

Electronic Supplementary Information

## An electron-deficient tris(triazole)-based discotic liquid crystal that exhibits fast electron transport

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## 1. Materials and characterization techniques

**1.1 Materials.** “All solvents and chemicals (AR quality) were used as received without any further modification. Silica gel (100–200 & 60-120 mesh) was used for column chromatographic separations. Pre-coated aluminium sheets with silica gel (Merck, Kieselgel 60, F254) were used for thin-layer chromatography (TLC).” These are similar, as reported in our earlier studies.<sup>1,2</sup>

### 1.2 Instrumentation

The instrumental details are similar to our previous works.<sup>1-4</sup>

## 2. Experimental procedures

**2.1 Synthesis of 2,5,8-tris(3,4,5-tris(dodecyloxy)phenyl)-5,8-dihydro-2H-benzo[1,2-*d*:3,4-*d'*:5,6-*d''*]tris([1,2,3]triazole) (1):** The procedure for the synthesis of compound **1** is similar, as reported elsewhere.<sup>5</sup> A round-bottom flask was charged with **2** (560 mg, 1 equiv.), pyridine (15 ml) and Cu(OAc)<sub>2</sub>·H<sub>2</sub>O (535.34 mg, 10 equiv.), and the resultant solution was kept stirring for 1 h at 80 °C. Water (30 ml) was then added to the reaction mixture and left for stirring for 30 minutes at the same temperature. It was then cooled to room temperature and extraction was done using dichloromethane (DCM). The purification using column chromatography (Silica Gel 100-200 mesh, hexane) afforded liquid crystal **1** as a beige solid in 72% yield.

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, δ in ppm):** δ 7.67 (s, 6H, Ar), 4.02-4.17 (m, 18H, 9 × OCH<sub>2</sub>), 1.27-1.93 (m, 180H, 90 × CH<sub>2</sub>), 0.87 (t, 27H, 9 × CH<sub>3</sub>).

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, δ in ppm):** δ 153.64, 138.54, 136.89, 135.33, 98.73, 73.70, 69.48, 31.98, 31.96, 30.40, 29.81, 29.79, 29.76, 29.74, 29.71, 29.66, 29.46, 29.44, 29.42, 26.16, 22.73, 14.16.

**MALDI-MS (m/z):** [M+H]<sup>+</sup> : 2087.7888 (calculated for C<sub>132</sub>H<sub>232</sub>N<sub>9</sub>O<sub>9</sub> [M+H] : 2087.7973).

**IR (Neat, KBr, ν<sub>max</sub>/cm<sup>-1</sup>):** 2920, 2850, 1605, 1505, 1463, 1450, 1384, 1341, 1280, 1231, 1153, 1119, 979, 884, 826, 720, 667, 613.

### 2.2 Synthesis of 2,4,6-tris((3,4,5-tris(dodecyloxy)phenyl)diazenyl)benzene-1,3,5-triamine (2):

In the ice-cold solution of 3,4,5-tridodecyloxyaniline **4** (1 g, 3 equiv.) in DCM, TFA (296.0 μl, 7.5 equiv.) was added dropwise under vigorous stirring. After 10 minutes of stirring, *t*-butyl nitrite (235.6 μl, 3.84 equiv.) was added slowly to the resulting solution and was stirred for 1 h at 0~5 °C. The formed reaction mixture of aniline was transferred to the stirred ice-cold solution of **3**

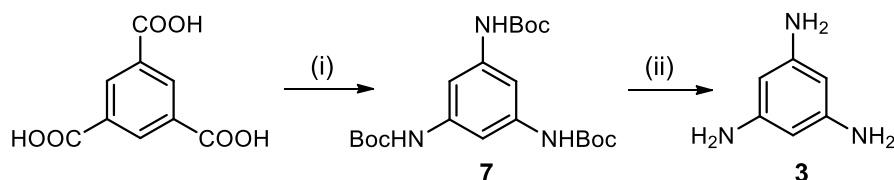
(63.50 mg, 1 equiv.), DCM and K<sub>2</sub>CO<sub>3</sub> (356.29 mg, 5 equiv.) within a duration of 10 minutes. The resulting reaction mixture was stirred for an additional 12 h at ambient temperature. The product was extracted using DCM, which was further purified using column chromatography (Silica Gel 60-120 mesh, ethyl acetate/hexane 10:90) furnished **2** as a red semi-solid dye in 79% yield.

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, δ in ppm):** δ 6.91 (s, 6H, Ar), 3.99-4.07 (m, 18H, 9 × OCH<sub>2</sub>), 1.26-1.86 (m, 180H, 90 × CH<sub>2</sub>), 0.88 (t, 27H, 9 × CH<sub>3</sub>).

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, δ in ppm):** δ 156.73, 153.54, 149.03, 138.55, 107.41, 99.63, 73.67, 69.66, 69.12, 63.11, 32.83, 31.99, 31.96, 31.94, 30.41, 29.81, 29.79, 29.76, 29.71, 29.67, 29.65, 29.57, 29.50, 29.47, 29.45, 29.42, 29.38, 29.25, 28.70, 28.19, 26.21, 26.19, 25.81, 25.77, 25.73, 22.73, 14.15.

**IR (Neat, KBr, ν<sub>max</sub>/cm<sup>-1</sup>):** 3499, 3441, 3382, 3222, 2921, 2851, 1596, 1494, 1467, 1439, 1347, 1330, 1226, 1121, 1032, 828, 778, 720, 613.

**2.3 Synthesis of 1,3,5-Triaminobenzene (3):** 1,3,5-Triaminobenzene **3** was prepared in two steps, as reported earlier.<sup>6</sup> Trimesic acid undergoes Curtius rearrangement reaction in the presence of diphenylphosphoryl azide, under heating conditions to obtain 1,3,5-Boc-amino-benzene **7** which was then deprotected to give 1,3,5-triaminobenzene **3** under acidic conditions.



**Scheme S1.** Synthesis of triaminobenzene, **3**. Reagents and conditions: (i) DPPA, triethylamine, toluene, *tert*-butanol, 80 °C, 4 h; (ii) Conc. HCl, ethanol, RT, 12 h.

**2.3.1 First Step: Synthesis of 1, 3, 5-Boc-amino-benzene (7):** The diphenylphosphoryl azide (6.54 ml, 3.2 equiv.) was added slowly to the solution of trimesic acid (2 g, 1 equiv.) and triethylamine (4.25 ml, 3.2 equiv.) in toluene (10 ml) and *tert*-butanol (6 ml) present in the volume ratio of 5:3. The resulting mixture was then stirred at 80 °C for 4 h followed by stirring at 110 °C for 2 h. The product was then extracted using ethyl acetate and was purified using column chromatography (Silica Gel 60-120 mesh, ethyl acetate/hexane 1:99) to give **7** as a white fluffy solid in 68% yield.

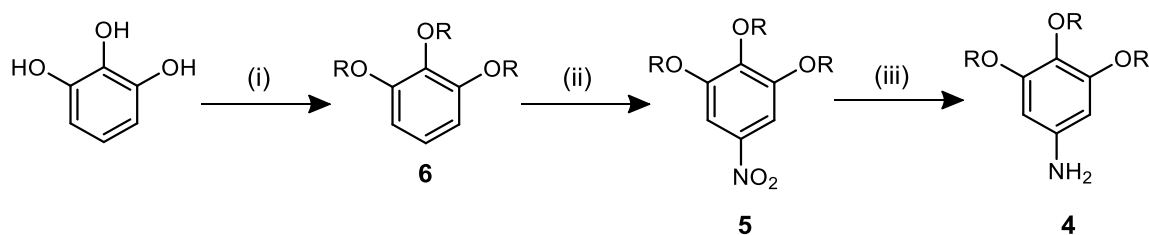
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, δ in ppm):** 7.17 (s, 3H), 6.49 (s, 3H), 1.48 (s, 27H)

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, δ in ppm):** 152.60, 139.52, 102.75, 80.58, 28.30.

**IR (Neat, KBr, ν<sub>max</sub>/cm<sup>-1</sup>):** 3396, 3339, 3276, 2982, 2933, 1739, 1711, 1684, 1614, 1534, 1451, 1422, 1369, 1237, 1158, 1089, 966, 849, 772, 681.

**2.3.2 Second Step: Synthesis of 1,3,5-Triaminobenzene (3):** 1,3,5-Boc-amino-benzene **7** (1g, 2.36 mmol) was added slowly to the mixed solution of ethanol (5 ml) and concentrated hydrochloric acid (5 ml) in the volume ratio of 1:1 and was stirred overnight (12 h) at ambient temperature. Ethanol was then added to induce precipitation and the mixture was filtered to give **3** as a white solid in 75% yield and was immediately used for the next step without further purification.

**2.4 Synthesis of 3,4,5-Trialkoxyaniline (4):** 3,4,5-Trialkoxyaniline **4** was prepared in three steps, as reported earlier.<sup>7</sup> 1,2,3-Trialkoxybenzene was synthesized by reacting pyrogallol with 1-bromoalkane in the presence of a base in DMF, which was nitrated using nitric acid (70 %) and sodium nitrite in DCM, and lastly, catalytic hydrogenation was done to get 3,4,5-Trialkoxyaniline **4**.



**Scheme S2.** Synthesis of trialkoxyaniline (**4**). Reagents and conditions: (i) K<sub>2</sub>CO<sub>3</sub>, dodecylbromide, DMF, 80 °C, 48 h; (ii) NaNO<sub>2</sub>, Conc. HNO<sub>3</sub>, DCM, RT, 12 h; (iii) Pd-C, dry THF, H<sub>2</sub> atm, 24 h.

**2.4.1 First Step: Synthesis of 1,2,3-Tridodecyloxybenzene (6):** Dodecylbromide (19.04 ml, 5 equiv.) was added to a stirring suspension of pyrogallol (2 g, 1 equiv.), anhydrous K<sub>2</sub>CO<sub>3</sub> (10.96 g, 5 equiv.) and potassium iodide (catalytic) in dry DMF, under nitrogen. The resulting reaction mixture was heated at 80 °C and stirred for 48 h under a nitrogen atmosphere. The crude product was extracted with diethyl ether, which was then purified by column chromatography (Silica Gel 100-200 mesh, hexane) furnished **6** as a white solid in 75% yield.

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, δ in ppm):** δ 6.90 (t, 1H, Ar), 6.54 (d, 2H, Ar), 3.93-3.98 (m, 6H, 3 × OCH<sub>2</sub>), 1.26-1.81 (m, 60H, alkyl protons), 0.88 (t, 9H, CH<sub>3</sub>).

