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## 1. Synthesis and Characterization

Melting points were taken on Opti-Melt (Automated melting point system). The FT-IR spectra were recorded as KBr pellet on Shimadzu in the range of 3800-600  $\text{cm}^{-1}$ . Microanalysis was performed on Perkin-Elmer PE 2400 CHN analyser. The texture images were studied on a trinocular optical polarising microscope (POM) equipped with a heating stage.  $^1\text{H}$  NMR spectra and  $^{13}\text{C}$  NMR was recorded on a 400 MHz in Bruker Advance 400 in the range of 0.5 ppm-16 ppm using  $\text{CDCl}_3$  solvent. Thermo gravimetric analysis (TGA) was performed using a Perkin Elmer-STA 6000 apparatus under high purity nitrogen. Mass Spectrometry was carried out using High Resolution Mass Spectrometer. The phase transition temperatures were measured using Shimadzu DSC-50 at heating and cooling rates of  $10^\circ\text{C min}^{-1}$ . The samples were heated from room temperature to  $550^\circ\text{C}$  at  $10^\circ\text{C/min}$ . X-ray diffraction (XRD) measurements were performed on a Rigaku-Ultima IV powder diffractometer equipped with a  $\text{Cu K}\alpha$  source ( $\lambda = 1.5418 \text{ \AA}$  and 1.6 kW, X-ray tube with applied voltage and current values as 40 kV and 30 mA power) and also Philips X'PERT MPD. The absorption spectra were studied by using Jasco V-570 UV-Vis recording spectrophotometer with a variable wavelength between 200 and 800 nm. The fluorescence spectra were recorded on a Jasco FP-6500 spectrofluorometer. Cyclic voltammetry (CV) experiments were performed on a CH Instruments electrochemical workstation. The reference electrode was calibrated with the ferrocene/ferrocenium ( $\text{Fc/Fc}^+$ ) redox couple (absolute energy level of  $-4.80 \text{ eV}$  to vacuum).

### Preparation of 3,6-diamino-9H-carbazole (2)

3,6-diamino-9H-carbazole (**2**) was synthesized by refluxing the reaction mixture of 3,6-dinitro-9H-carbazole (**1**) with 10% Pd/C in methanol and glacial acetic acid was hydrogenated at atmospheric pressure under a balloon for 6 h.<sup>1</sup> Yield 79 %, FT-IR (KBr) in  $\text{cm}^{-1}$ : 3303, 2918,

2850, 1240, 1126.  $^1\text{H}$  NMR  $\text{CDCl}_3$  (400 MHz): 7.41 (s, 2H, Ar), 6.96 (d, 2H, Ar), 7.86 (d, 2H, Ar), 8.43 (s, 1H, -NH), 4.62 (s, 4H, -NH<sub>2</sub>).  $^{13}\text{C}$  NMR: 144.6, 131.2, 113.2, 106.4, 101.3.

### **Preparation of 3,4,5-trihexyloxy benzaldehyde (3a)**

3,4,5-trihexyloxy benzaldehyde (**3a**) was synthesized by refluxing the reaction mixture of 3,4,5-trihydroxy benzaldehyde (1 equiv.) with hexyl bromide (3 equiv.) and anhydrous  $\text{K}_2\text{CO}_3$  (3 equiv.) in dry acetone for 2 hr.<sup>2</sup> Yield 86 %, FT-IR (KBr) in  $\text{cm}^{-1}$ : 2970, 2861, 1664, 1234, 876, 771.  $^1\text{H}$  NMR  $\text{CDCl}_3$  (400 MHz): 0.89 (t, 9H,  $\text{CH}_3$ ), 1.26-1.47 (m, 18H,  $\text{CH}_2$ ), 1.71 (p, 6H,  $\text{CH}_2$ ), 4.06 (t, 6H,  $\text{CH}_2$ ), 7.10 (s, 2H, Ar), 10.03 (s, 1H, CHO).  $^{13}\text{C}$  NMR: 177.6, 164.1, 144.6, 108.1, 77.8, 31.4, 29.8, 22.7.

### **Preparation of 3,4,5-trioctyloxy benzaldehyde (3b)**

3,4,5-trioctyloxy benzaldehyde (**3b**) was synthesized by refluxing the reaction mixture of 3,4,5-trihydroxy benzaldehyde (1 equiv.) with octyl bromide (3 equiv.) and anhydrous  $\text{K}_2\text{CO}_3$  (3 equiv.) in dry acetone for 2 hr.<sup>2</sup> Yield 82 %, FT-IR (KBr) in  $\text{cm}^{-1}$ : 2943, 2801, 1660, 1234, 872, 776, 663.  $^1\text{H}$  NMR  $\text{CDCl}_3$  (400 MHz): 0.89 (t, 9H,  $\text{CH}_3$ ), 1.26-1.47 (m, 30 H,  $\text{CH}_2$ ), 1.71 (p, 6H,  $\text{CH}_2$ ), 4.06 (t, 6H,  $\text{CH}_2$ ), 7.10 (s, 2H, Ar), 10.03 (s, 1H, CHO).  $^{13}\text{C}$  NMR: 177.6, 164.1, 144.6, 141.5, 108.1, 77.8, 31.4, 29.8, 22.7, 19.4.

### **Preparation of 3,4,5-tridecyloxy benzaldehyde (3c)**

3,4,5-tridecyloxy benzaldehyde (**3c**) was synthesized by refluxing the reaction mixture of 3,4,5-trihydroxy benzaldehyde (1 equiv.) with decyl bromide (3 equiv.) and anhydrous  $\text{K}_2\text{CO}_3$  (3 equiv.) in dry acetone for 2 hr.<sup>2</sup> Yield 87 %, FT-IR (KBr) in  $\text{cm}^{-1}$ : 2905, 2867, 1650, 1442, 1210, 1120, 872, 776, 663.  $^1\text{H}$  NMR  $\text{CDCl}_3$  (400 MHz): 0.89 (t, 9H,  $\text{CH}_3$ ), 1.26-1.47 (m, 42 H,  $\text{CH}_2$ ),

1.71 (p, 6H, CH<sub>2</sub>), 4.08 (t, 6H, CH<sub>2</sub>), 7.34 (s, 2H, Ar), 10.06 (s, 1H, CHO). <sup>13</sup>C NMR: 177.6, 164.1, 144.6, 141.5, 108.1, 77.8, 31.4, 29.8, 22.7, 19.4.

#### **Preparation of 3,4,5-tridodecyloxy benzaldehyde (3d)**

3,4,5-tridodecyloxy benzaldehyde (**3d**) was synthesized by refluxing the reaction mixture of 3,4,5-trihydroxy benzaldehyde (1 equiv.) with decyl bromide (3 equiv.) and anhydrous K<sub>2</sub>CO<sub>3</sub> (3 equiv.) in dry acetone for 2 hr.<sup>2</sup> Yield 78 %, FT-IR (KBr) in cm<sup>-1</sup>: 2915, 2867, 1640, 1440, 1212, 1121, 821, 756, 663, 632. <sup>1</sup>H NMR CDCl<sub>3</sub> (400 MHz): 0.89 (t, 9H, CH<sub>3</sub>), 1.26-1.47 (m, 48 H, CH<sub>2</sub>), 1.71 (p, 6H, CH<sub>2</sub>), 4.08 (t, 6H, CH<sub>2</sub>), 7.34 (s, 2H, Ar), 10.06 (s, 1H, CHO). <sup>13</sup>C NMR: 177.6, 164.1, 144.6, 141.5, 108.1, 77.8, 31.4, 29.8, 22.7, 19.4.

#### **Preparation of 9H-Carbazole-bis-(trihexyloxy phenyl schiff-base) (4a)**

9H-Carbazole-bis-(trihexyloxy phenyl schiff-base) (**4a**) was synthesized by refluxing the reaction mixture of 9H-Carbazole-bis-(trihexyloxy phenyl schiff-base) (**2**) (1 equiv.) with 3,4,5-trihexyloxy benzaldehyde (**3a**) (2 equiv.) in ethanol with presence of few drops of acetic acid for 3 hr.<sup>3</sup> Yield 72 %, FT-IR (KBr) in cm<sup>-1</sup>: 3321, 3068, 2906, 2860, 1440, 1241, 884, 761. <sup>1</sup>H NMR CDCl<sub>3</sub> (400 MHz): 0.89 (t, 18H, CH<sub>3</sub>), 1.36-1.46 (m, 36H, CH<sub>2</sub>), 1.71 (p, 12H, CH<sub>2</sub>), 4.04 (t, 12H, CH<sub>2</sub>), 7.22 (d, 4H, Ar), 7.43 (s, 2H, Ar), 6.41 (s, 2H, Ar), 7.61 (s, 2H, Ar), 8.08 (s, 2H, -CH=N), 8.62 (s, 1H, -NH). <sup>13</sup>C NMR: 166.4, 144.6, 140.8, 133.4, 131.2, 112.8, 108.3, 73.6, 31.8, 29.6.

