Supporting Information For:

The first examples of room temperature liquid crystal dimers based-on cholesterol and pentaalkynylbenzene

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1. Materials and Reagents

Chemicals and solvents were all of AR quality and were used without further purification. Pentabromophenol, 1-ethynyl-4-pentylbenzene, copper iodide, bis(triphenylphosphine) palladium(II) dichloride, potassium carbonate, 5-bromovaleric acid, potassium hydroxide and tetraoctyl ammonium bromide were all purchased from Sigma–Aldrich (Bangalore, India). Cholesterol & Ethyl-11-bromoundecanoate were purchased from alfaaesar & TCI (India) respectively. Column chromatographic separations were performed on silica gel (60-120 & 230-400 mesh). Thin layer chromatography (TLC) was performed on aluminium sheets pre-coated with silica gel (Merck, Kieselgel 60, F254).

2. Instrumental

Structural characterization. Structural characterization of the compound was carried out through a combination of infrared spectroscopy (Perkin Elmer Spectrum AX3), ^{1}H NMR and ^{13}C NMR (BrukerBiospin Switzerland Avance-iii 400 MHz and 100 MHz spectrometers respectively), UV-VIS-NIR spectrophotometer (LABINDIA UV-Vis Spectrophotometer

3000+) and mass spectrometry (Waters synapt g2s). NMR spectra were recorded using deuteriated chloroform ($CDCl_3$) as solvent and tetramethylsilane (TMS) as an internal standard.

Differential Scanning Calorimetry. DSC measurements were performed on Perkin Elmer DSC 8000 coupled to a Controlled Liquid Nitrogen Accessory (CLN 2) with a scan rate of 5°C/min.

Polarized Optical Microscopy. Textural observations of the mesophase were performed with Nikon Eclipse LV100POL polarising microscope provided with a Linkam heating stage (LTS 420). All images were captured using a Q-imaging camera.

X-ray Diffraction. X-ray diffraction (XRD) was carried out on powder samples using Cu Kα (λ=1.54 Å) radiation from DY 1042-Empyrean XRD with Polymer Control System and Pixel system (Diffractometer System-Empyrean, Measuring program-Focusing mirror, scans axis-gonioKAlpha-1.54060, Goniometer Radius-240mm and Modification editor-Panalytical).

3. Spectroscopic data for the synthesised compounds

Compound **4**:

FT-IR (cm^{-1}): 3082.2, 3031.7, 2932.72, 2208.78, 1903.3, 1731.74, 1606.79, 1513.63, 1465.5, 1425.80, 1378, 1346.69, 1266.8, 1177.91, 1084.86, 1019.84, 963.64, 837.96, 733.27, 551.42.

UV-Vis (nm): 233, 268, 339, 383, 418.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 (m, 10H), 7.21 (m, 10H), 5.37 (m, 1H), 4.63 (m, 1H), 4.42 (t, 2H, J = 8, 4 Hz), 2.67 (t, 10H, J = 8 Hz), 2.15 (t, 2H, J = 8, 4 Hz), 2.31 (d, 2H, J = 8 Hz), 2.01 (m, 5H), 1.84 (m, 3H), 1.67 - 0.93 (m, 76H).

^{13}C NMR (400 MHz, $CDCl_3$): δ 172.95, 159.92, 144.05, 143.97, 143.74, 131.80, 131.62, 128.62, 128.60, 124.22, 122.58, 120.70, 120.48, 120.07, 99.62, 99.52, 97.39, 87.09, 86.61,

84.04, 74.0, 73.83, 56.69, 56.14, 50.02, 42.31, 39.75, 39.54, 36.20, 36.02, 35.84, 31.85, 31.56, 31.52, 30.98, 28.28, 28.05, 24.31, 23.82, 22.87, 22.60, 21.98, 19.33, 18.74, 14.11, 11.86.

MS: m/z for $C_{103}H_{128}O_3$ 1413.99; found 1413.03

Compound **8**:

FT-IR (cm^{-1}): 3027.22, 2929.23, 2856.75, 2208.51, 1732.68, 1605.80, 1513.06, 1466.50, 1424.84, 1378.26, 1347.54, 1252.04, 1175.53, 1085.02, 1019.71, 838.10, 725.79, 552.22.