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, δ in ppm):** δ 161.26, 153.43, 138.38, 123.13, 106.73, 73.39, 69.08, 64.16, 31.97, 31.95, 31.93, 30.37, 29.79, 29.77, 29.73, 29.68, 29.57, 29.52, 29.45, 29.43, 29.40, 29.37, 29.21, 28.52, 26.17, 26.13, 25.83, 22.73, 14.15.

**IR (Neat, KBr, ν<sub>max</sub>/cm<sup>-1</sup>):** 2916, 2850, 1604, 1469, 1392, 1305, 1257, 1179, 1115, 956, 772, 714.

**2.4.2 Second Step: Synthesis of 3,4,5-Tridodecyloxynitrobenzene (5):** To the solution of 1,2,3-tridodecyloxybenzene **6** (2 g, 1 equiv.) in DCM, sodium nitrite (30.61 mg, 0.14 equiv.) was added and the resultant solution was cooled to 0 °C. To this ice-cold suspension, 70% HNO<sub>3</sub> (421.88 μl, 3 equiv.) was added dropwise and stirred at room temperature for 12 h. The crude product was extracted with DCM and then purified by column chromatography (Silica Gel 100-200 mesh, ethyl acetate/hexane 2:98), yielding **5** as a pale-yellow solid in 65% yield.

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, δ in ppm):** δ 7.46 (s, 2H, Ar), 4.01-4.07 (m, 6H, 3 × OCH<sub>2</sub>), 1.26-1.85 (m, 60H, alkyl protons), 0.88 (t, 9H, CH<sub>3</sub>).

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, δ in ppm):** δ 152.70, 143.77, 143.14, 102.09, 73.83, 69.43, 31.95, 30.31, 29.77, 29.74, 29.71, 29.68, 29.63, 29.54, 29.45, 29.42, 29.39, 29.36, 29.10, 26.04, 26.00, 22.72, 14.15.

**IR (Neat, KBr, ν<sub>max</sub>/cm<sup>-1</sup>):** 2915, 2850, 1617, 1510, 1468, 1434, 1381, 1351, 1215, 1126, 966, 850, 720.

**2.4.3 Third Step: Synthesis of 3,4,5-Tridodecyloxyaniline (4):** To the solution of **5** (1.5 g, 1 equiv.) in dry THF, 10% palladium-charcoal (150 mg, 10 wt% of **5**) was added. The reaction mixture was stirred under a hydrogen atmosphere (H<sub>2</sub> gas-filled balloon) for 12 h. Then, the reaction mixture was filtered and concentrated to get **4** as a dark grey solid in 90% yield.

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, δ in ppm):** δ 5.91 (s, 2H, Ar), 3.82-3.92 (m, 6H, 3 × OCH<sub>2</sub>), 3.46 (bd s, 2H, NH<sub>2</sub>), 1.26-1.80 (m, 60H, 30 × CH<sub>2</sub>), 0.88 (t, 9H, 3 × CH<sub>3</sub>).

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, δ in ppm):** δ 153.72, 142.32, 131.05, 94.42, 73.60, 68.96, 31.97, 31.96, 30.32, 29.80, 29.77, 29.73, 29.69, 29.45, 29.43, 29.40, 26.22, 26.13, 22.73, 14.15.

**IR (Neat, KBr, ν<sub>max</sub>/cm<sup>-1</sup>):** 3418, 3334, 2920, 2850, 1599, 1510, 1463, 1396, 1242, 1115, 1031, 819, 720, 624.

### 3. NMR Spectra

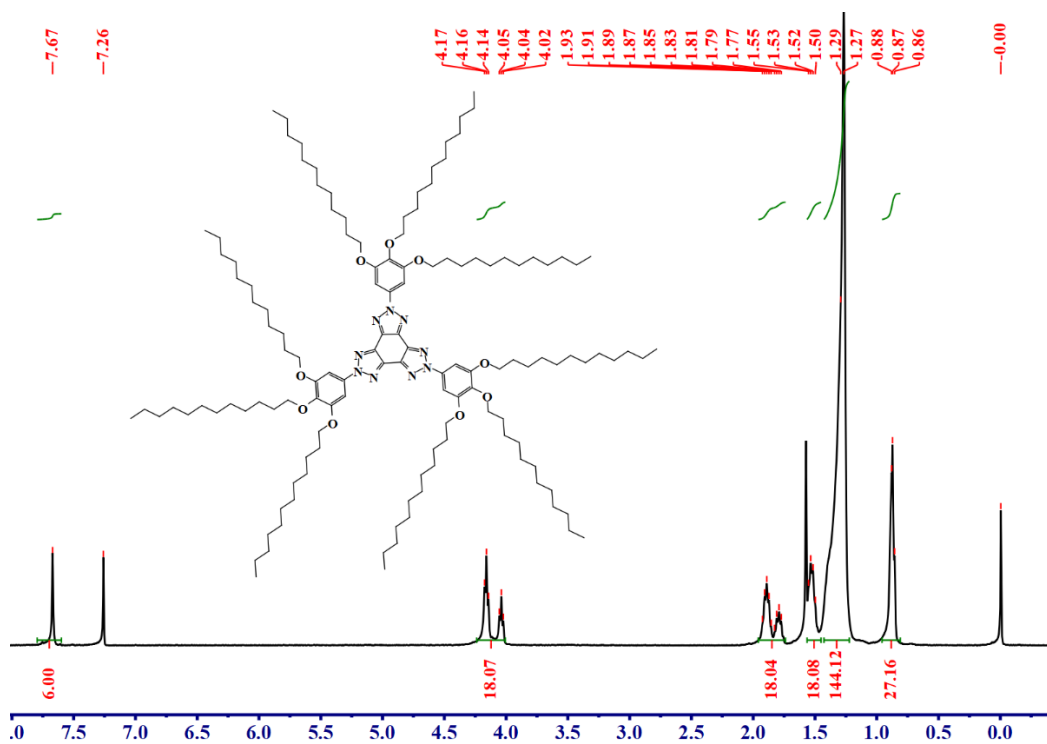


Figure S1. <sup>1</sup>H NMR spectrum of compound 1.

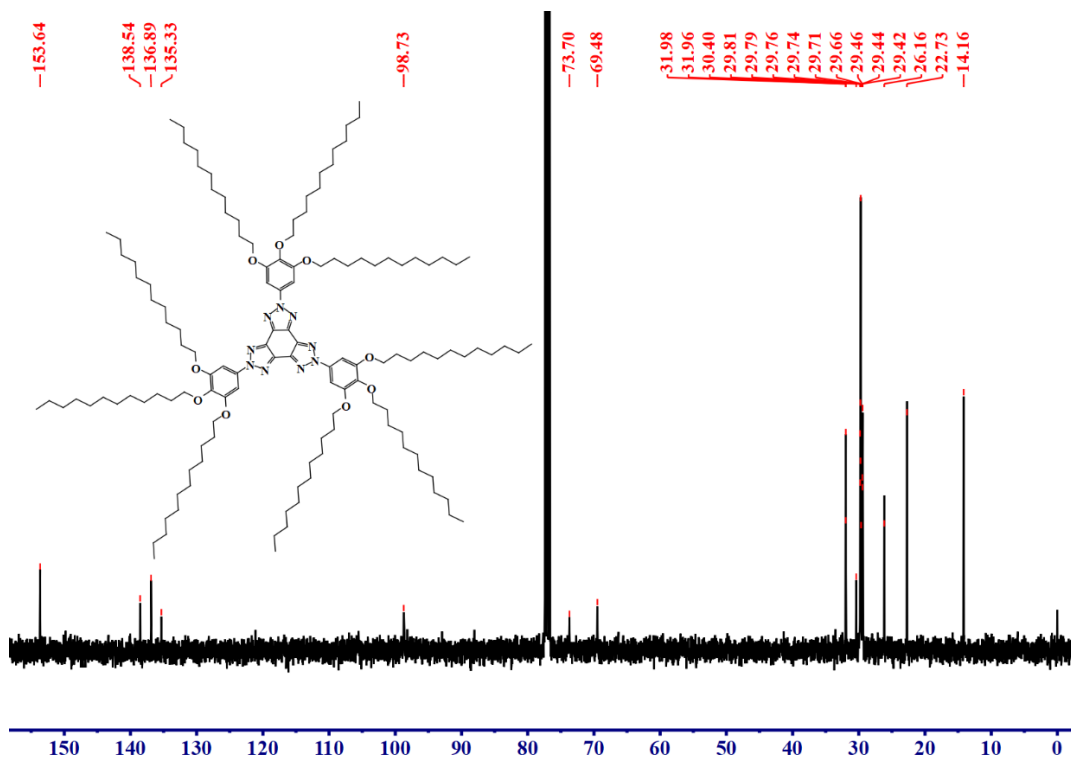
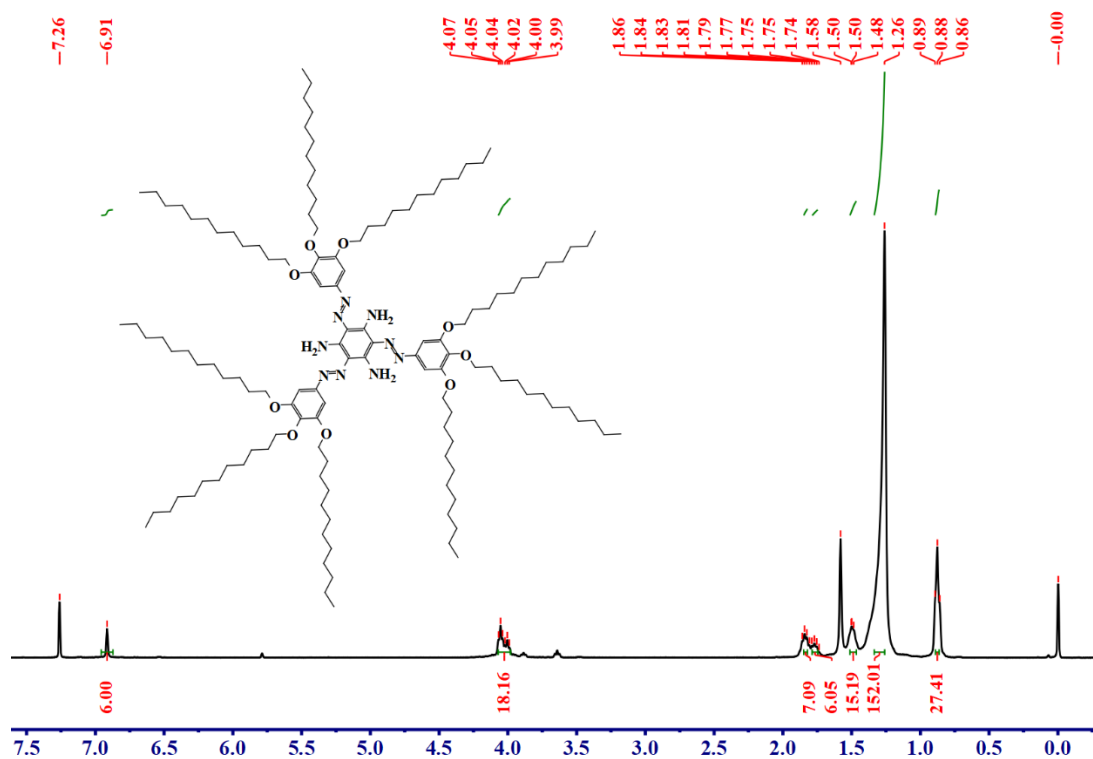
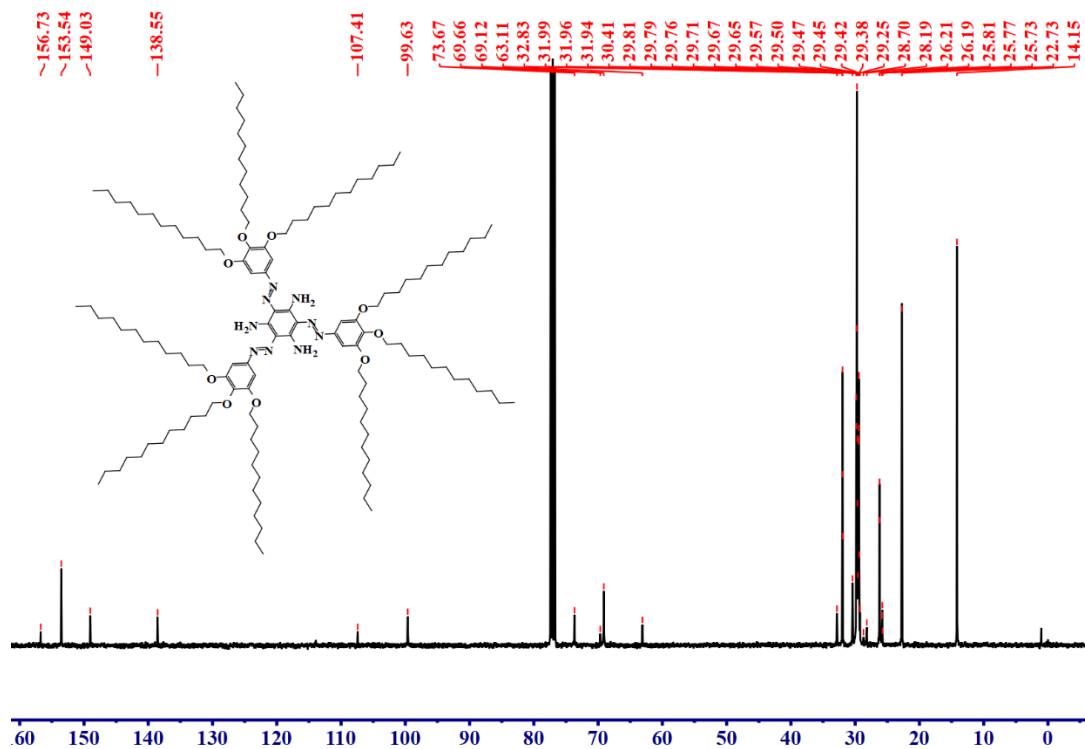