#### **Preparation of 9H-Carbazole-bis-(trioctyloxy phenyl schiff-base) (4b)**

9H-Carbazole-bis-(trioctyloxy phenyl schiff-base) (**4b**) was synthesized by refluxing the reaction mixture of 9H-Carbazole-bis-(trihexyloxy phenyl schiff-base) (**2**) (1 equiv.) with 3,4,5-

trioctyloxy benzaldehyde (**3b**) (2 equiv.) in ethanol with presence of few drops of acetic acid for 3 hr.<sup>3</sup> Yield 76 %, FT-IR (KBr) in  $\text{cm}^{-1}$ : 3320, 3018, 2936, 2861, 1430, 1240, 896, 760, 664.  $^1\text{H}$  NMR  $\text{CDCl}_3$  (400 MHz): 0.89 (t, 18H,  $\text{CH}_3$ ), 1.36-1.46 (m, 52H,  $\text{CH}_2$ ), 1.73 (p, 12H,  $\text{CH}_2$ ), 4.04 (t, 12H,  $\text{CH}_2$ ), 7.22 (d, 4H,  $J = 6$  Hz, Ar), 7.43 (s, 2H,  $J = 2.6$  Hz, Ar), 6.41 (s, 2H,  $J = 2.4$  Hz, Ar), 7.63 (s, 2H, Ar), 8.10 (s, 2H,  $-\text{CH}=\text{N}$ ), 8.61 (s, 1H,  $-\text{NH}$ ).  $^{13}\text{C}$  NMR: 166.4, 144.6, 140.8, 133.4, 131.2, 114.7, 112.8, 108.3, 73.6, 31.6, 29.6.

#### **Preparation of 9H-Carbazole-bis-(tridecyloxy phenyl schiff-base) (4c)**

9H-Carbazole-bis-(tridecyloxy phenyl schiff-base) (**4c**) was synthesized by refluxing the reaction mixture of 9H-Carbazole-bis-(trihexyloxy phenyl schiff-base) (**2**) (1 equiv.) with 3,4,5-trioctyloxy benzaldehyde (**3c**) (2 equiv.) in ethanol with presence of few drops of acetic acid for 3 hr.<sup>3</sup> Yield 78 %, FT-IR (KBr) in  $\text{cm}^{-1}$ : 3321, 3018, 2930, 2836, 1440, 1241, 890, 730, 668.  $^1\text{H}$  NMR  $\text{CDCl}_3$  (400 MHz): 0.89 (t, 18H,  $\text{CH}_3$ ), 1.36-1.46 (m, 62H,  $\text{CH}_2$ ), 1.73 (p, 12H,  $\text{CH}_2$ ), 4.04 (t, 12H,  $\text{CH}_2$ ), 7.21 (d, 4H,  $J = 6.2$  Hz, Ar), 7.44 (s, 2H,  $J = 2.8$  Hz, Ar), 6.84 (s, 2H,  $J = 2.6$  Hz, Ar), 7.63 (s, 2H, Ar), 8.12 (s, 2H,  $-\text{CH}=\text{N}$ ), 8.61 (s, 1H,  $-\text{NH}$ ).  $^{13}\text{C}$  NMR: 166.4, 144.6, 140.8, 133.4, 131.2, 114.7, 112.8, 108.3, 73.6, 31.6, 29.6.

#### **Preparation of 9H-Carbazole-bis-(tridodecyloxy phenyl schiff-base) (4d)**

9H-Carbazole-bis-(tridodecyloxy phenyl schiff-base) (**4d**) was synthesized by refluxing the reaction mixture of 9H-Carbazole-bis-(trihexyloxy phenyl schiff-base) (**2**) (1 equiv.) with 3,4,5-trioctyloxy benzaldehyde (**3d**) (2 equiv.) in ethanol with presence of few drops of acetic acid for 3 hr.<sup>3</sup> Yield 69 %, FT-IR (KBr) in  $\text{cm}^{-1}$ : 3330, 3018, 2930, 2861, 1430, 1240, 896, 734, 661.  $^1\text{H}$  NMR  $\text{CDCl}_3$  (400 MHz): 0.89 (t, 18H,  $\text{CH}_3$ ), 1.36-1.46 (m, 74H,  $\text{CH}_2$ ), 1.71 (p, 12H,  $\text{CH}_2$ ), 4.04 (t, 12H,  $\text{CH}_2$ ), 7.22 (d, 4H,  $J = 6$  Hz, Ar), 7.43 (s, 2H,  $J = 2.6$  Hz, Ar), 6.41 (s, 2H,  $J = 2.4$  Hz,

Ar), 7.67 (s, 2H, Ar), 8.12 (s, 2H, -CH=N), 8.63 (s, 1H, -NH).  $^{13}\text{C}$  NMR: 166.4, 144.6, 140.8, 133.4, 131.2, 114.7, 112.8, 108.3, 73.6, 31.6, 29.6.

**Preparation of 4,4'-(bis (trihexyloxy benzyldiene amino)-9H-carbazole-9-yl) benzaldehyde (5a)**

4,4'-(bis (trihexyloxy benzyldiene amino)-9H-carbazole-9-yl) benzaldehyde (**5a**) were prepared by the Ullman reaction of compound (**4a**) with 4-bromo benzaldehyde in 1,2-dichloro benzene solution in the presence of anhydrous  $\text{K}_2\text{CO}_3$  and CuI catalyst at  $180^\circ\text{C}$  for 18 h.<sup>4</sup> Yield 71 %, FT-IR (KBr) in  $\text{cm}^{-1}$ : 3018, 2930, 2861, 1630, 1430, 1310, 1240, 891, 734, 668.  $^1\text{H}$  NMR  $\text{CDCl}_3$  (400 MHz): 0.89 (t, 18H,  $\text{CH}_3$ ), 1.36-1.46 (m, 36H,  $\text{CH}_2$ ), 1.71 (p, 12H,  $\text{CH}_2$ ), 4.04 (t, 12H,  $\text{CH}_2$ ), 7.58 (d, 4H,  $J = 6.2$  Hz, Ar), 7.83 (s, 2H,  $J = 2.8$  Hz, Ar), 6.41 (s, 2H,  $J = 3.6$  Hz, Ar), 7.67 (s, 2H,  $J = 6.0$  Hz, Ar), 7.22-7.26 (s, 4H, Ar), 8.10 (s, 2H, -CH=N), 9.13 (s, 1H, -CHO).  $^{13}\text{C}$  NMR: 171.5, 166.4, 146.6, 133.7, 129.9, 126.2, 114.7, 112.8, 108.3, 73.6, 69.0, 31.6, 25.6.

**Preparation of 4,4'-(bis (trioctyloxy benzyldiene amino)-9H-carbazole-9-yl) benzaldehyde (5b)**

4,4'-(bis (trioctyloxy benzyldiene amino)-9H-carbazole-9-yl) benzaldehyde (**5b**) were prepared by the Ullman reaction of compound (**4b**) with 4-bromo benzaldehyde in 1,2-dichloro benzene solution in the presence of anhydrous  $\text{K}_2\text{CO}_3$  and CuI catalyst at  $180^\circ\text{C}$  for 18 h.<sup>4</sup> Yield 74 %, FT-IR (KBr) in  $\text{cm}^{-1}$ : 3018, 2932, 2860, 1630, 1440, 1310, 1240, 891, 734, 634.  $^1\text{H}$  NMR  $\text{CDCl}_3$  (400 MHz): 0.89 (t, 18H,  $\text{CH}_3$ ), 1.36-1.46 (m, 52H,  $\text{CH}_2$ ), 1.73 (p, 12H,  $\text{CH}_2$ ), 4.06 (t, 12H,  $\text{CH}_2$ ), 7.54 (d, 4H,  $J = 6.4$  Hz, Ar), 7.81 (s, 2H,  $J = 2.8$  Hz, Ar), 6.47 (s, 2H,  $J = 3.8$  Hz, Ar), 7.67 (s, 2H,  $J = 6.0$  Hz, Ar), 7.22-7.26 (s, 4H, Ar), 8.12 (s, 2H, -CH=N), 9.10 (s, 1H, -CHO).  $^{13}\text{C}$  NMR: 171.5, 166.4, 146.6, 133.7, 129.9, 126.2, 114.7, 112.8, 108.3, 73.6, 69.1, 31.8, 25.6.

**Preparation of 4,4'-(bis (tridecyloxy benzylidene amino)-9H-carbazole-9-yl) benzaldehyde (5c)**

4,4'-(bis (tridecyloxy benzylidene amino)-9H-carbazole-9-yl) benzaldehyde (**5c**) were prepared by the Ullman reaction of compound (**4c**) with 4-bromo benzaldehyde in 1,2-dichloro benzene solution in the presence of anhydrous  $K_2CO_3$  and CuI catalyst at  $180^\circ C$  for 18 h.<sup>4</sup> Yield 67 %, FT-IR (KBr) in  $cm^{-1}$ : 3018, 2932, 2860, 1630, 1460, 1320, 1243, 896, 734, 710, 639.  $^1H$  NMR  $CDCl_3$  (400 MHz): 0.89 (t, 18H,  $CH_3$ ), 1.36-1.46 (m, 62H,  $CH_2$ ), 1.73 (p, 12H,  $CH_2$ ), 4.06 (t, 12H,  $CH_2$ ), 7.57 (d, 4H,  $J = 6.4$  Hz, Ar), 7.82 (s, 2H,  $J = 2.8$  Hz, Ar), 6.32 (s, 2H,  $J = 3.8$  Hz, Ar), 7.67 (s, 2H,  $J = 6.0$  Hz, Ar), 7.22-7.24 (s, 4H, Ar), 8.10 (s, 2H,  $-CH=N$ ), 9.12 (s, 1H,  $-CHO$ ).  $^{13}C$  NMR: 171.5, 166.4, 146.6, 133.3, 129.8, 126.2, 114.7, 112.8, 108.3, 73.2, 69.4, 31.6, 25.6.