UV-Vis (nm): 232, 267, 339, 384, 415.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55 (m, 10H), 7.20 (m, 10H), 5.39 (m, 1H), 4.64 (m, 1H), 4.37 (t, 2H, J = 8, 4 Hz), 4.09 (t, 2H, J = 8, 4 Hz), 2.66 (t, 10H, J = 4, 8 Hz), 2.31 (m, 6H), 1.92 (m, 5H), 1.66 (m, 15H), 1.56 – 0.86 (m, 86H).

^{13}C NMR (400 MHz, $CDCl_3$): δ 173.95, 172.73, 160.25, 144.02, 143.90, 143.70, 139.57, 131.79, 131.62, 128.76, 128.56, 128.53, 122.71, 120.73, 120.56, 120.50, 120.13, 99.55, 99.39, 97.33, 87.13, 86.65, 84.12, 74.78, 73.96, 63.61, 56.63, 56.14, 49.97, 42.29, 39.70 39.53, 38.16, 36.58, 36, 34.59, 31.85, 31.52, 31.01, 29.67, 28.05, 26.43, 23.93, 22.66, 22.59, 21.59, 21.04, 19.33, 18.71, 14.09, 11.85.

MS: m/z for $C_{114}H_{148}O_5$ 1598.14; found 1598.14

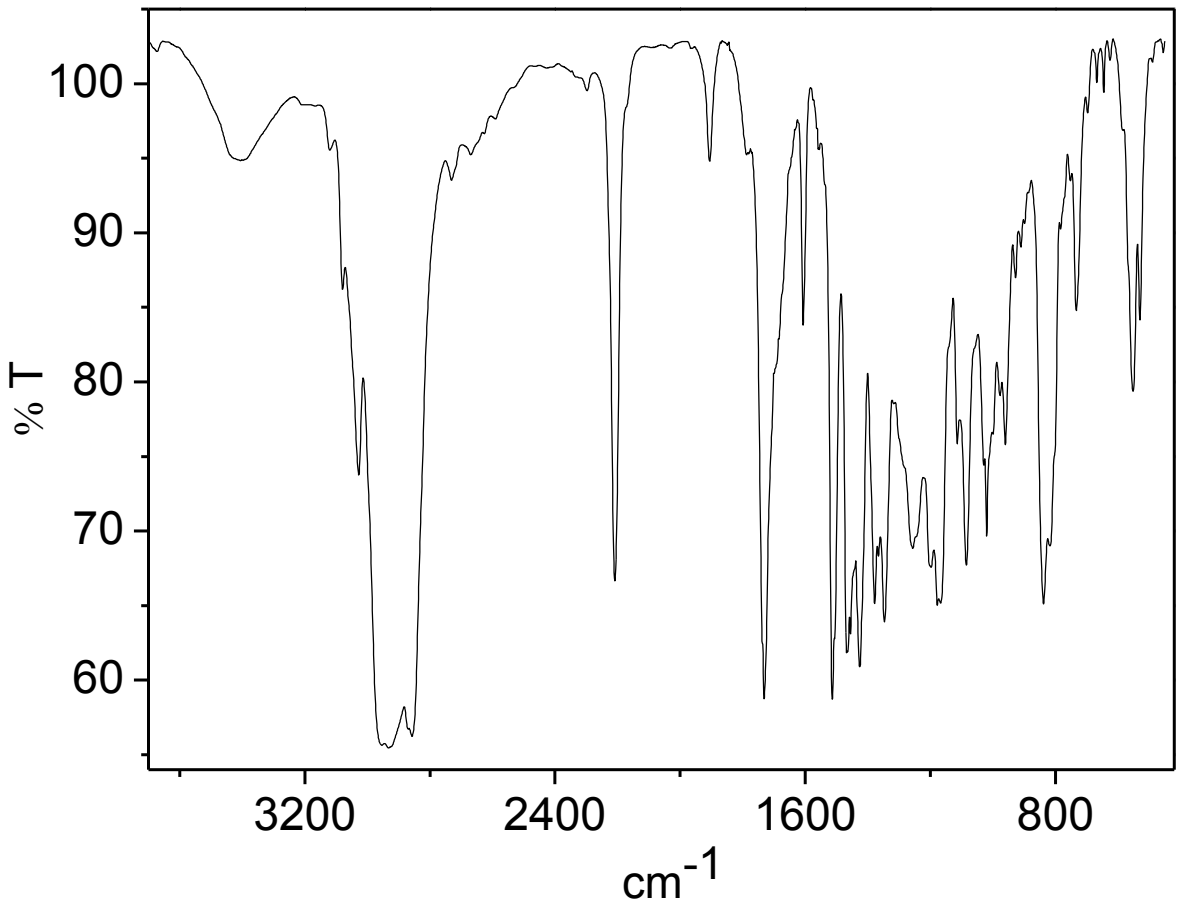

Figure S1. IR spectrum of compound **4**.