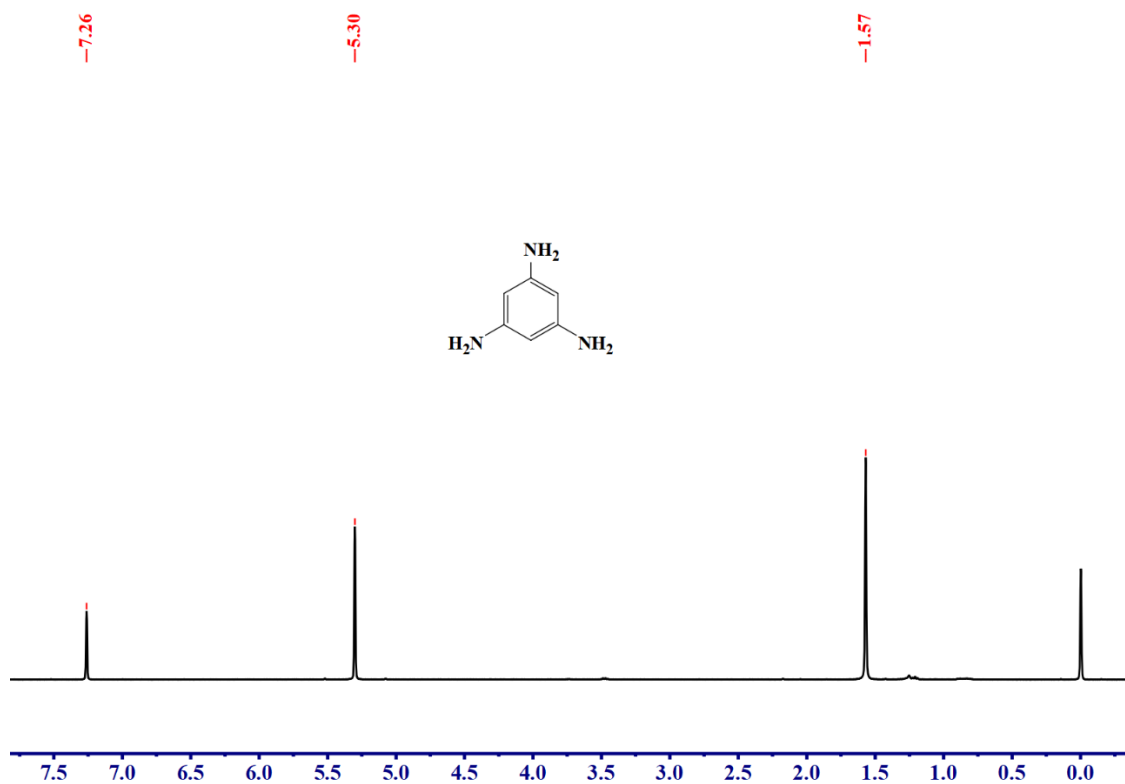
Figure S2. <sup>13</sup>C NMR spectrum of compound 1.



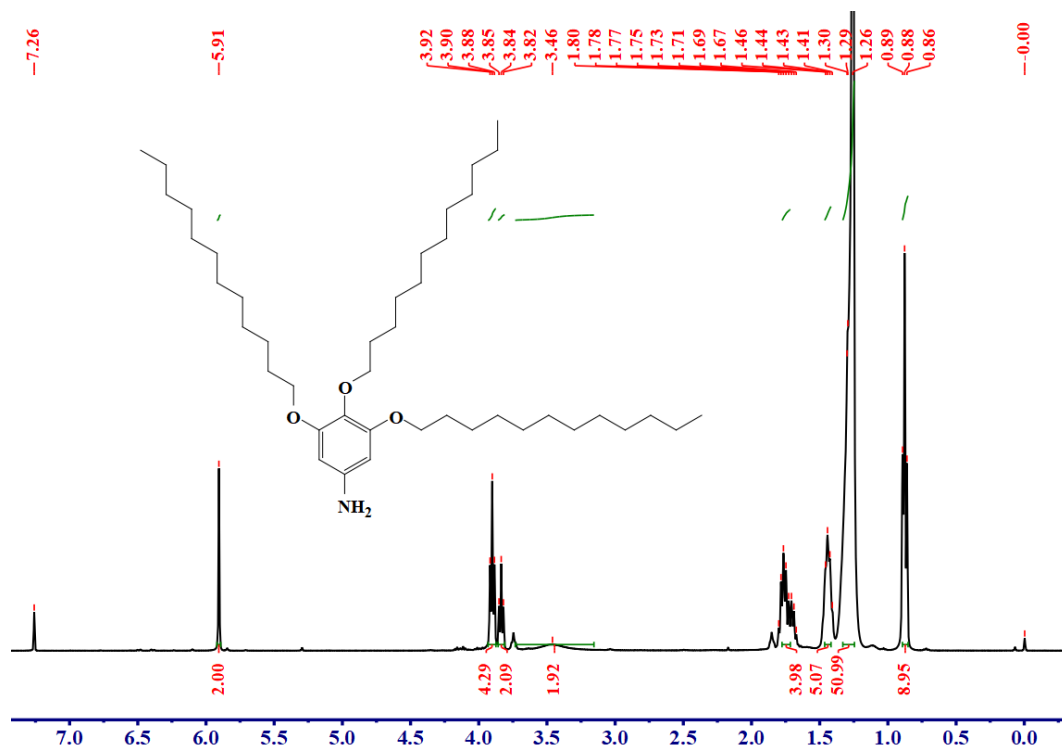
**Figure S3.**  $^1\text{H}$  NMR spectrum of compound **2**.