**Preparation of 4,4'-(bis (tridodecyloxy benzylidene amino)-9H-carbazole-9-yl) benzaldehyde (5d)**

4,4'-(bis (tridodecyloxy benzylidene amino)-9H-carbazole-9-yl) benzaldehyde (**5d**) were prepared by the Ullman reaction of compound (**5d**) with 4-bromo benzaldehyde in 1,2-dichloro benzene solution in the presence of anhydrous  $K_2CO_3$  and CuI catalyst at  $180^\circ C$  for 18 h.<sup>4</sup> Yield 64 %, FT-IR (KBr) in  $cm^{-1}$ : 3018, 2932, 2860, 1630, 1440, 1310, 1240, 891, 734, 634.  $^1H$  NMR  $CDCl_3$  (400 MHz): 0.89 (t, 18H,  $CH_3$ ), 1.36-1.46 (m, 74H,  $CH_2$ ), 1.73 (p, 12H,  $CH_2$ ), 4.06 (t, 12H,  $CH_2$ ), 7.52 (d, 4H,  $J = 6.2$  Hz, Ar), 7.80 (s, 2H,  $J = 2.6$  Hz, Ar), 6.48 (s, 2H,  $J = 3.6$  Hz, Ar), 7.63 (s, 2H,  $J = 6.0$  Hz, Ar), 7.22-7.26 (s, 4H, Ar), 8.10 (s, 2H,  $-CH=N$ ), 9.12 (s, 1H,  $-CHO$ ).  $^{13}C$  NMR: 171.5, 166.4, 146.6, 133.7, 129.9, 126.2, 114.7, 112.8, 108.3, 73.6, 69.1, 31.8, 25.6.

**Preparation of 4,4'-(bis(trihexyloxy benzylideneamino)-9H-carbazole-butoxy phenthroimidazole (6a)**

4,4'-(bis(trihexyloxy benzylideneamino)-9H-carbazole-butoxy phenthroimidazole (**6a**) is prepared by the one pot synthesis of derivative (**5a**) with 9, 10-phenanthrene quinone and 4-butoxy aniline in presence of ammonium acetate and acetic acid under N<sub>2</sub> (gas).<sup>5</sup> The resultant final crude was purified by using column chromatography on silica gel using methanol: chloroform (1:4, v/v) as the eluent. Yield: 64 %; FT-IR (KBr pellet) in cm<sup>-1</sup>: 3013, 2920, 2866, 1508, 1440, 1234, 713, 686, 563; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): 0.89-0.91 (t, 21H, CH<sub>2</sub>), 1.27-1.47 (m, 39H, CH<sub>2</sub>), (q, 4H), 1.71 (t, 14H, CH<sub>2</sub>), 4.08 (t, 14H, CH<sub>2</sub>), 8.61 (s, 1H, Ar), 8.71 (s, 2H, -CH=N), 7.02 (d, 4H, *J* = 6.2 Hz, Ar), 7.62 (d, 6H, *J* = 6.0 Hz, Ar), 7.51 (d, 4H, *J* = 6.6 Hz, Ar), 7.22 (s, 2H, Ar). <sup>13</sup>C NMR: 158.6, 153.6, 146.4, 141.8, 133.5, 128.1, 125.5, 122.4, 114.4, 77.4, 77.0, 68.7, 31.8, 22.6. MALDI ToF MS for compound **6a** (M+1) Calculated: 1414.8814 Found 1415.5838.

**Preparation of 4,4'-(bis(trioctyloxy benzylideneamino)-9H-carbazole-butoxy phenthroimidazole (6b)**

4,4'-(bis(trioctyloxy benzylideneamino)-9H-carbazole-butoxy phenthroimidazole (**6b**) is prepared by the one pot synthesis of derivative (**5b**) with 9, 10-phenanthrene quinone and 4-butoxy aniline in presence of ammonium acetate and acetic acid under N<sub>2</sub> (gas).<sup>5</sup> The resultant final crude was purified by using column chromatography on silica gel using methanol: chloroform (1:4, v/v) as the eluent. Yield: 67 %; FT-IR (KBr pellet) in cm<sup>-1</sup>: 3010, 2903, 2826, 1508, 1440, 1310, 1234, 794, 563; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): 0.89-0.91 (t, 21H, CH<sub>2</sub>), 1.27-1.47 (m, 76H, CH<sub>2</sub>), (q, 4H), 1.71 (t, 12H, CH<sub>2</sub>), 4.04 (t, 14H, CH<sub>2</sub>), 8.61 (s, 1H, Ar), 8.75 (s, 2H, -CH=N), 7.43 (d, 4H, *J* = 6.0 Hz, Ar), 7.61 (d, 6H, *J* = 6.2 Hz, Ar), 7.56 (d, 4H, *J* = 6.8 Hz, Ar), 7.22 (s, 2H, Ar). <sup>13</sup>C NMR: 158.6, 152.6, 144.4, 141.8, 133.5, 128.1, 125.5, 122.4, 114.4,



77.4, 77.0, 68.7, 31.8, 22.6. MALDI ToF MS for compound **6b** (M+1) Calculated: 1583.0712  
Found 1584.3492.

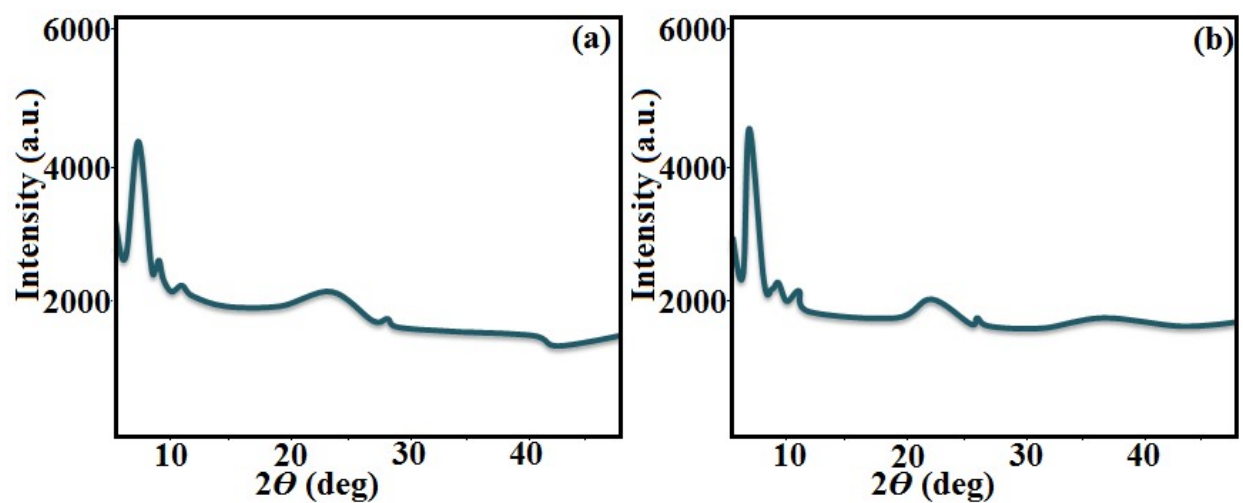
**Preparation of 4,4'-(bis(tridecyloxy benzylideneamino)-9H-carbazole-butoxy phenthroimidazole (6c)**

4,4'-(bis(tridecyloxy benzylideneamino)-9H-carbazole-butoxy phenthroimidazole (**6c**) is prepared by the one pot synthesis of derivative (**5c**) with 9, 10-phenanthrene quinone and 4-butoxy aniline in presence of ammonium acetate and acetic acid under N<sub>2</sub> (gas).<sup>5</sup> The resultant final crude was purified by using column chromatography on silica gel using methanol: chloroform (1:4, v/v) as the eluent. Yield: 61 %; FT-IR (KBr pellet) in cm<sup>-1</sup>: 3012, 2920, 2866, 1508, 1440, 1234, 713, 686, 563; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): 0.89-0.91 (t, 21H, CH<sub>2</sub>), 1.27-1.43 (m, 87H, CH<sub>2</sub>), (q, 4H), 1.73 (t, 14H, CH<sub>2</sub>), 4.08 (t, 14H, CH<sub>2</sub>), 8.43 (s, 1H, Ar), 8.63 (s, 2H, -CH=N), 7.08 (d, 4H, *J* = 6.2 Hz, Ar), 7.62 (d, 6H, *J* = 6.0 Hz, Ar), 7.51 (d, 4H, *J* = 6.6 Hz, Ar), 7.26 (s, 2H, Ar). <sup>13</sup>C NMR: 155.8, 153.6, 144.4, 141.8, 133.5, 128.1, 125.5, 122.4, 114.4, 77.4, 77.0, 68.7, 31.8, 22.6. MALDI ToF MS for compound **6c** (M+1) Calculated: 1751.2642  
Found 1752.4241.