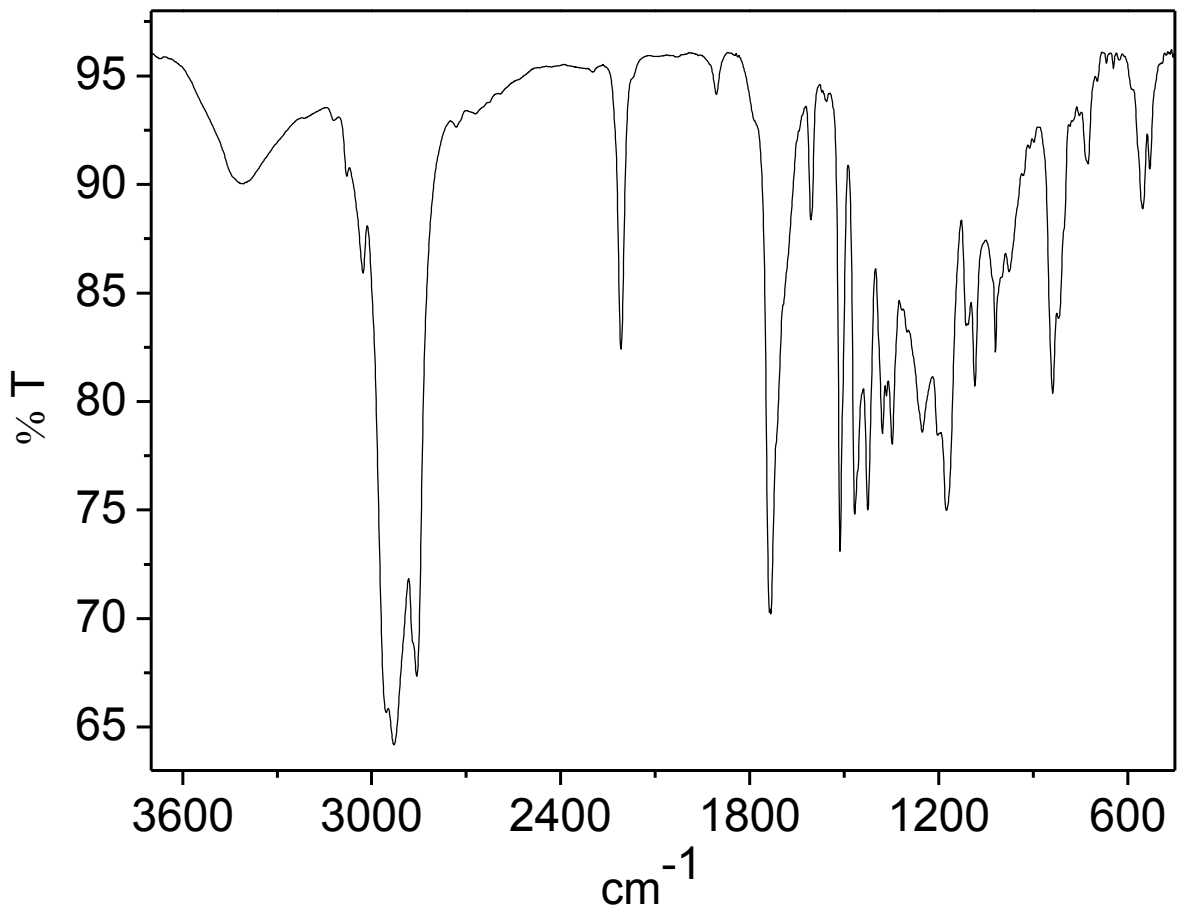

Figure S2. IR spectrum of compound **8.**

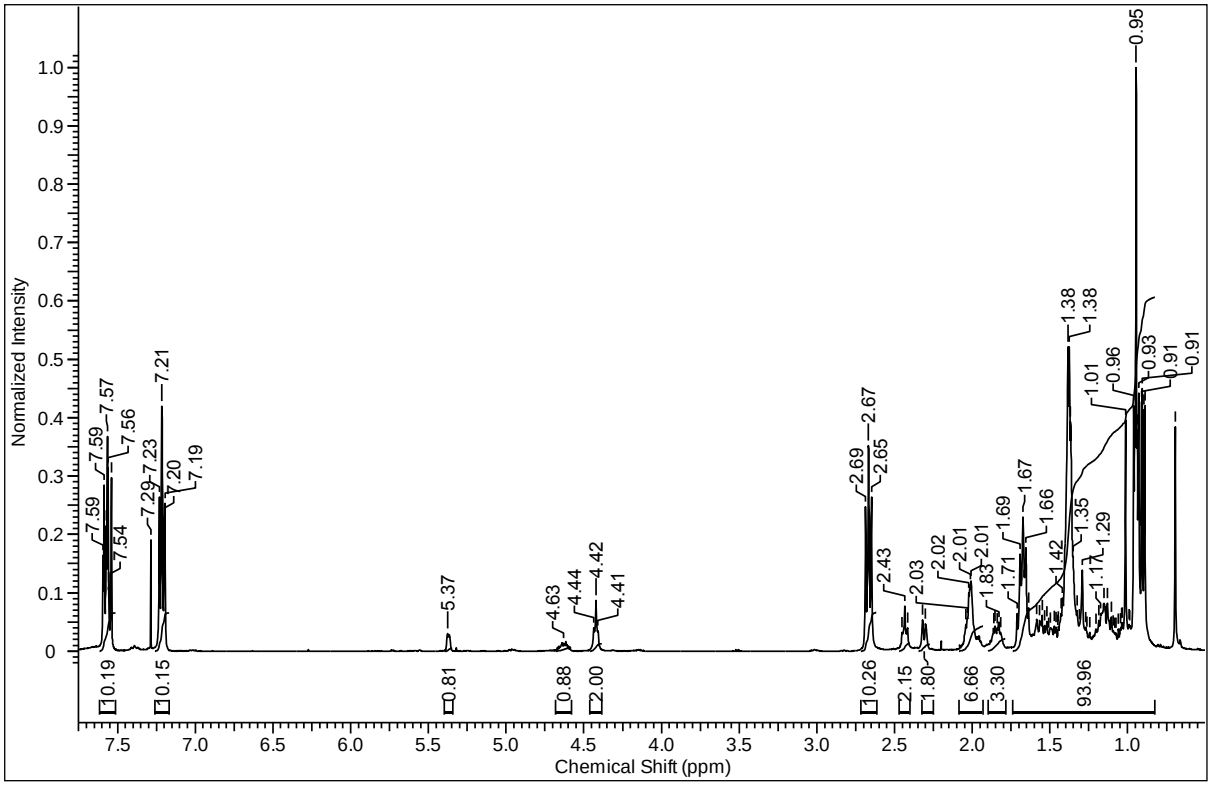

Figure S3. ^{1}H NMR