**Figure S4.**  $^{13}\text{C}$  NMR spectrum of compound **2**.



**Figure S5.** <sup>1</sup>H NMR spectrum of compound 3.



**Figure S6.** <sup>1</sup>H NMR spectrum of compound 4.

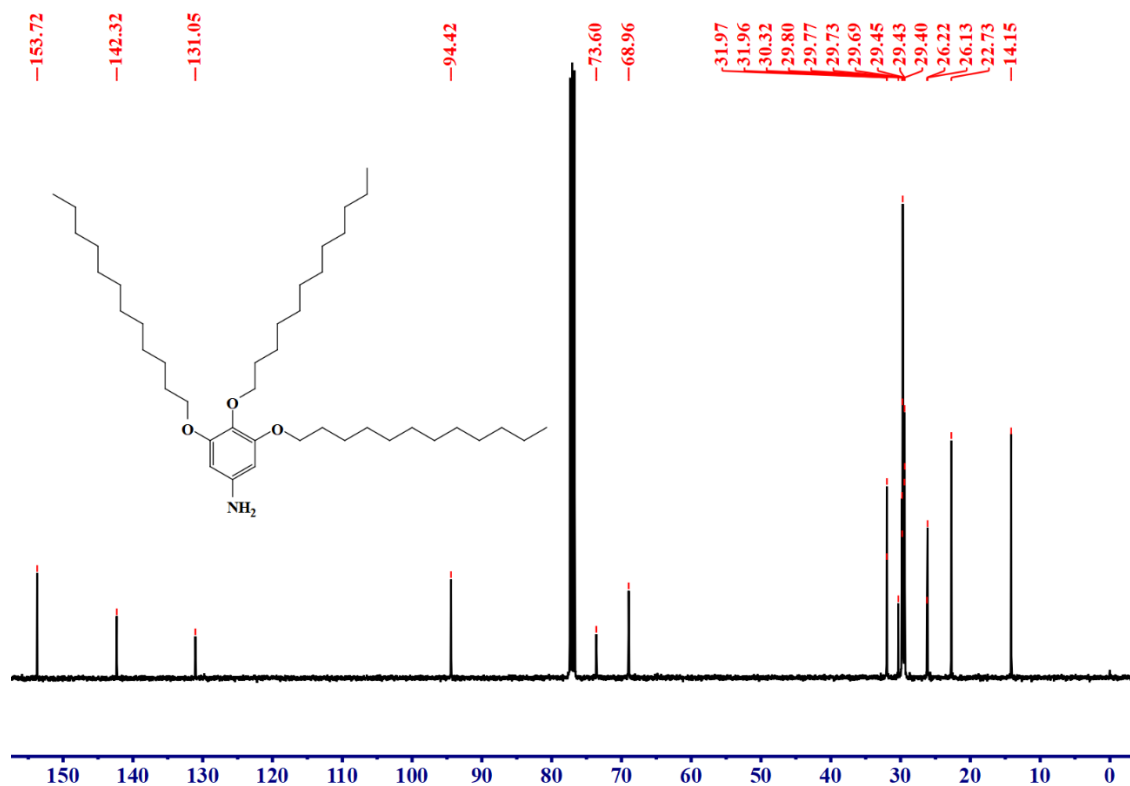


Figure S7. <sup>13</sup>C NMR spectrum of compound 4.

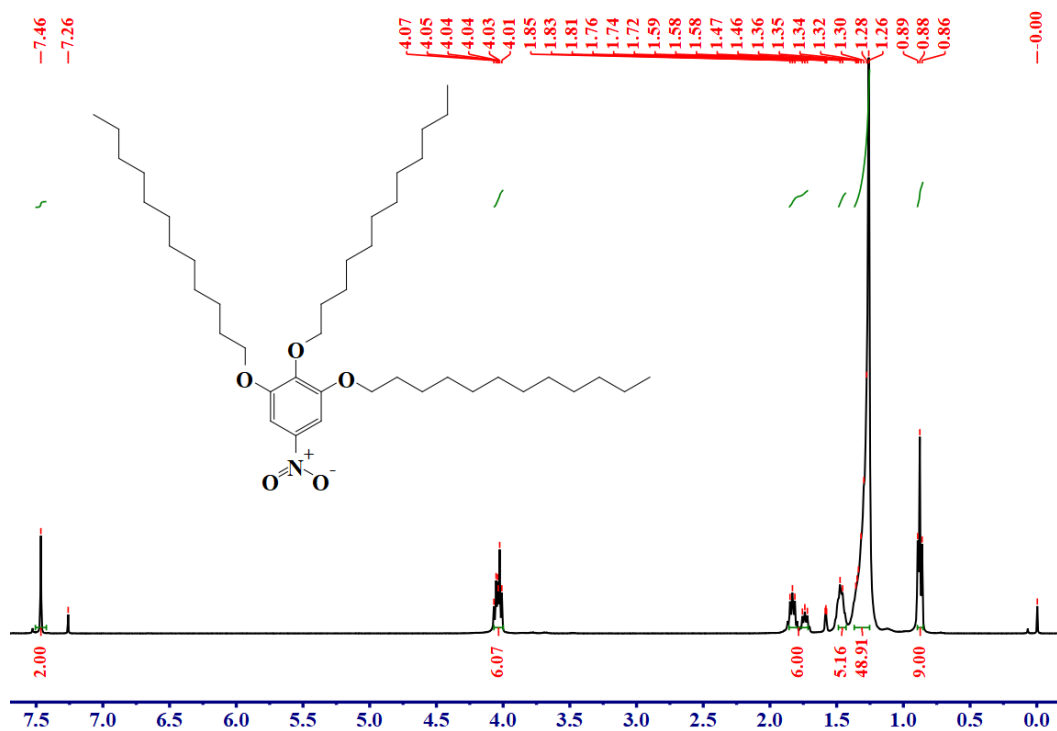


Figure S8. <sup>1</sup>H NMR spectrum of compound 5.

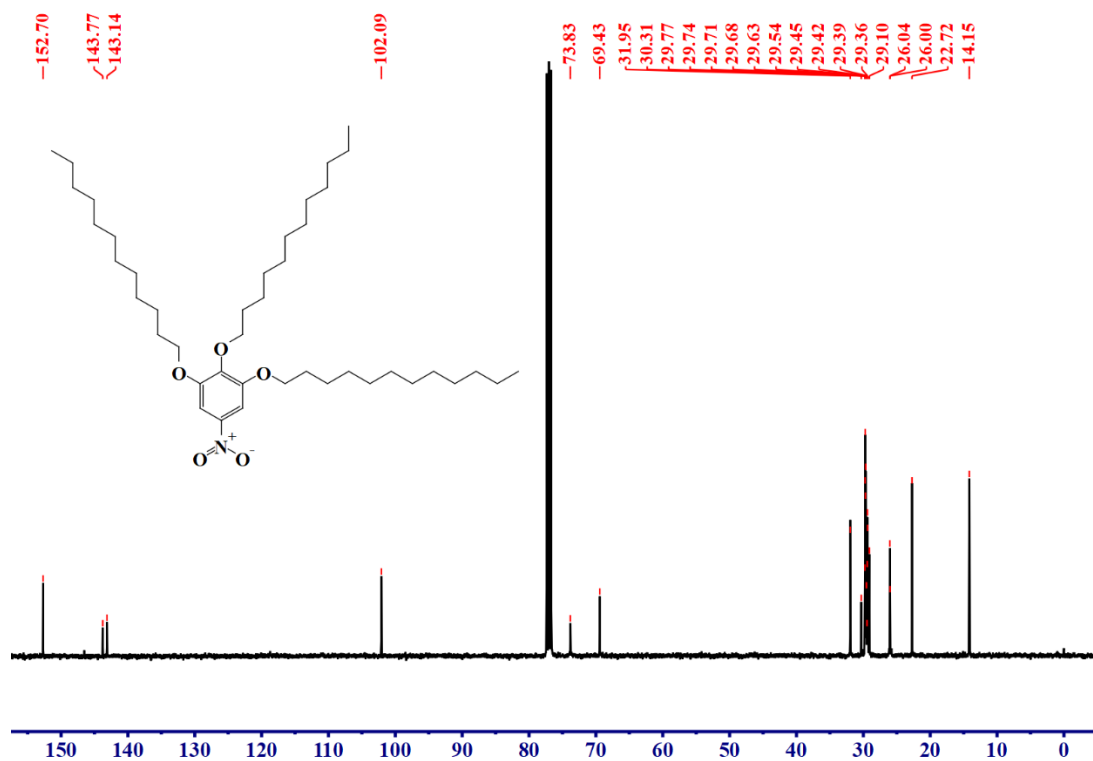


Figure S9. <sup>13</sup>C NMR spectrum of compound 5.

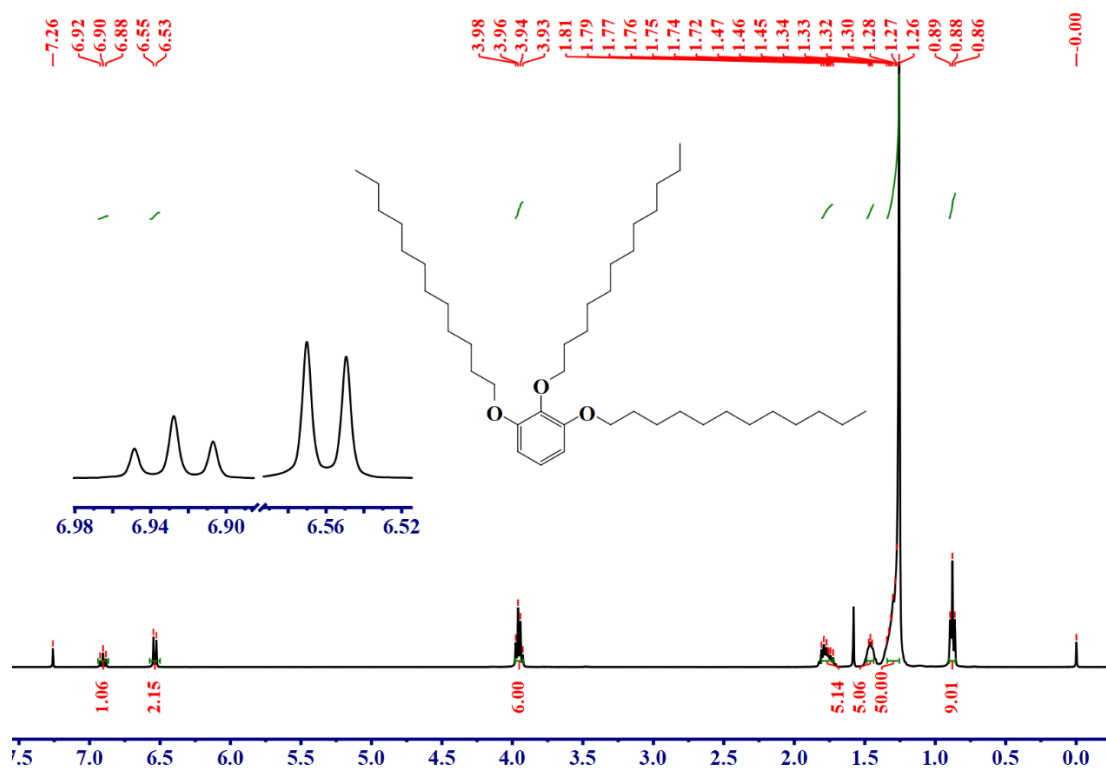


Figure S10. <sup>1</sup>H NMR spectrum of compound 6.