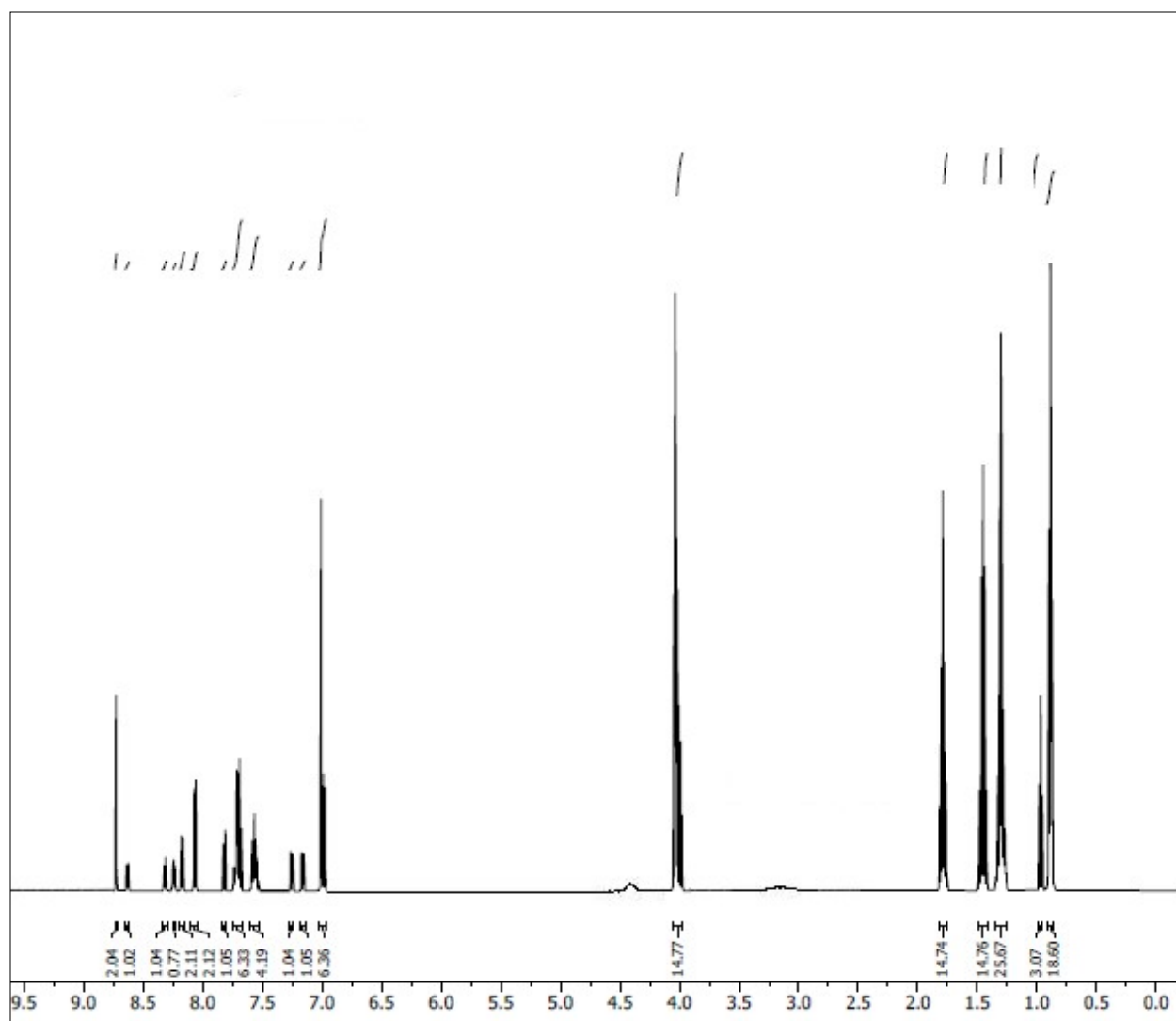
**Preparation of 4,4'-(bis(tridodecyloxy benzylideneamino)-9H-carbazole-butoxy phenthroimidazole (6d)**

4,4'-(bis(trihexyloxy benzylideneamino)-9H-carbazole-butoxy phenthroimidazole (**6a**) is prepared by the one pot synthesis of derivative (**5a**) with 9, 10-phenanthrene quinone and 4-butoxy aniline in presence of ammonium acetate and acetic acid under N<sub>2</sub> (gas).<sup>5</sup> The resultant final crude was purified by using column chromatography on silica gel using methanol: chloroform (1:4, v/v) as the eluent. Yield: 64 %; FT-IR (KBr pellet) in cm<sup>-1</sup>: 3013, 2990, 2861, 1508, 1446, 1234, 913, 742, 686, 577; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): 0.93 (t, 21H, CH<sub>2</sub>), 1.27-1.47 (m, 104H, CH<sub>2</sub>), (q, 4H), 1.71 (t, 14H, CH<sub>2</sub>), 4.04 (t, 14H, CH<sub>2</sub>), 8.61 (s, 1H, Ar), 8.71 (s, 2H, -

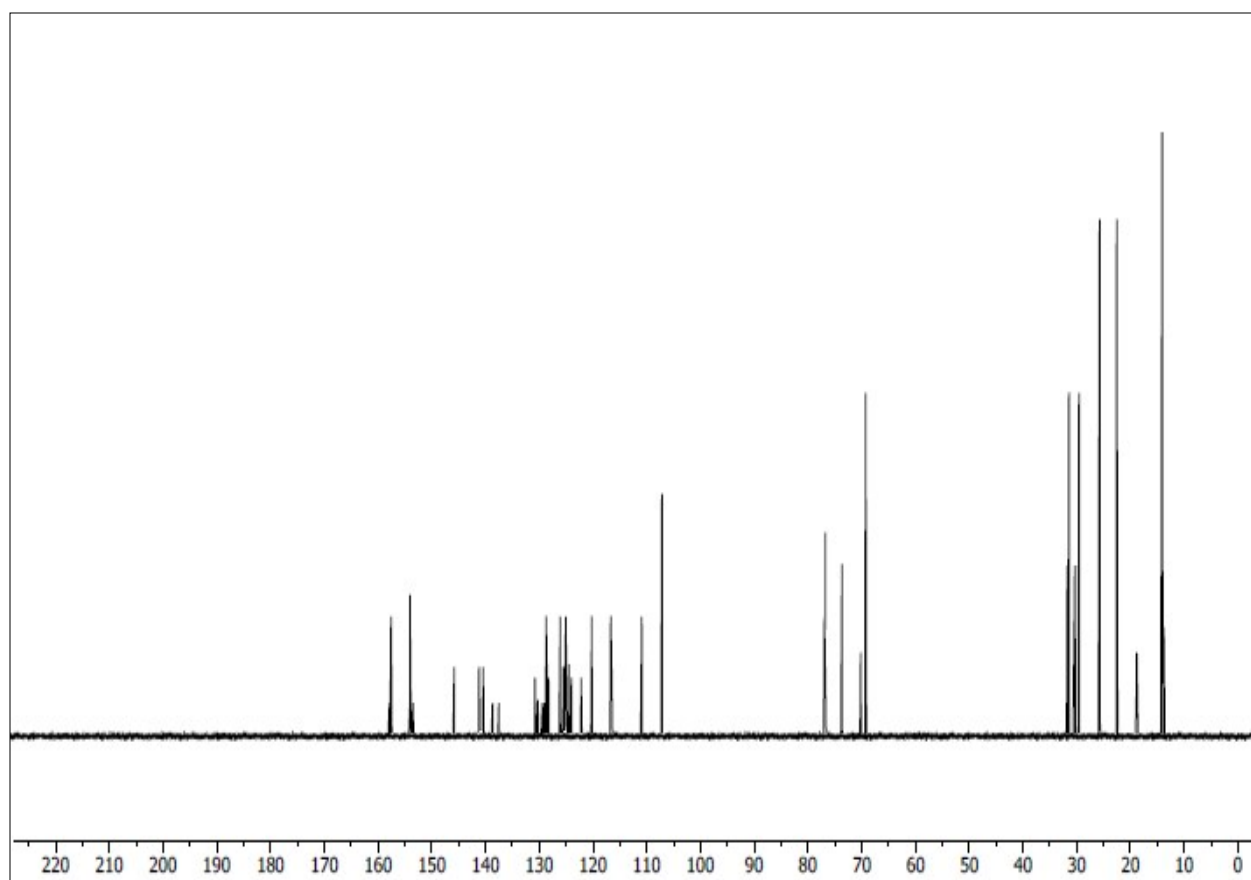
CH=N), 7.02 (d, 4H,  $J = 6.2$  Hz, Ar), 7.62 (d, 6H,  $J = 6.0$  Hz, Ar), 7.51 (d, 4H,  $J = 6.6$  Hz, Ar), 7.22 (s, 2H, Ar).  $^{13}\text{C}$  NMR: 155.8, 151.6, 144.4, 141.8, 133.5, 128.1, 125.5, 122.4, 114.4, 77.4, 77.0, 68.7, 31.8, 22.7. MALDI ToF MS for compound **6d** ( $M+1$ ) Calculated: 1919.4514 Found 1920.8244.



