0.98315100
C	9.72730800	-0.43961400	0.98379500
C	10.53879600	-0.21398600	-0.31636100
H	9.98354000	-1.42134300	1.39227700
H	10.03410200	0.30192800	1.72903300
H	10.24758200	-0.96099600	-1.06118800
H	10.26493800	0.76518300	-0.72839400
C	12.02237900	-0.26696100	-0.08633000
C	12.85390300	-1.14247300	-0.64308900
H	12.42293900	0.47642400	0.60226700
H	13.91767400	-1.13069300	-0.43383100
H	12.50056100	-1.90160800	-1.33488800
C	-2.78126600	0.55192100	-1.23513500
C	-3.62082900	0.45097100	0.05510200
H	-3.09960500	-0.22003900	-1.94195300
H	-2.98117300	1.51708200	-1.71418500
H	-3.44172700	-0.52466500	0.52483900
H	-3.25907500	1.20276200	0.76604400
C	-5.13036500	0.64348400	-0.15598700
C	-5.89402700	0.65293700	1.17779500
C	-5.74260700	-0.42544500	-1.10020400
C	-7.37395400	1.05391500	0.99222000
H	-5.41050500	1.33214200	1.88712900
C	-7.24184200	-0.68801700	-0.83097100
H	-5.60765100	-0.11212300	-2.14037100
C	-7.95947900	0.58908900	-0.36552100
H	-7.47493800	2.14232700	1.06531500
H	-7.34783600	-1.46359100	-0.06468100
C	-9.49721600	0.47359200	-0.35218100
C	-10.09406100	-0.67221600	0.47678400
H	-9.84339800	0.36749500	-1.38833000

H	-9.91227800	1.42475600	0.00648300
C	-11.62804300	-0.67994100	0.46252400
H	-9.73197500	-1.63395000	0.09511200
H	-9.75101800	-0.60846000	1.51629200
H	-11.99739600	0.27599700	0.85334000
H	-11.97784300	-0.73796100	-0.57537600
H	-0.96029100	2.52190800	-0.70751900
H	-1.26912400	-1.72528900	-1.20177900
H	1.14086400	-1.95706800	-0.73764500
H	-7.96006800	0.63837900	1.81783500
H	-5.83013900	-0.34709600	1.62422800
H	-5.18948400	-1.36599300	-0.98949300
H	-7.71623300	-1.08608100	-1.73428000
H	-5.27067800	1.63049600	-0.61899000
H	-7.72480300	1.36666300	-1.10470300
C	2.86300100	0.02652300	-0.19556200
C	4.05032000	-0.06216200	0.02080600
C	-12.23607400	-1.83011100	1.27013100
H	-11.93255900	-1.78007100	2.32061000
H	-11.91424900	-2.80085000	0.88008600
H	-13.32889200	-1.80645300	1.23955700
H	1.45221300	2.29440200	-0.24384500
F	5.62865300	2.16665800	0.57211500

Optimized geometry for molecular **4FTV**

C	6.26867300	-1.39756800	0.18373000
C	7.63481300	-1.48599000	0.41558900
C	8.38558400	-0.36171400	0.77776800
C	7.71654700	0.86155000	0.90607300
C	6.35152900	0.96518800	0.67727700
C	5.60170900	-0.16627400	0.30842200
H	5.70360100	-2.27958100	-0.09307300
H	8.12881400	-2.44762900	0.31831100
H	8.27420000	1.74687100	1.19542500
H	5.84844800	1.91868900	0.78376500
C	1.62581100	0.16827900	-0.38659500
C	0.97196700	1.40409800	-0.28221400

C	0.83262200	-0.93213700	-0.76159200
C	-0.37909600	1.55883800	-0.53204700
C	-0.52392100	-0.78877400	-1.01505800
C	-1.15466900	0.45720100	-0.90638200
C	9.87885900	-0.45747700	0.98490500
C	10.68310900	-0.15453200	-0.30391500
H	10.14274900	-1.45963400	1.33573600
H	10.18731800	0.24187600	1.76943100
H	10.39220100	-0.85972500	-1.08874100
H	10.40133700	0.84471100	-0.65868900
C	12.16820100	-0.21194100	-0.08528400
C	13.00202400	-1.04803200	-0.69670200
H	12.56820700	0.49147400	0.64447700
H	14.06679000	-1.04259400	-0.49207500
H	12.64925900	-1.76689300	-1.43054400
C	-2.63734000	0.60758500	-1.15436700
C	-3.48404000	0.40955300	0.12009900
H	-2.94699300	-0.11250700	-1.91718700
H	-2.83896100	1.60407400	-1.56272400
H	-3.30233500	-0.59611600	0.51995400
H	-3.13280900	1.11130900	0.88535700
C	-4.99243200	0.60883600	-0.09235800
C	-5.77017700	0.52875300	1.23070800
C	-5.58978900	-0.39853000	-1.11114600
C	-7.24894300	0.93774600	1.05420000
H	-5.29685300	1.16133300	1.98835600
C	-7.08953600	-0.68662100	-0.87321400
H	-5.44838800	-0.01599900	-2.12706200
C	-7.81933600	0.55443900	-0.33571900
H	-7.35254000	2.01967300	1.19122900
H	-7.19805900	-1.51041100	-0.15945800
C	-9.35623900	0.43001200	-0.34464000
C	-9.95430200	-0.76906700	0.40414500
H	-9.69194800	0.38822000	-1.38876300
H	-9.78026300	1.35423800	0.06958600
C	-11.48820500	-0.77843900	0.38118300
H	-9.58808600	-1.70310000	-0.03767200