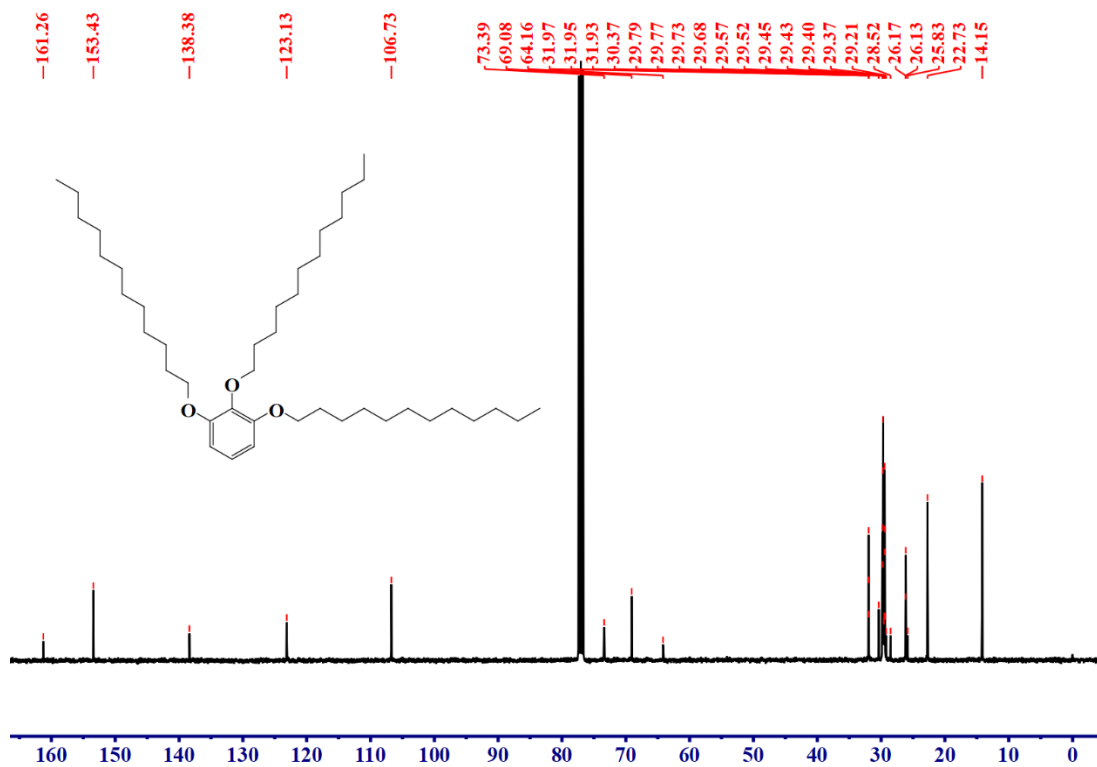


Figure S11. <sup>13</sup>C NMR spectrum of compound 6.

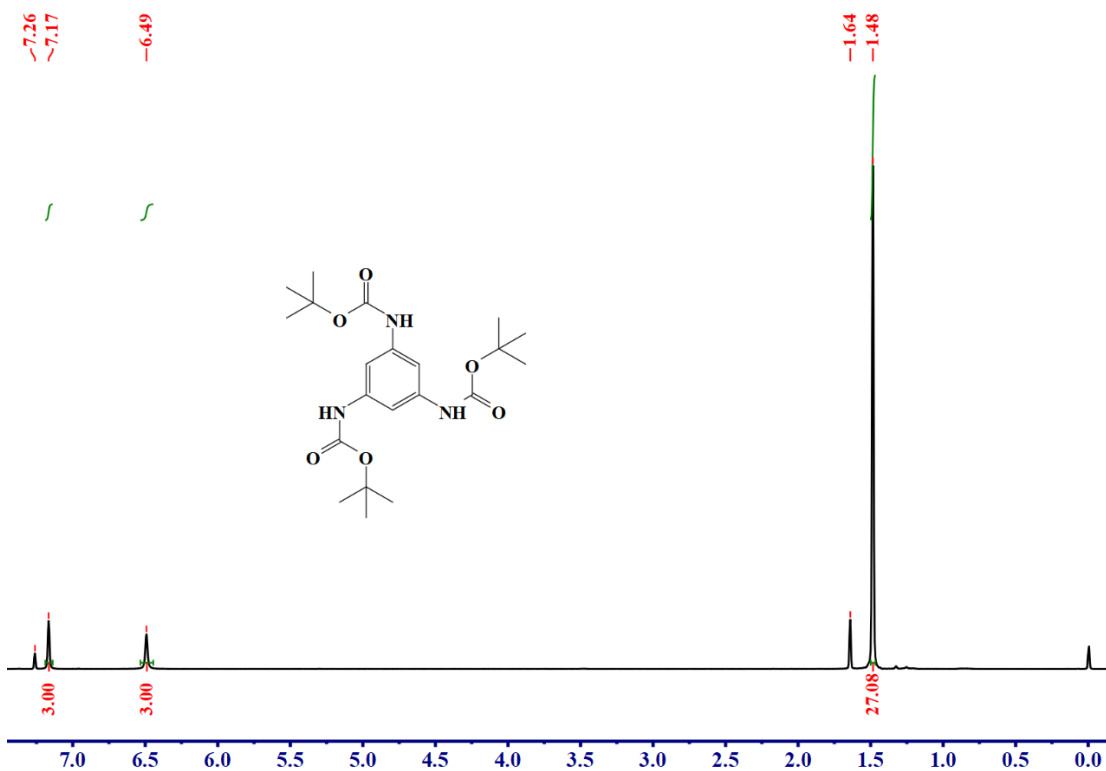


Figure S12. <sup>1</sup>H NMR spectrum of compound 7.

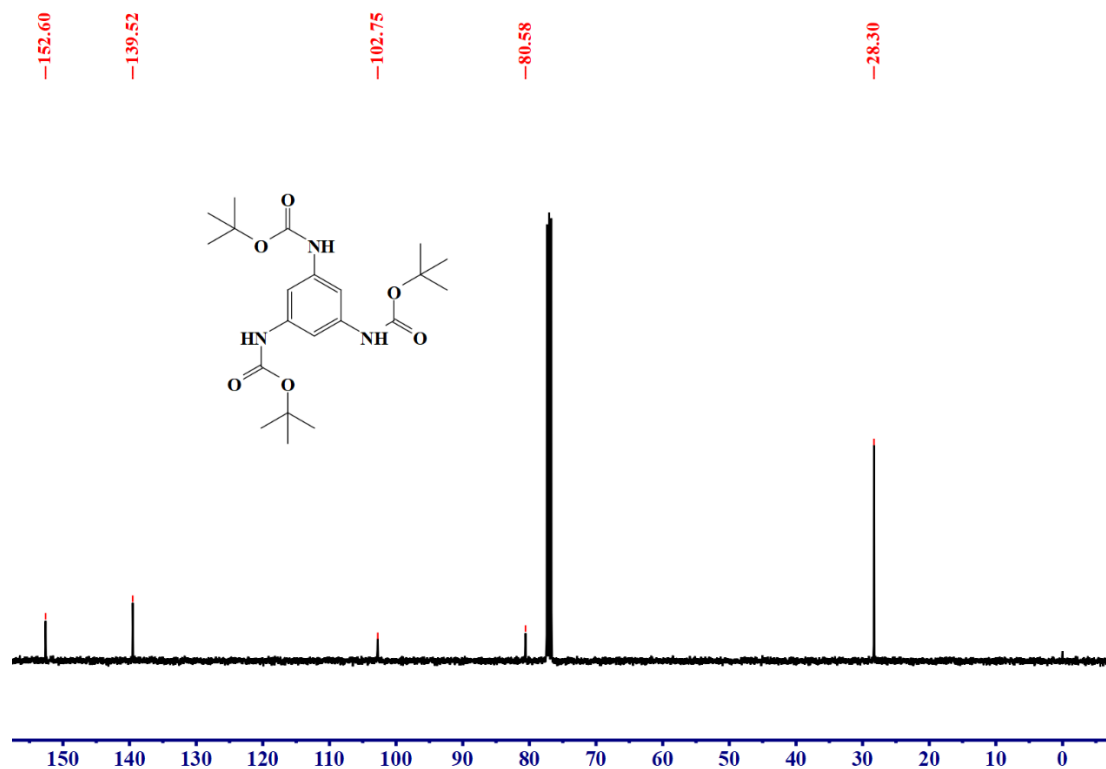


Figure S13. <sup>13</sup>C NMR spectrum of compound 7.