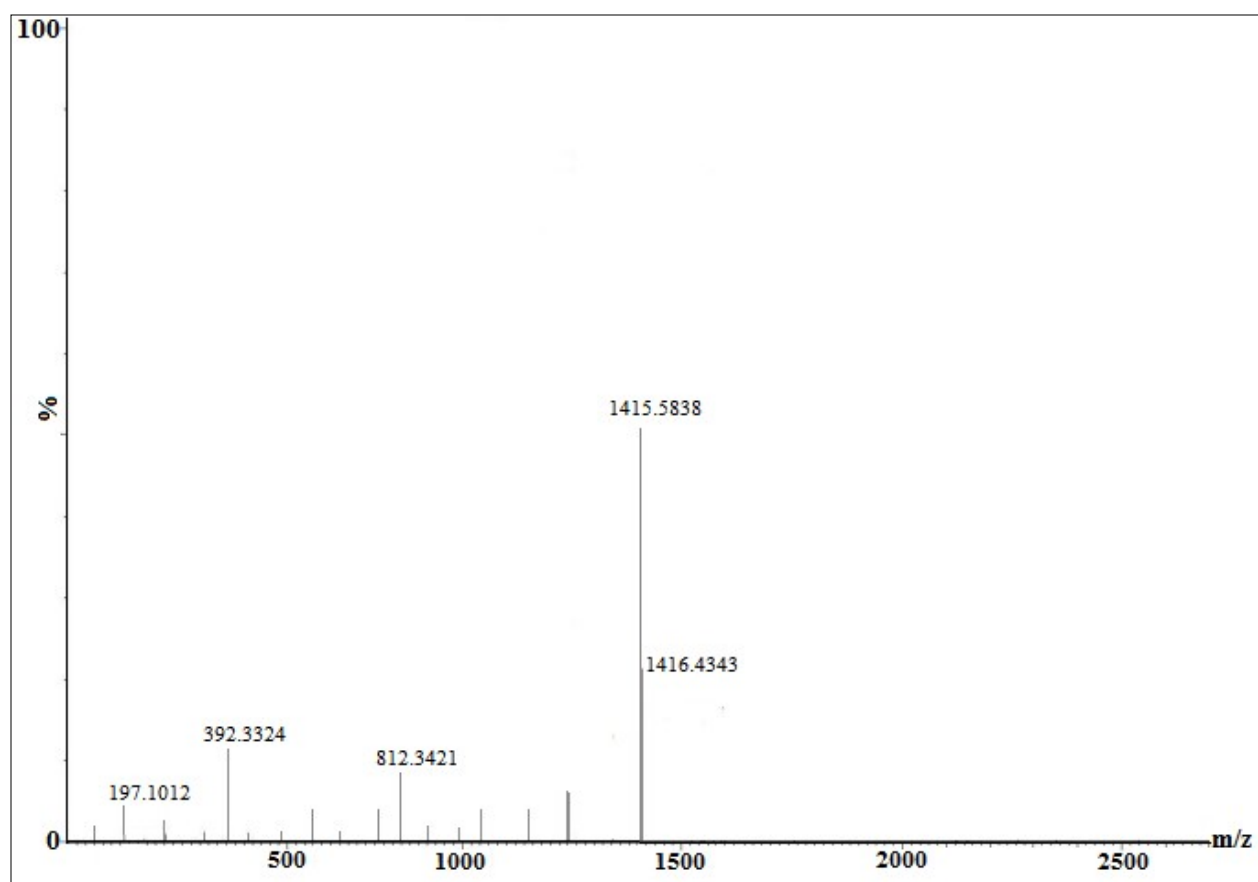
**Figure S1.** XRD profiles depicting the intensity against the  $2\theta$  obtained for the Col<sub>h</sub> phase of compound **6c** at 46.0 °C (a); Col<sub>h</sub> phase of compound **6d** at 36.0 °C (b) on cooling from isotropic temperature; the insert shows the image pattern obtained.



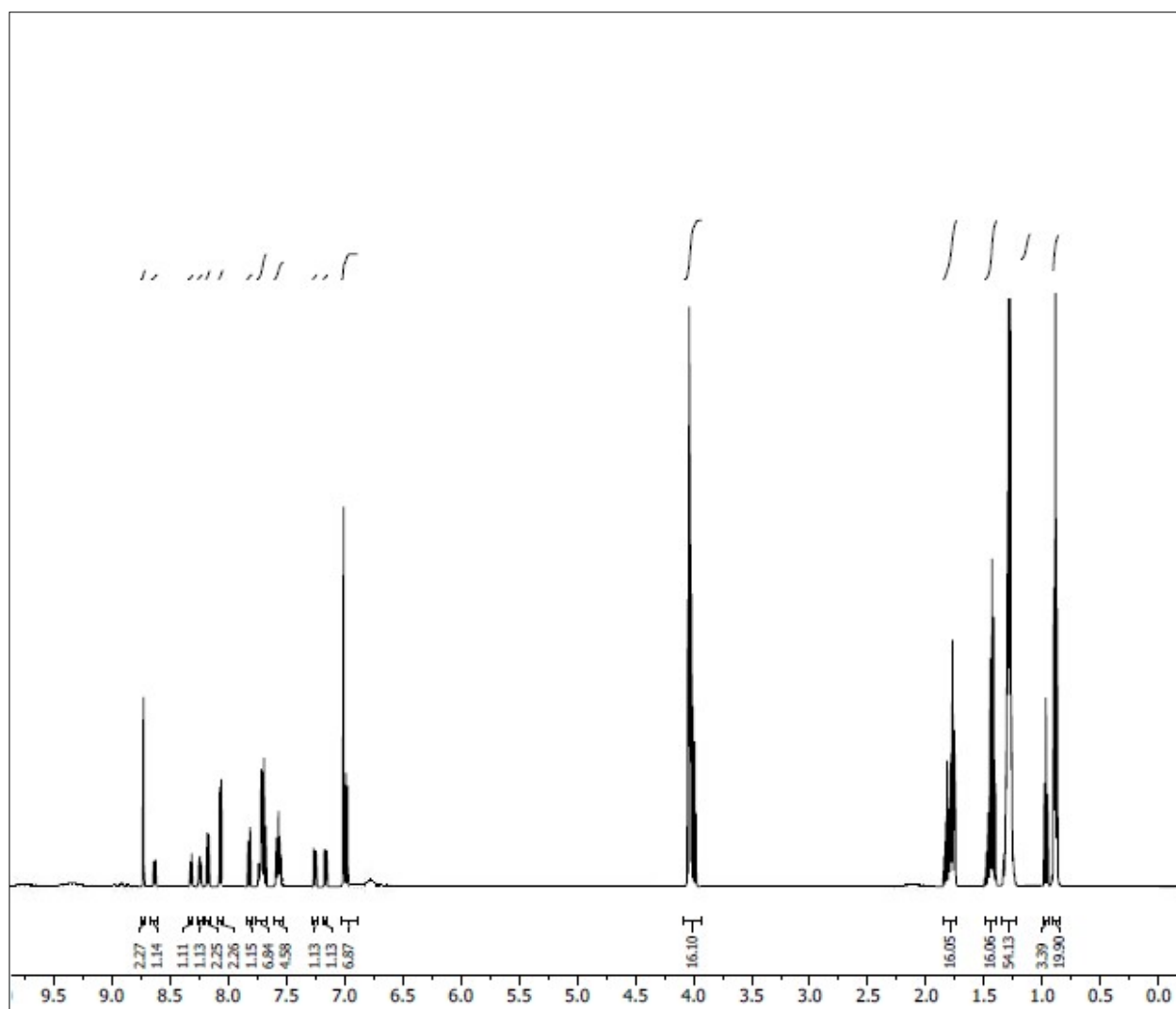
**Figure S2.**  $^1\text{H}$  NMR of compound 6a