spectrum of compound **4**

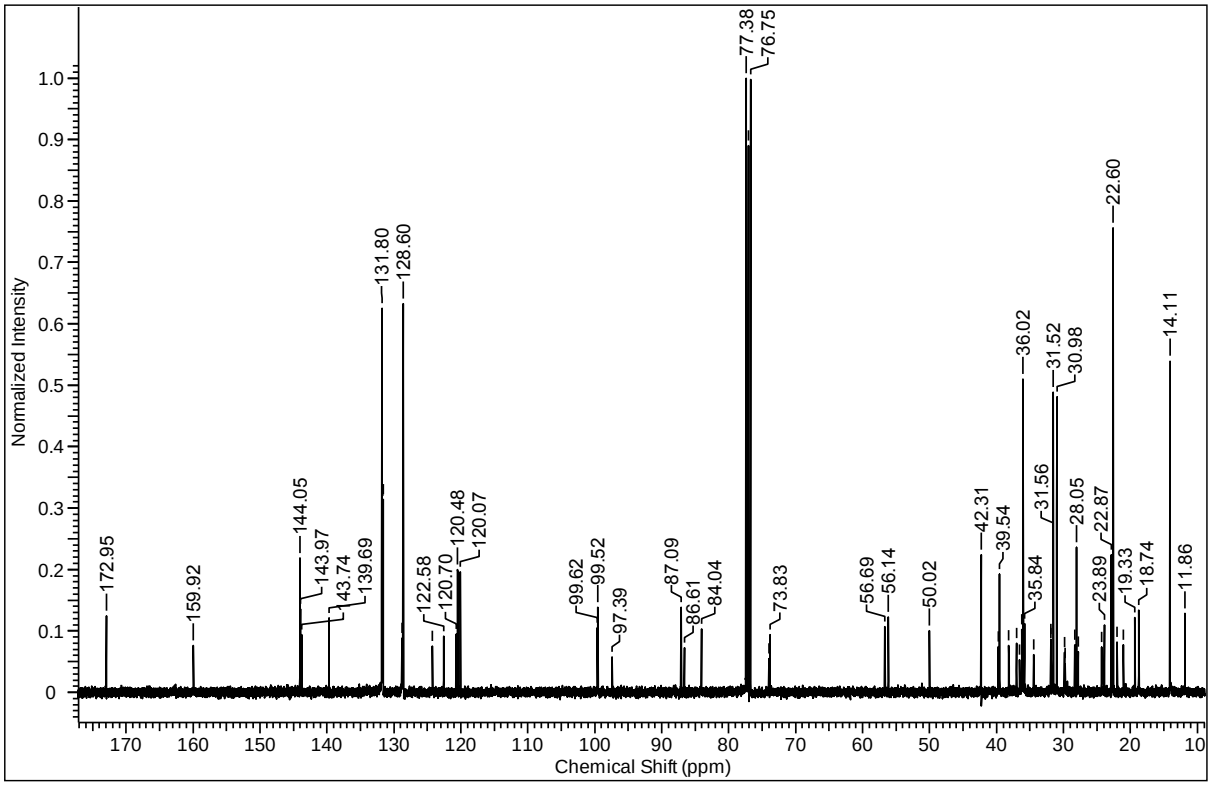

Figure S4. ^{13}C NMR spectrum of compound **4**

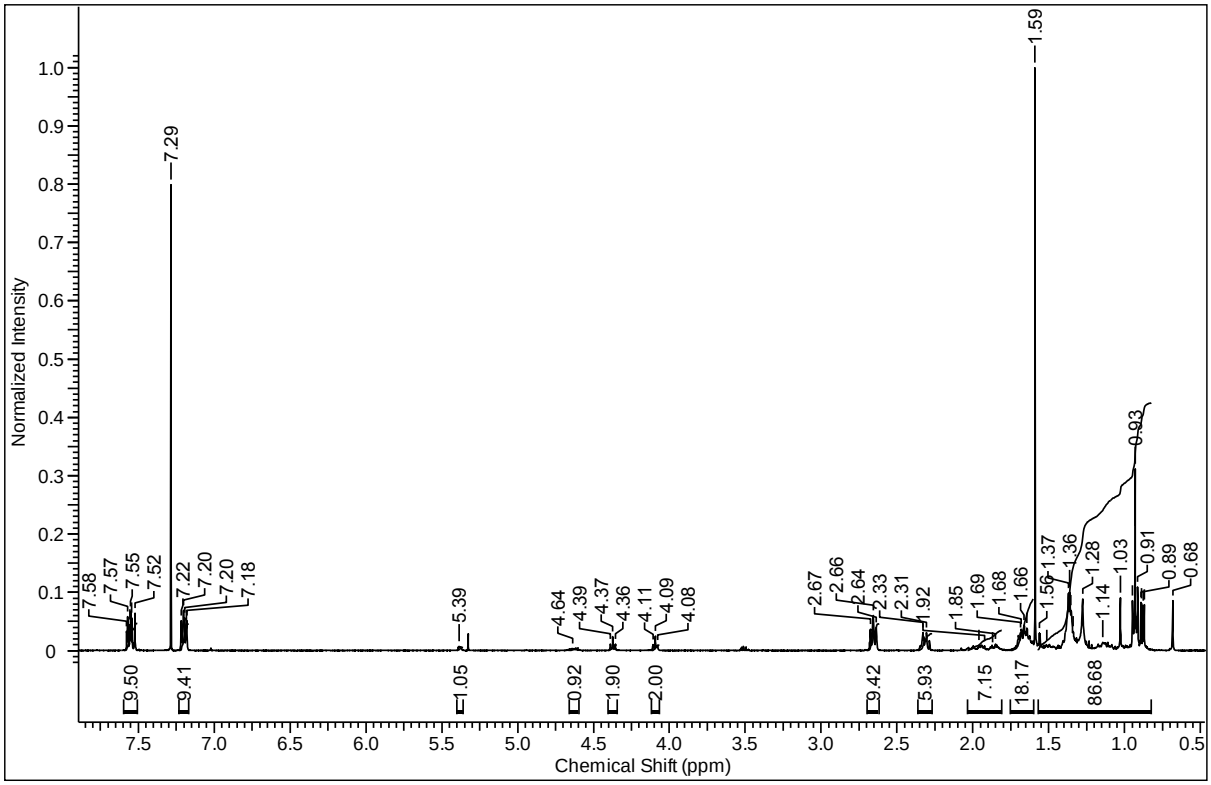