H	-9.61701700	-0.77266400	1.44744100
H	-11.86101400	0.14958700	0.83143100
H	-11.83259600	-0.76926700	-0.66012000
H	-0.81257800	2.54803800	-0.43870000
H	-1.10408400	-1.65649400	-1.31020200
H	1.30789400	-1.90086000	-0.85549900
H	-7.84232000	0.47267700	1.84761600
H	-5.70860400	-0.49818600	1.61141100
H	-5.03179100	-1.34125600	-1.05855200
H	-7.55288000	-1.02880500	-1.80466700
H	-5.13279900	1.62351300	-0.49115600
H	-7.58258800	1.37785300	-1.02279100
C	3.01657700	0.04784200	-0.13647100
C	4.20395400	-0.06121000	0.06998100
F	1.69051800	2.48996400	0.06985800
C	-12.09827200	-1.97946700	1.10924500
H	-11.79991700	-1.99739700	2.16220200
H	-11.77319300	-2.92244900	0.65855200
H	-13.19095300	-1.95511900	1.07495400

Optimized geometry for molecular **4FTFV**

C	6.04510900	-1.49776900	0.23016200
C	7.40801400	-1.60700500	0.46691500
C	8.18442500	-0.47931000	0.76060700
C	7.54990700	0.76574600	0.81298800
C	6.19131100	0.86314600	0.57528800
C	5.39387700	-0.25125100	0.27621700
H	5.45600500	-2.37883300	0.00706400
H	7.87856000	-2.58346800	0.42815800
H	8.09994700	1.67090900	1.04398900
C	1.42600700	0.09308000	-0.43202400
C	0.77734600	1.33613400	-0.41993000
C	0.62915100	-1.03058900	-0.72076200
C	-0.57436300	1.47445900	-0.67727600
C	-0.72742200	-0.90290400	-0.98098800
C	-1.35379700	0.35005200	-0.96504000
C	9.67534400	-0.59202800	0.97431200

C	10.48575700	-0.34340700	-0.32233000
H	9.91979400	-1.58722400	1.35655700
H	9.99378900	0.12614200	1.73729900
H	10.18240600	-1.06684100	-1.08540200
H	10.22381100	0.64973400	-0.70776900
C	11.96919800	-0.42238000	-0.09884100
C	12.78684300	-1.29329100	-0.68271900
H	12.38196400	0.29627800	0.60850100
H	13.85139900	-1.30167100	-0.47735900
H	12.42069000	-2.02806300	-1.39387300
C	-2.83724500	0.48553100	-1.21676400
C	-3.67671400	0.37288100	0.07277900
H	-3.15134100	-0.28326100	-1.92849000
H	-3.03929600	1.45300000	-1.68956200
H	-3.49753600	-0.60674300	0.53384500
H	-3.31649200	1.11901100	0.79029000
C	-5.18586400	0.56672900	-0.13958400
C	-5.95218500	0.56143900	1.19265500
C	-5.79560400	-0.49213100	-1.09655200
C	-7.43148900	0.96521600	1.00785700
H	-5.47009500	1.23232400	1.91078200
C	-7.29609700	-0.75560900	-0.83502600
H	-5.65683400	-0.16860900	-2.13311900
C	-8.01331800	0.51710100	-0.35706500
H	-7.53222600	2.05265300	1.09393600
H	-7.40568300	-1.54016200	-0.07847800
C	-9.55122900	0.40398500	-0.35039900
C	-10.15327500	-0.75024900	0.46294300
H	-9.89373400	0.31056900	-1.38897200
H	-9.96593900	1.35165900	0.01768900
C	-11.68721800	-0.75505700	0.44186100
H	-9.79120600	-1.70821300	0.07187200
H	-9.81472900	-0.69888000	1.50459400
H	-12.05654600	0.19701800	0.84198600
H	-12.03246400	-0.80050000	-0.59818500
H	-1.00531900	2.46890700	-0.65737100
H	-1.31124600	-1.78849400	-1.20776100

H	1.10138600	-2.00511300	-0.74203700
H	-8.01980000	0.53978200	1.82678600
H	-5.88991000	-0.44370400	1.62763200
H	-5.24390300	-1.43440800	-0.99318900
H	-7.76809400	-1.14217800	-1.74450700
H	-5.32545400	1.55864300	-0.59211400
H	-7.77506500	1.30287600	-1.08637600
C	2.81656300	-0.01537600	-0.17646800
C	4.00265300	-0.11866000	0.03637400
C	-12.30086400	-1.91326600	1.23353900
H	-12.00224700	-1.87562500	2.28592200
H	-11.97886600	-2.88008600	0.83402400
H	-13.39347000	-1.88734900	1.19812700
F	5.61209100	2.07707500	0.63717100
F	1.49888800	2.44166100	-0.15393400