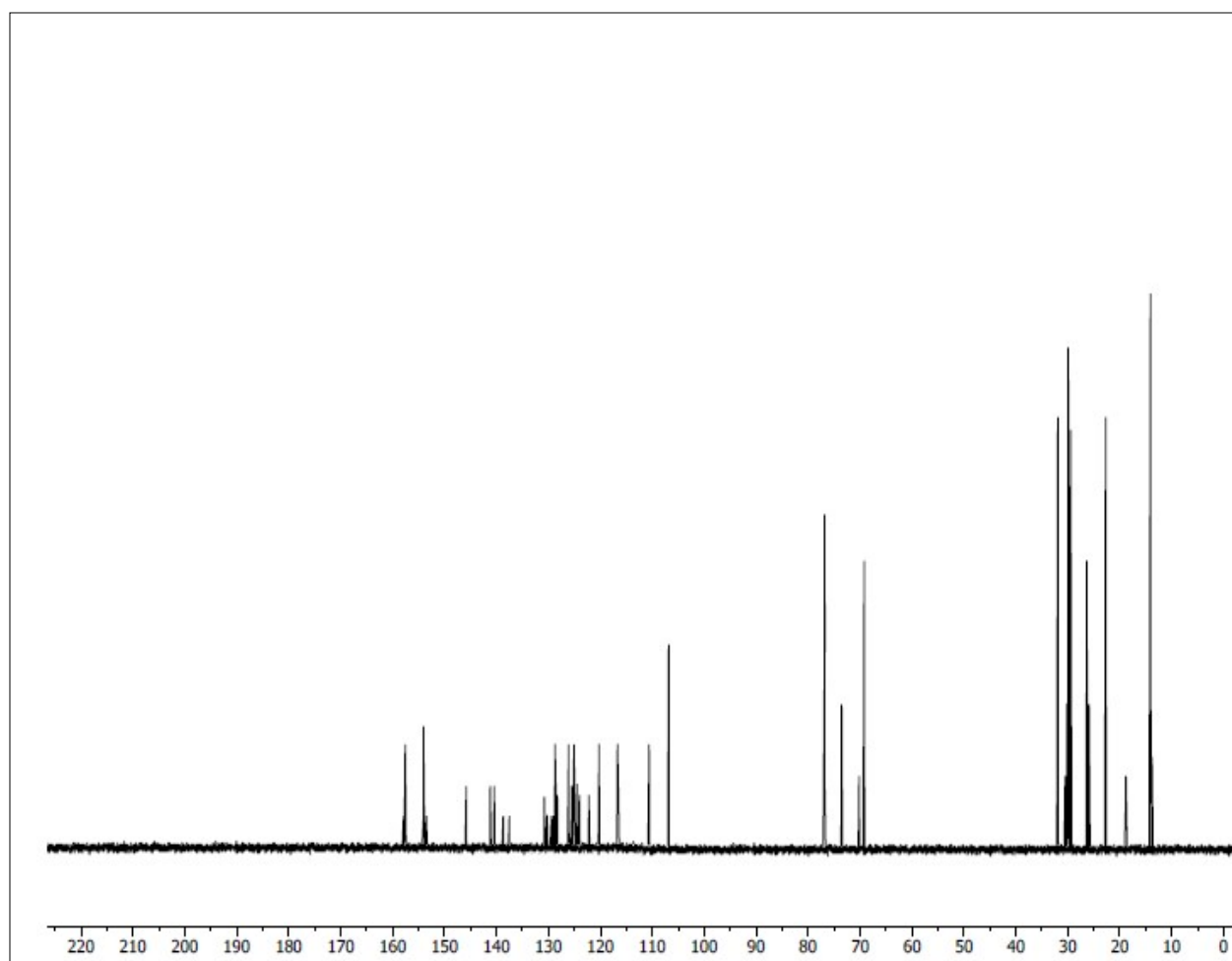
**Figure S<sub>3</sub>.**  $^{13}\text{C}$  NMR of compound **6a**