Figure S5. ^{1}H NMR spectrum of compound **8.**

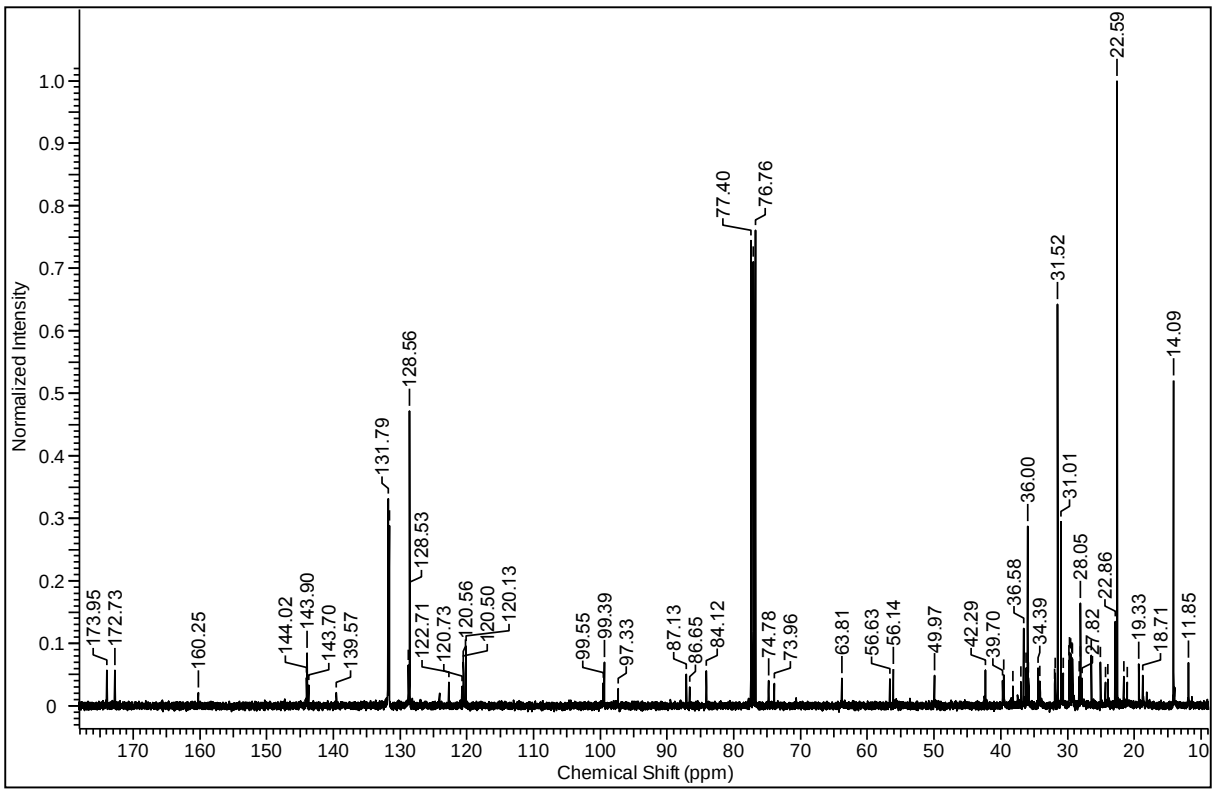

Figure S6. ^{13}C NMR spectrum of compound **8**.