#### 4. HRMS data

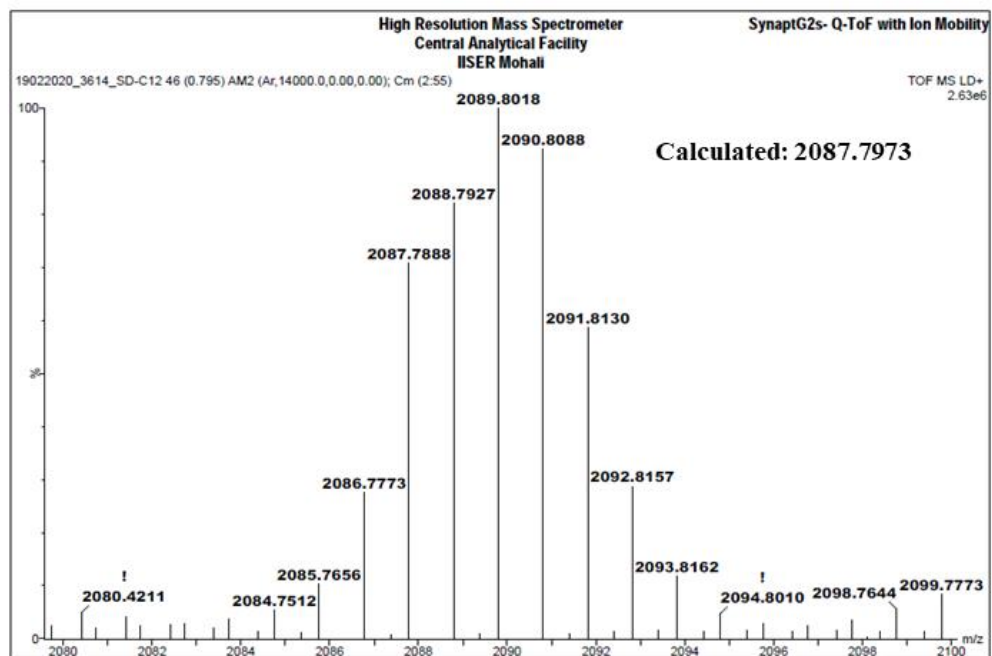
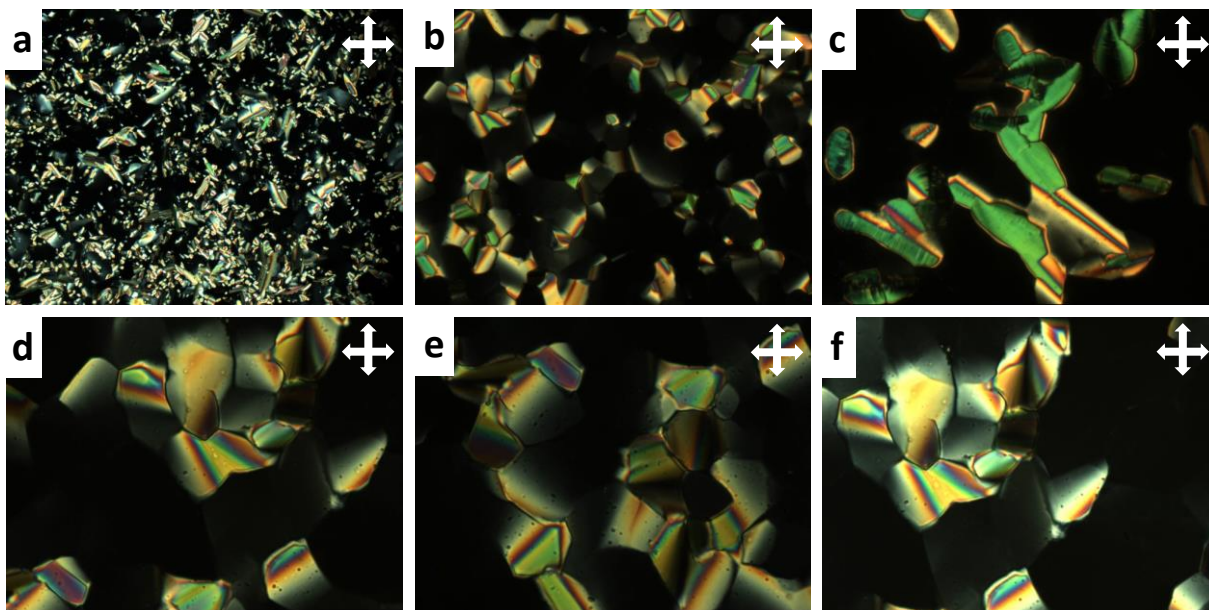


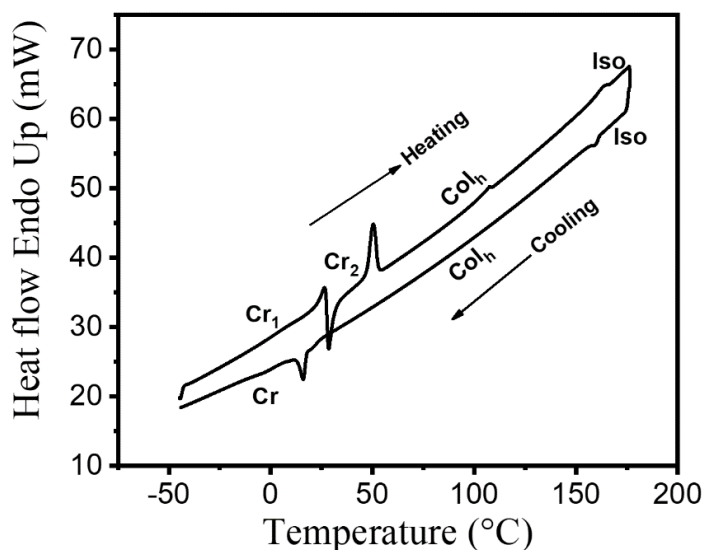
Figure S14. HRMS spectrum of 1.

## 5. Polarized optical images (POM) images



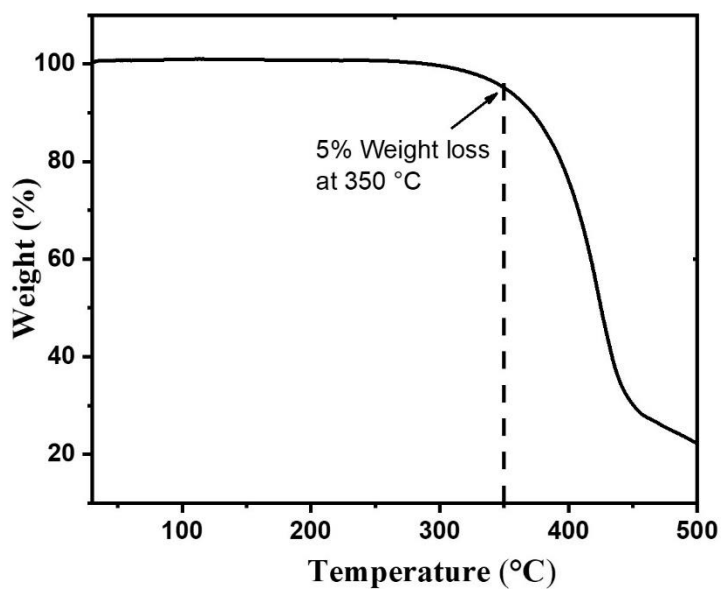
**Figure S15.** POM images of compound **1** under crossed polarizer at (a) 155.4 °C (magnification  $\times 50$ ), (b) 115.9 °C (magnification  $\times 200$ ), (c) 66.6 °C (magnification  $\times 200$ ), (d) 60.5 °C (magnification  $\times 500$ ), (e) 59.1 °C (magnification  $\times 500$ ) (also shown in Figure 1a in main manuscript), and (f) 41.9 °C (magnification  $\times 500$ ), on cooling from isotropic liquid kept between a glass slide and coverslip.

## 6. Differential scanning calorimetry (DSC) thermogram



**Figure S16.** Thermogram from DSC studies with a scanning rate of 10 °C/min of compound **1**.

## 7. Thermogravimetric analysis (TGA) curve



**Figure S17.** TGA curve of compound **1** recorded with heating rate of 10 °C/min under a nitrogen atmosphere.

<b>Table S1.</b> Thermal behaviour of compound <sup>a</sup>			
<b>C</b>	<b>Heating Scan</b>	<b>Cooling Scan</b>	<b><math>T_d^b</math> (°C)</b>
<b>1</b>	Cr <sub>1</sub> 28.5 (24.7) Cr <sub>2</sub> 50.4 (56.4) Col <sub>h</sub> 163.3 (5.8) Iso	Iso 159.5 (4.6) Col <sub>h</sub> 16.0 (27.1) Cr	350
<sup>a</sup> Enthalpy values in parentheses in kJ/mol and temperatures in °C. <sup>b</sup> Decomposition temperature corresponding to 5% weight loss. Abbreviations: C = compound; Cr = crystalline solid; Col <sub>h</sub> = columnar hexagonal; Iso = isotropic liquid.			

## 8. X-ray diffraction studies

<b>Table S2.</b> The following data corresponds to the observed and calculated $d$ -spacings and planes of the diffraction peaks obtained for the hexagonal lattice at 60 °C.					
Col <sub>h</sub> phase with lattice parameter $a = 37.04 \text{ \AA}$					
Miller Indices ( $hk$ )	$d_{\text{obs}} (\text{\AA})^a$	$d_{\text{cal}} (\text{\AA})^b$	Relative Intensity $I(hk)$	Multiplicity	Phase $\Phi(hk)$
<b>10</b>	32.08	32.08	100.00	6	0
<b>11</b>	18.41	18.52	2.97	6	$\pi$
<b>20</b>	15.99	16.04	2.46	6	0
<b>30</b>	10.62	10.69	3.14	6	0
<b>h<sub>a</sub></b>	4.93	Fluid alkyl chain			
<b>h<sub>c</sub></b>	3.69	$\pi$ - $\pi$ interaction			
<sup>a</sup> $d_{\text{obs}}$ : experimental $d$ -spacing. <sup>b</sup> $d_{\text{cal}}$ : calculated $d$ -spacing by using the relation: $\frac{1}{d^2} = \frac{4}{3} \left( \frac{h^2 + hk + k^2}{a^2} \right)$ . h <sub>a</sub> is due to chain-chain correlation. h <sub>c</sub> due to core to core (face to face) correlations.					

**Electron density map:** The procedure for reconstructing the electron density map has been adopted from our previous reports.<sup>1-4</sup> Briefly, we reproduced here for the readers' convenience.

“The electron density  $\rho(x,y)$  of a liquid crystal is related to its structure factor  $F(hk)$  by inverse Fourier transformation,  $\rho(x,y) = \sum_{h,k} F(hk)e^{2\pi i(hx+ky)}$

where  $(hk)$  are the Miller Indices and  $x, y$  are the fractional coordinates of the unit cell.