**Figure S<sub>4</sub>.** HRMS of compound **6a**

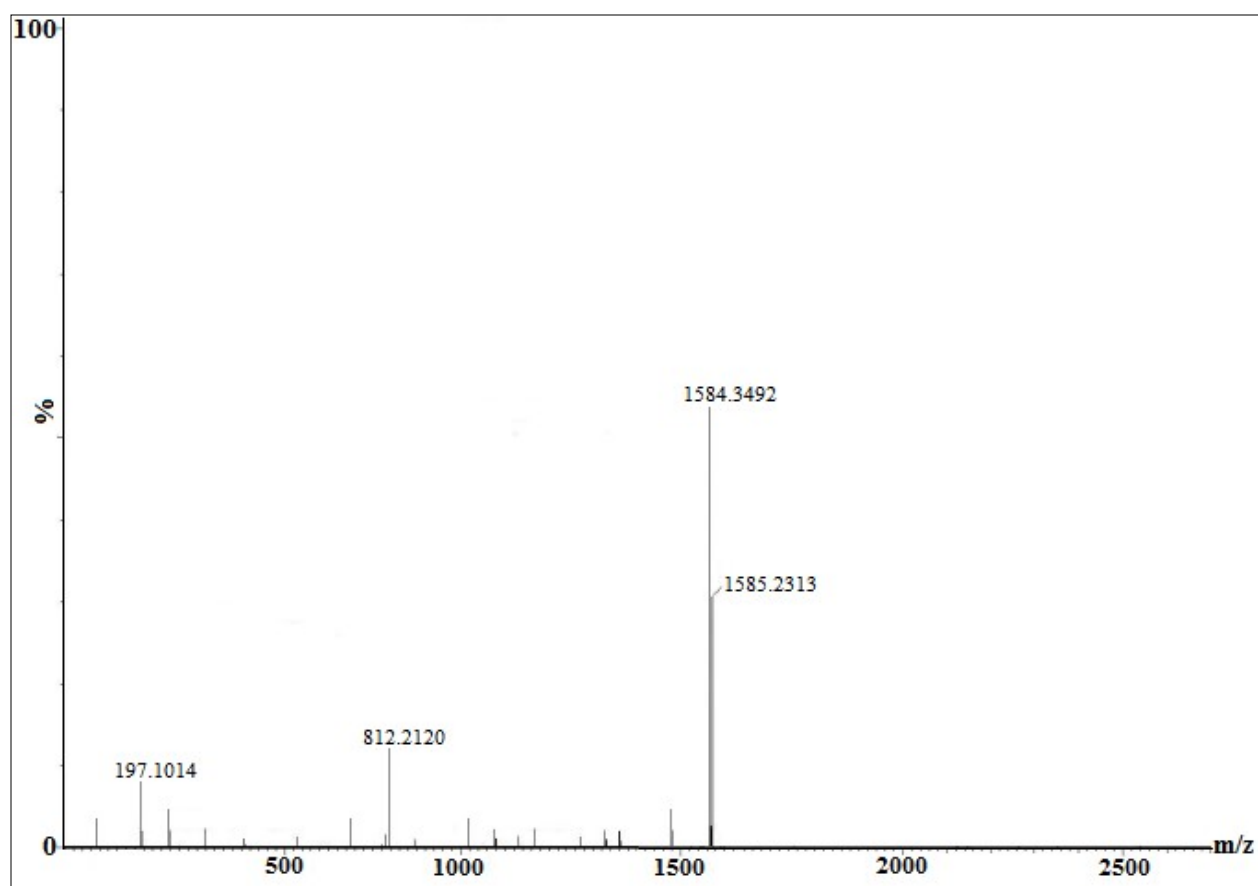


**Figure S<sub>5</sub>.** <sup>1</sup>H NMR of compound **6b**

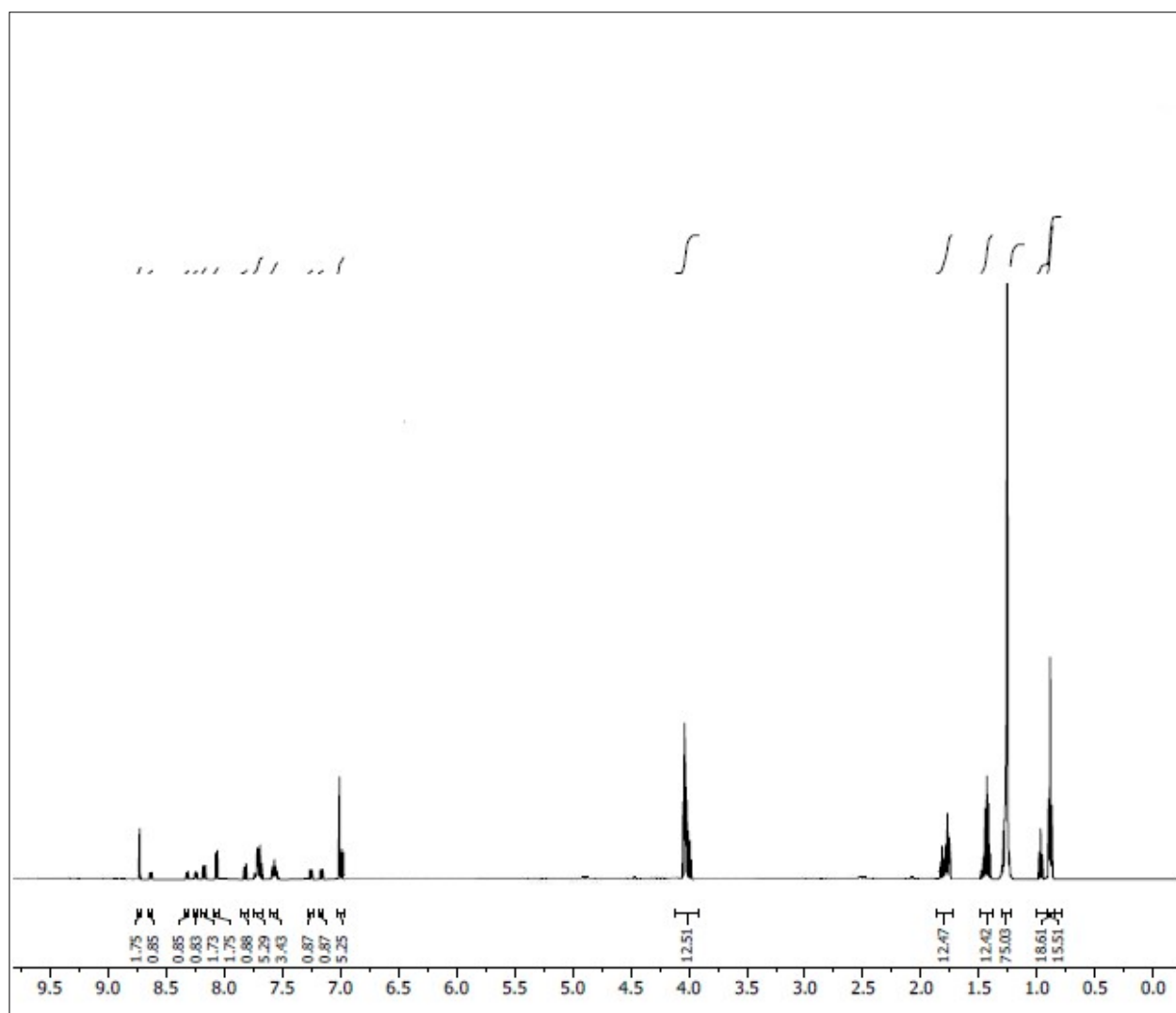


**Figure S<sub>6</sub>.**  $^{13}\text{C}$  NMR of compound **6b**





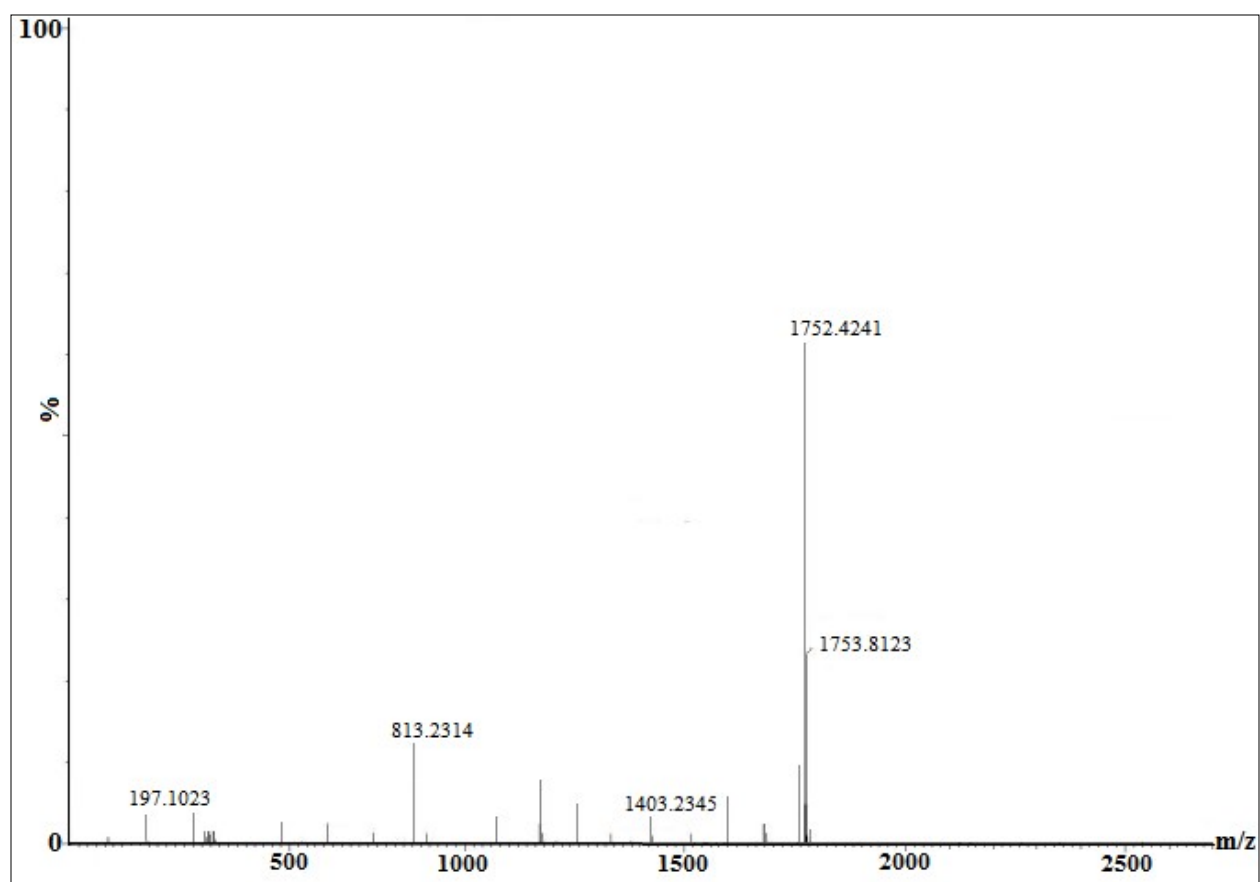
**Figure S7.** HRMS of compound **6b**



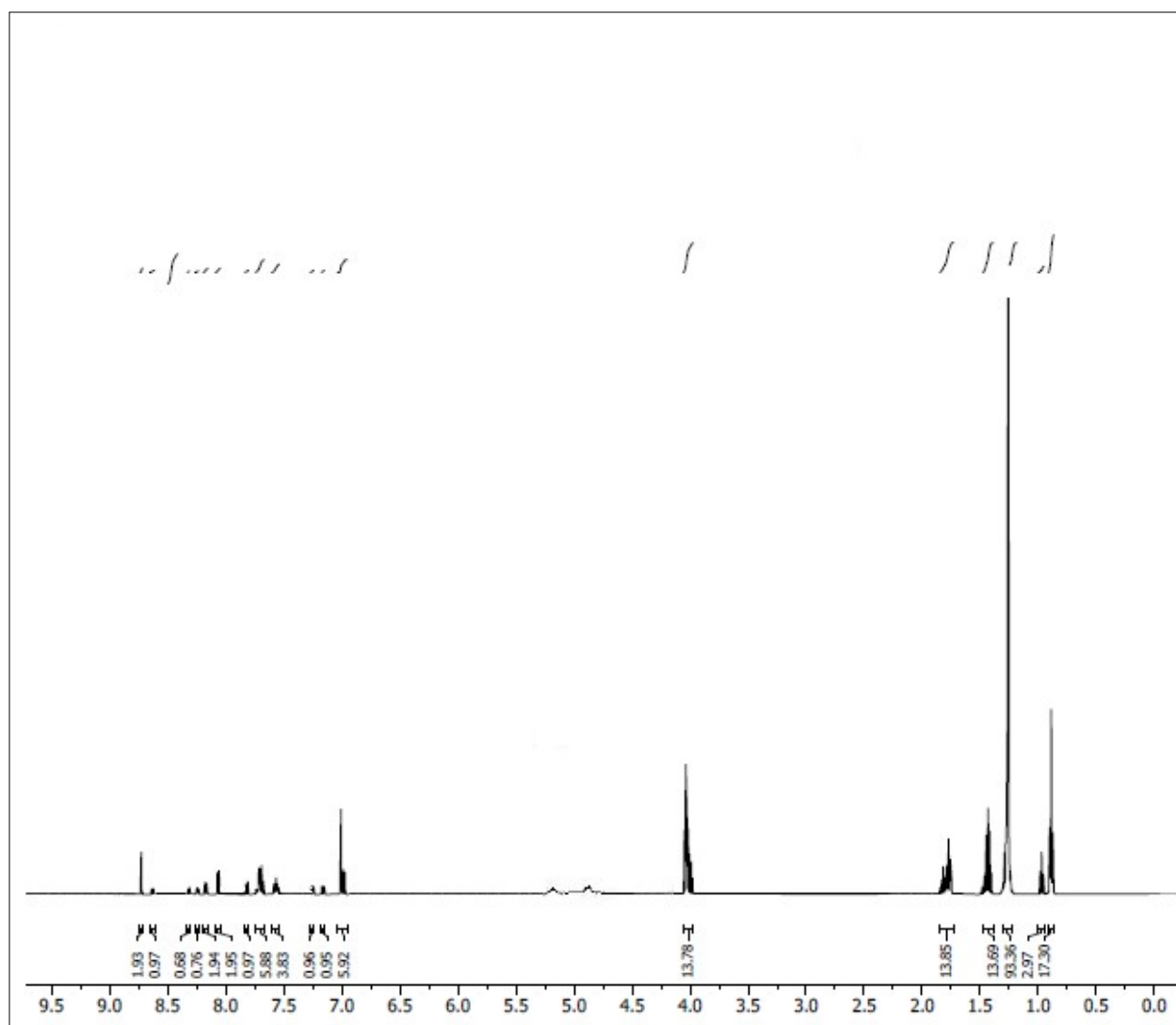
**Figure S8.**  $^1\text{H}$  NMR of compound **6c**