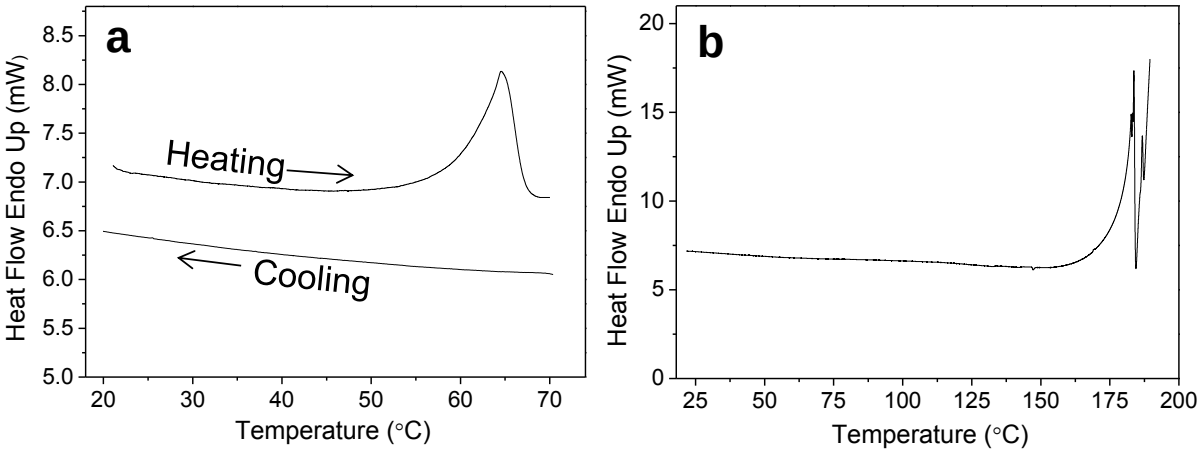

Figure S7. DSC traces of compound **4** & **8** (heating/cooling rate: 5 °C/min).

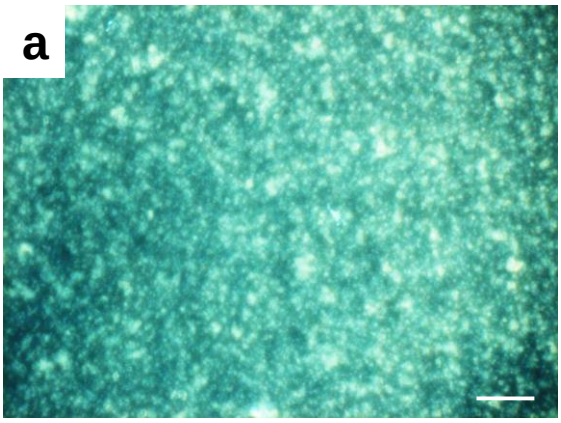

Figure S8. POM image showing increased birefringence on shearing for compound **8** at 25 °C (Crossed polarizers, scale bar = 20 μm)