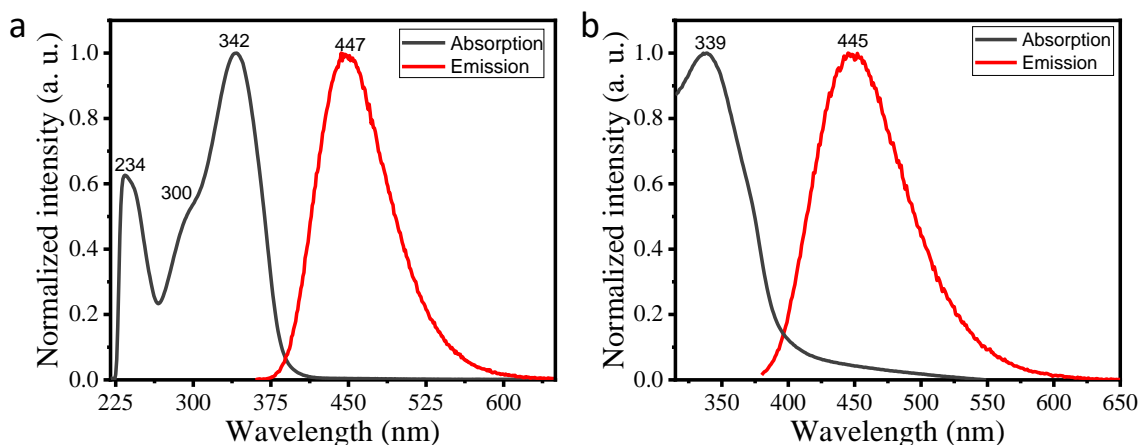
The complex structure factor  $F(hk)$  is equal to the product of the phase  $\Phi(hk)$  and the modulus  $|F(hk)|$  which is proportional to the square root of the intensity  $I(hk)$  of the observed reflection as

$$F(hk) = |F(hk)| e^{i\Phi(hk)} = \sqrt{I(hk)} e^{i\Phi(hk)}$$

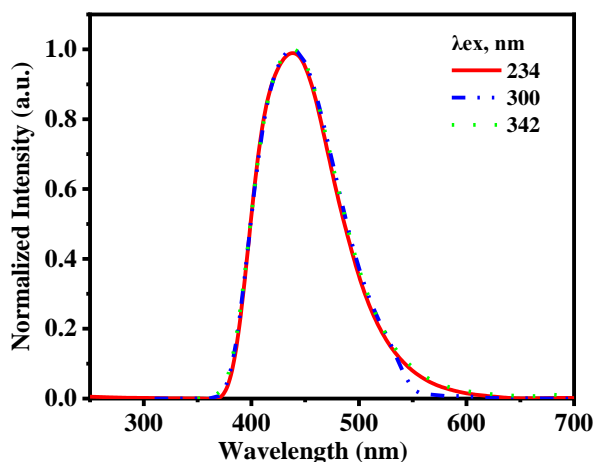
While the intensity  $I(hk)$  can be easily obtained from the X-ray diffraction experiment, the only information that cannot be obtained directly from the experiment is the phase  $\Phi(hk)$  for each diffraction peak. However, this problem becomes easily tractable when the structure under study is centro-symmetric, that is  $\rho(x,y) = \rho(-x,-y)$ , and  $F(hk)$  can only be real hence,  $\phi(hk)$  can only be

0 or  $\pi$ . For non centro-symmetric groups, the phase may take every value between 0 and  $2\pi$ . The observed columnar phases in compound **1** is centro-symmetric and also having few reflections in the small-angle region. Therefore, it is easy to reconstruct electron density maps of all possible phase combinations. The “correct” map is subsequently chosen on the merit of the reconstructed maps and other physical and chemical knowledge of the system such as chemical constituents and their sizes etc.”

## 9. Photophysical, electrochemical and theoretical studies



**Figure S18.** Absorption (left) and emission spectra (right) of compound **1** in (a) solution state (10<sup>-5</sup> M in HPLC DCM); (b) solid-state.



**Figure S19.** Emission spectra of compound **1** (10<sup>-5</sup> M) at different excitation wavelengths.

Relative quantum yield was obtained according to the well-known procedure using quinine sulfate in a 0.1 M H<sub>2</sub>SO<sub>4</sub> solution as the standard. Quantum yield values were calculated according to the following equation:

$$Q_S = Q_R \times \left(\frac{m_S}{m_R}\right) \times \left(\frac{n_S}{n_R}\right)^2$$

Where, Q: Quantum yield, m: the slope of the plot of integrated fluorescence intensity vs. absorbance, n = refractive index (1.407 for THF and 1.33 for distilled water). Subscript R refers to the reference fluorophore i.e., quinine sulfate in 0.1 M H<sub>2</sub>SO<sub>4</sub>, and subscript S refers to the sample under investigation.

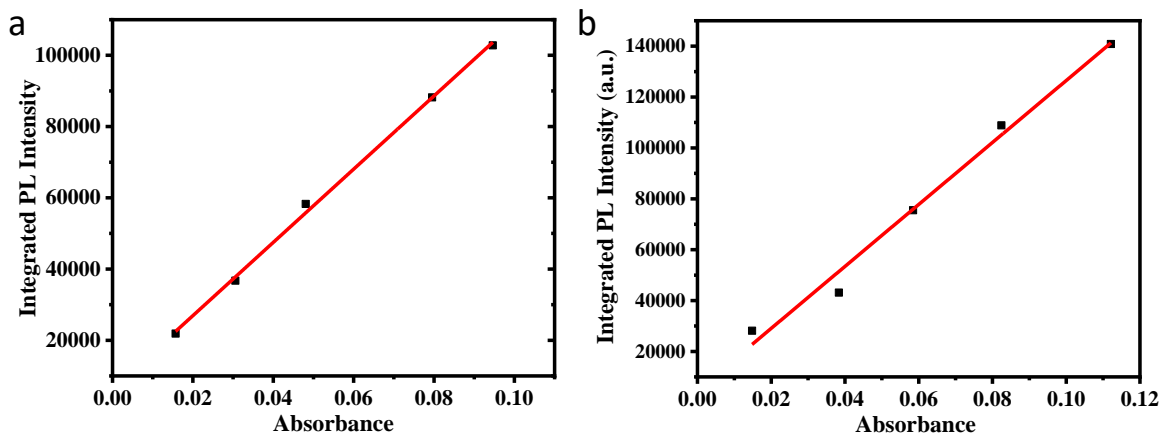
To minimize the re-absorption effects, the absorbance value was kept below 0.15.

The quantum yield of quinine sulfate in 0.1 M H<sub>2</sub>SO<sub>4</sub> solution is 0.54. After substituting the appropriate values, the simplified equation is:

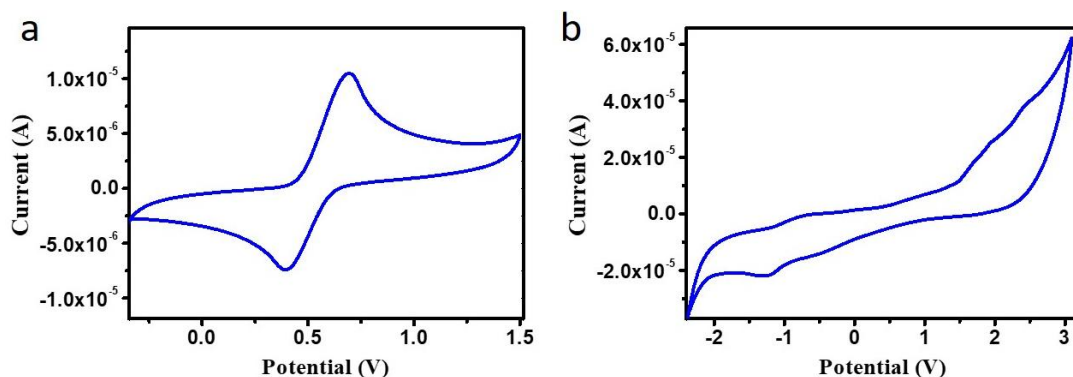
$$Q_S = 0.54 \times \left(\frac{m_S}{m_R}\right) \times \left(\frac{1.407}{1.33}\right)^2$$

$$Q_S = 0.60434 \times \left(\frac{m_S}{m_R}\right)$$

<b>Table S3.</b> Quantum yield measurement. <sup>a,b,c</sup>		
<b>m<sub>S</sub></b>	<b>m<sub>R</sub></b>	<b>Q<sub>S</sub></b>
1.21779 x 10 <sup>6</sup>	1.02802 x 10 <sup>6</sup>	0.716
<sup>a</sup> Measured in THF. <sup>b</sup> Excited at absorption maxima. <sup>c</sup> Standard Quinine sulphate (Q <sub>R</sub> = 0.54) in 0.1 M H <sub>2</sub> SO <sub>4</sub> .		

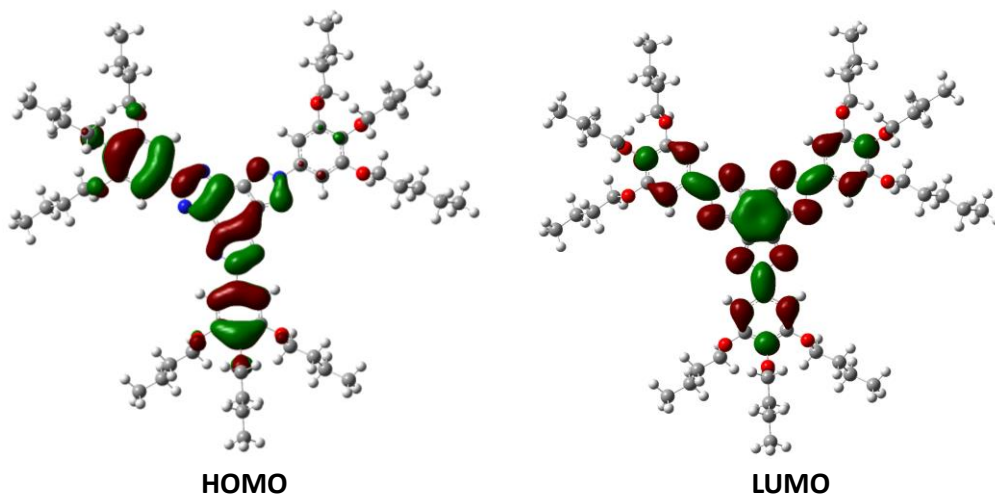


**Figure S20.** Plots of integrated photoluminescence (PL) intensity vs. absorbance of (a) quinine sulfate (0.1 M H<sub>2</sub>SO<sub>4</sub> solution); (b) compound **1**.



**Figure S21.** Cyclic voltammograms of (a) ferrocene; (b) compound **1** in HPLC DCM solution of TBAP (0.1 M) at a scanning rate 50 mVs<sup>-1</sup>.