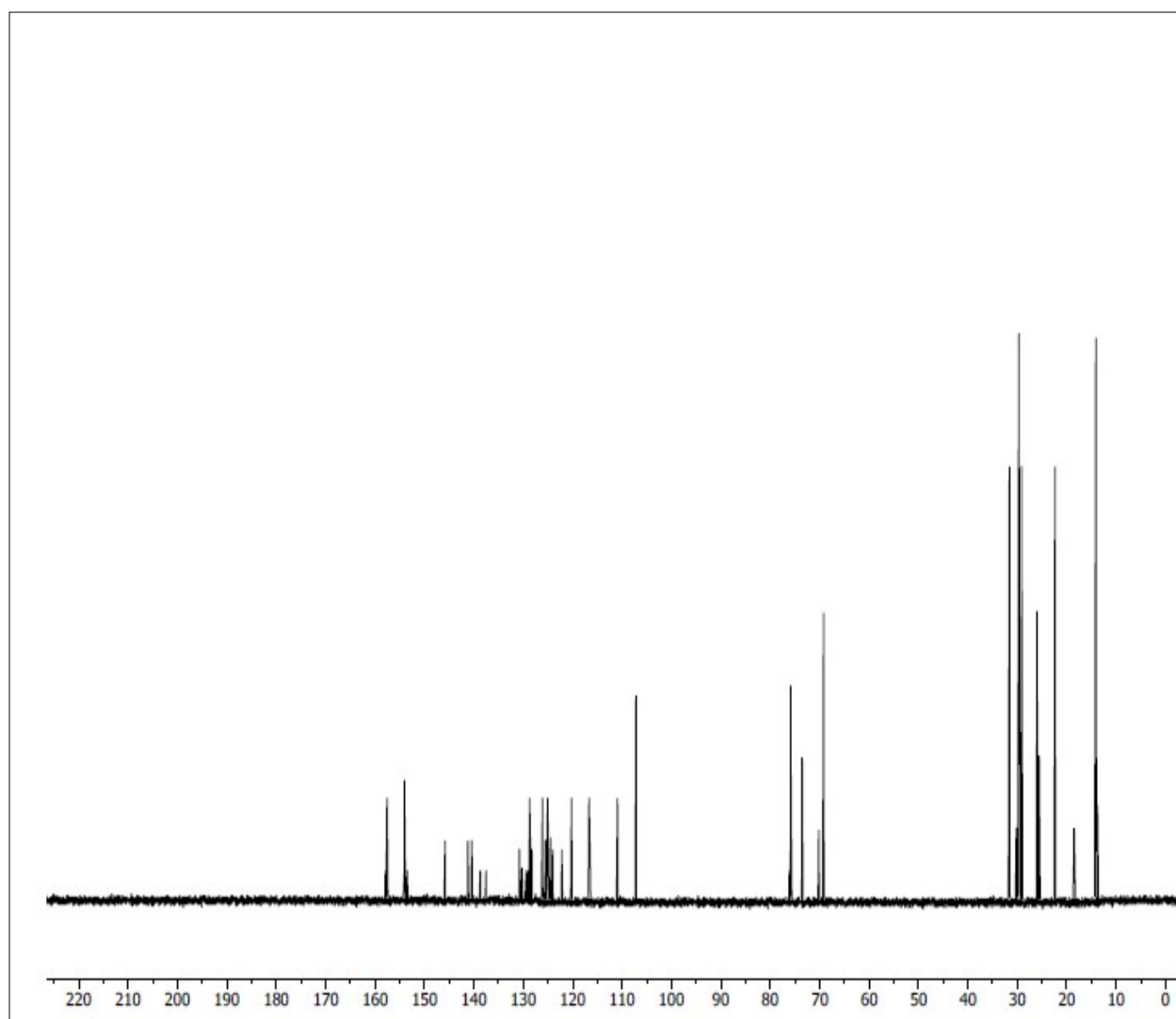
**Figure S<sub>9</sub>.**  $^{13}\text{C}$  NMR of compound **6c**



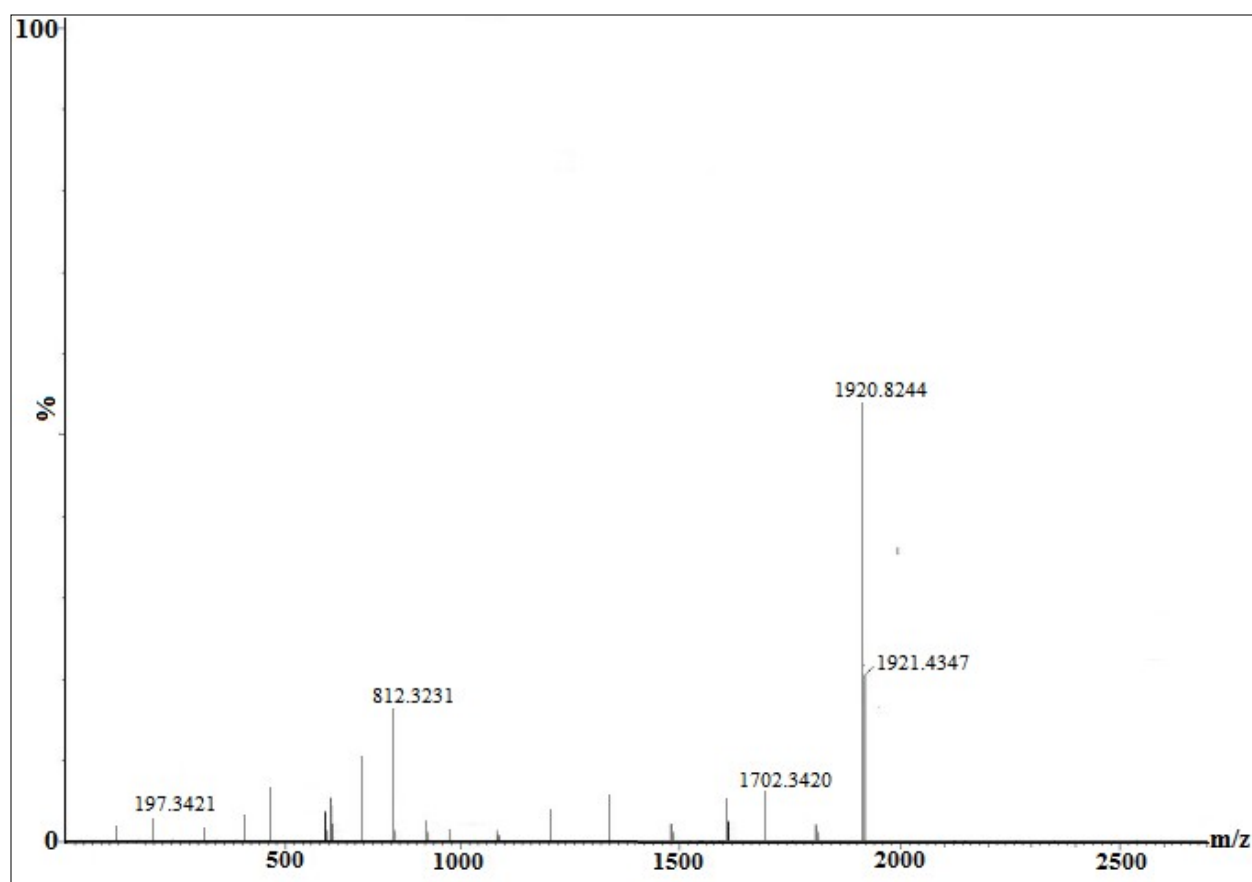
**Figure S<sub>10</sub>.** HRMS of compound **6c**



**Figure S11.**  $^1\text{H}$  NMR of compound 6d



**Figure S<sub>12</sub>.**  $^{13}\text{C}$  NMR of compound **6d**



**Figure S<sub>13</sub>.** HRMS of compound **6d**

## References

1. Camerel, F.; Donnio, B.; Ziessel, R. Liquid-crystalline functional carbazole and naphthalene platforms. *Soft Matter*. **2011**, 7, 412-428.
2. Sharma, V.S.; Patel, R.B. Synthesis and mesomorphic properties of new chalconyl-linkage-based liquid crystal compounds: The effect of flexibility. *Mol.Cryst.Liq.Cryst.* **2017**, 643, 129-140.
3. Sharma, V.S.; Sharma, A.S.; Jadeja, U.H.; Suthar, D. New chalcone based liquid crystals with allylidene amino linking unit: Synthesis and characterization. *Mol.Cryst.Liq.Cryst.* **2018**, 665, 64-81.
4. Gao, Z.; Wang, Z.; Shen, T.; Liu, Y.; Shen, F. High-efficiency deep blue fluorescent emitters based on phenanthro[9,10-d]imidazole substituted carbazole and their applications in organic light emitting diodes. *Organic Electronics*. **2014**, 15, 2667-2676.
5. Wang, Z.M.; Lu, P.; Chen, S.M.; Gao, Z.; Shen, F.Z. Phenanthro[9,10-d]imidazole as a new building block for blue light emitting materials. *J.Mater.Chem.* **2011**, 21, 5451-5456