<b>Table S4.</b> Electrochemical properties of compounds <b>1</b> . <sup>a</sup>							
Mesogen	$\lambda_{\text{onset,UV}}$ (nm)	$\Delta E_{\text{g,UV}}^b$ (eV)	$E_{\text{ox,onset}}$ (V)	$E_{\text{red,onset}}$ (V)	$E_{\text{HOMO}}^c$ (eV)	$E_{\text{LUMO}}^d$ (eV)	$\Delta E_{\text{g,CV}}^e$ (eV)
<b>1</b>	426	2.91	+1.46	-0.89	-5.71	-3.36	2.35
<sup>a</sup> Recorded in DCM solution (mM). Experimental conditions: reference electrode used was Ag/AgNO <sub>3</sub> , counter electrode used was platinum wire, glassy carbon used as working electrode, tetrabutylammonium perchlorate (TBAP) (0.1 M) acts as supporting electrolyte. <sup>b</sup> Optical Band gap obtained from the red edge of the longest wavelength in the UV-vis absorption spectra of thin film, Calculated as: $\Delta E_{\text{g,UV}}$ (optical band gap) = 1240/ $\lambda_{\text{onset,UV}}$ . <sup>c</sup> Estimated from the formula $E_{\text{HOMO}} = -(4.8 - E_{1/2,\text{Fc,Fc}^+} + E_{\text{oxd,onset}})$ eV, where $E_{1/2,\text{Fc,Fc}^+} = 0.55$ V. <sup>d</sup> Obtained from the formula $E_{\text{LUMO}} = -(4.8 - E_{1/2,\text{Fc,Fc}^+} + E_{\text{red,onset}})$ eV. <sup>e</sup> Electrochemical band gap: $\Delta E_{\text{g,CV}} = E_{\text{LUMO}} - E_{\text{HOMO}}$ .							



**Figure S22.** Frontier molecular orbitals of a homologue of compound **1** with R = C<sub>4</sub>H<sub>9</sub>, obtained by DFT calculations at B3LYP/6-31G (d,p) level of theory.

## **10. Mobility studies by space charge limited current (SCLC) technique**

### **10.1 Sample fabrication**

SCLC cells for electron and hole mobility measurement were fabricated using patterned ITO (Xinyan Technologies, Taiwan,  $15 \Omega/\text{cm}^2$ ) and Gold (Au) Electrodes. Patterned ITO substrates were first sequentially cleaned for 20 min each using 10% soap solution (Hellmanex<sup>TM</sup> III, Sigma Aldrich), distilled water, acetone, and isopropyl alcohol (IPA) in an ultrasonicator.  $\text{Cs}_2\text{CO}_3$  spin-coated (3 mg/ml in 2 methoxy ethanol, annealed at 120 °C for 10 min, 4500 rpm for 60 sec) ITO substrates were used to fabricate 3- 4  $\mu\text{m}$  thick cells for electron mobility measurement using mylar sheet. However, for hole mobility extraction in SCLC, Au electrodes were found suitable with the reported compound as both Au work function and HOMO level of the material were found suitable to obtain Ohmic contact. UV ozone (Nova Scan PSD- Pro Series) treated ITO substrate was used as a counter electrode in SCLC cells of hole mobility to ensure minimal or no contribution from electrons in charge carrier mobility. Au electrodes were prepared by sputtering unit (Tecport sputtering unit) using a mask during sputtering of 10 nm Ti/Ni followed by 100 nm of Au. Before cell fabrication, 20 min UV ozone was performed on both FTO and Au electrodes. The thickness of different cells was measured from the interference maxima and minima in the visible to NIR region by recording the transmitted light using Perkin Elmer (Lambda 35) UV-vis spectrophotometer. The thicknesses of samples used in this work were ranging from 3 to 5  $\mu\text{m}$ . The active area of the cells was 4  $\text{mm}^2$ . SCLC cells were filled using a capillary technique by melting the compound above (+15 °C) their isotropic transition temperature (well below decomposition temperature). Once filled, samples were allowed to cool down slowly to room temperature. Current-voltage (*J-V*) characteristics and dielectric constant (from 1 kHz to 2 MHz) was measured using Keithley 2436 B dual-channel source meter.

### **10.2 Space charge limited current (SCLC) technique**

Space charge limited current (SCLC) technique details for *J-V* characterization and subsequently mobility extraction is similar to as mentioned in our earlier published papers and reproduced below for the reader's convenience.<sup>8</sup>

“In SCLC measurement at low applied voltages, the current is a linear function of voltage (current follows the Ohm’s law) and the resistive behavior is Ohmic which is given by the following equation:

$$J = ne\mu \frac{V}{d} \quad (a)$$

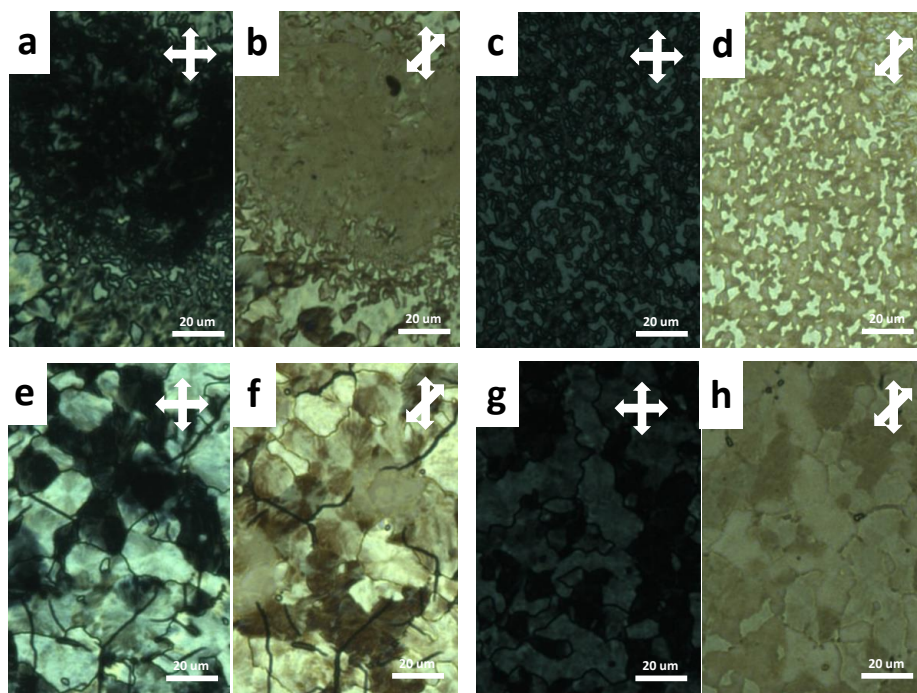
where  $J$  is the current density,  $n$  is the charge carrier density,  $e$  is the elementary charge,  $\mu$  is the charge carrier drift mobility,  $V$  is the applied voltage and  $d$  is the thickness of the sample.

At higher voltages, when the applied voltage crosses the threshold voltage ( $V_T$ ), the space charge builds up takes place across the sample due to injected charges and the voltage dependence of the current can be approximated by the Mott-Gurney equation given by:

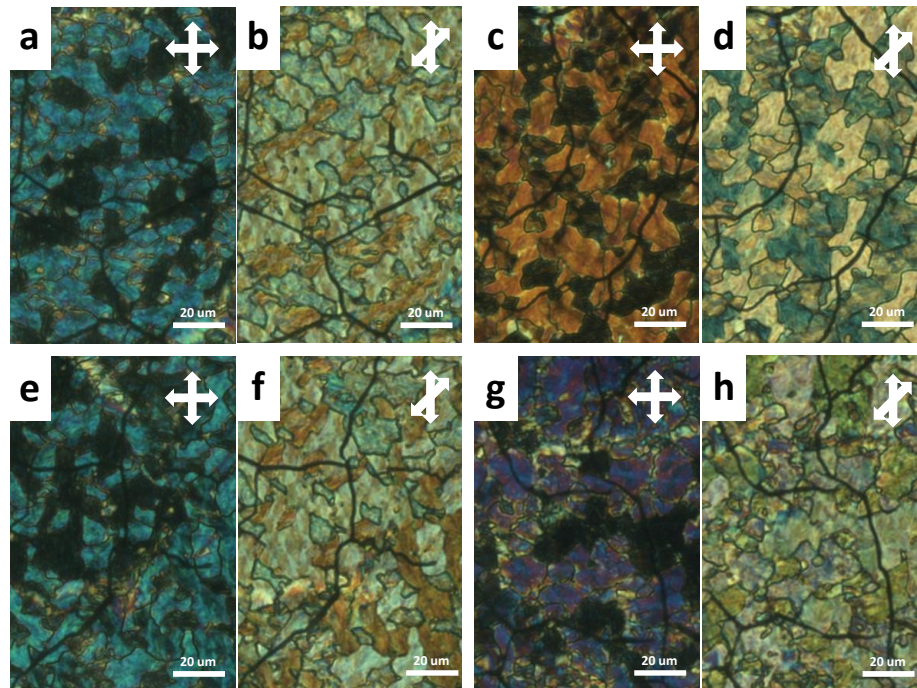
$$J = \frac{9}{8} \epsilon \epsilon_0 \mu \frac{V^2}{d^3} \quad (b)$$

where  $\epsilon_0$  is the free space permittivity and  $\epsilon$  is the relative dielectric constant of the material. By knowing the thickness ( $d$ ) and dielectric constant ( $\epsilon$ ) of the samples we can calculate the mobility.”

<b>Table S5.</b> Statistic table of all mobility values (hole and electron) for compound <b>1</b> .		
<b>Device No.</b>	<b><math>\mu_e</math> (cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup>)</b>	<b><math>\mu_h</math> (cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup>)</b>
<b>1</b>	2.71 x 10 <sup>-3</sup>	1.49 x 10 <sup>-6</sup>
<b>2</b>	2.47 x 10 <sup>-3</sup>	7.38 x 10 <sup>-7</sup>
<b>3</b>	1.71 x 10 <sup>-3</sup>	2.05 x 10 <sup>-6</sup>
<b>4</b>	1.09 x 10 <sup>-3</sup>	1.57 x 10 <sup>-6</sup>
<b>5</b>	1.26 x 10 <sup>-3</sup>	1.21 x 10 <sup>-6</sup>
<b>6</b>	1.61 x 10 <sup>-2</sup> §	1.06 x 10 <sup>-6</sup>
<b>Average</b>	1.85 x 10 <sup>-3</sup>	1.38 x 10 <sup>-6</sup>
<b>Std. Dev.</b>	0.719 x 10 <sup>-3</sup>	0.504 x 10 <sup>-6</sup>
<b>Final</b>	(1.85 ± 0.72) x 10 <sup>-3</sup>	(1.38 ± 0.50) x 10 <sup>-6</sup>
§Champion Device is not included in Averaging and Std. Deviation calculation		



**Figure S23.** POM textures obtained in electron-only SCLC cell under crossed polarizer (a, c, e, g) at 90° angle & (b, d, f, h) at 45° angle for compound **1**.



**Figure S24.** POM textures obtained in hole-only SCLC cell under crossed polarizer (a, c, e, g) at 90° angle & (b, d, f, h) at 45° angle for compound **1**.

## 11. References

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