

Supplementary Information:

Novel Phenazine Fused Triphenylene Discotic Liquid Crystals: Synthesis, Characterisation, Thermal, Optical and Nonlinear Optical Properties

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1. General methods

The AR-grade quality of reagents and solvents were acquired from Sigma-Aldrich and Spectrochem respectively. The solvents used in the reaction were dried and double distilled using standard experimental procedure prior to use. The progress, completion of the reactions and purity of all the compounds were primarily determined by thin layered chromatography. The crude compounds were purified by column chromatography using silica gel as a stationary phase. The molecular structure and purity of all compounds were determined using data recorded from spectroscopic and elemental analysis methods. Fourier transform infrared spectroscopy (FT-IR) spectra were recorded using Shimadzu – 8400; only major peaks were reported in cm^{-1} (wave number). Nuclear magnetic resonance spectroscopy (^1H NMR and ^{13}C NMR) were recorded on Bruker 500 MHz machine using deuterated chloroform (CDCl_3) as a solvent and chemical shifts are given in parts per million (ppm) relative to tetramethylsilane (TMS) as an internal standard (CDCl_3 : ^1H NMR: $\delta = 7.23$ ppm; ^{13}C NMR = 77.0 ppm). The patterns (splitting or multiplicity) of the ^1H NMR signals are represented as s = singlet, d = doublet, t = triplet, m = multiplet and coupling constants (J) are mentioned in Hz. Elemental analysis was carried out using Elementar Vario MICRO Select instrument. The microscopic textures were recorded on sample placed between ordinary glass slides using Olympus BX51 polarising optical microscope attached with a digital camera (Olympus, Tokyo, Japan) in conjunction with Mettler FP82HT hot stage controlled by Mettler FP90 central processor. The phase transition temperature and associated enthalpy values for all the liquid crystalline compounds were determined by METTLER TOLEDO DSC 3 STAR^e system with PC system operating on STAR^e software using 2–4 mg of samples. Prior to the use, the instrument was calibrated using pure indium and zinc. DSC traces were recorded at scan rate of $10\text{ }^\circ\text{C min}^{-1}$ under continues flow of nitrogen gas. X-ray diffraction studies were performed on powder samples in Lindemann capillaries with $\text{Cu K}\alpha$ ($\lambda = 1.54060\text{ \AA}$)

radiation using DY 1042-Empyrean (PANalytical) X-ray diffractometer comprising a programmable divergence slit and PIXcel 3D detector.

2. Polarising optical microscopy textures

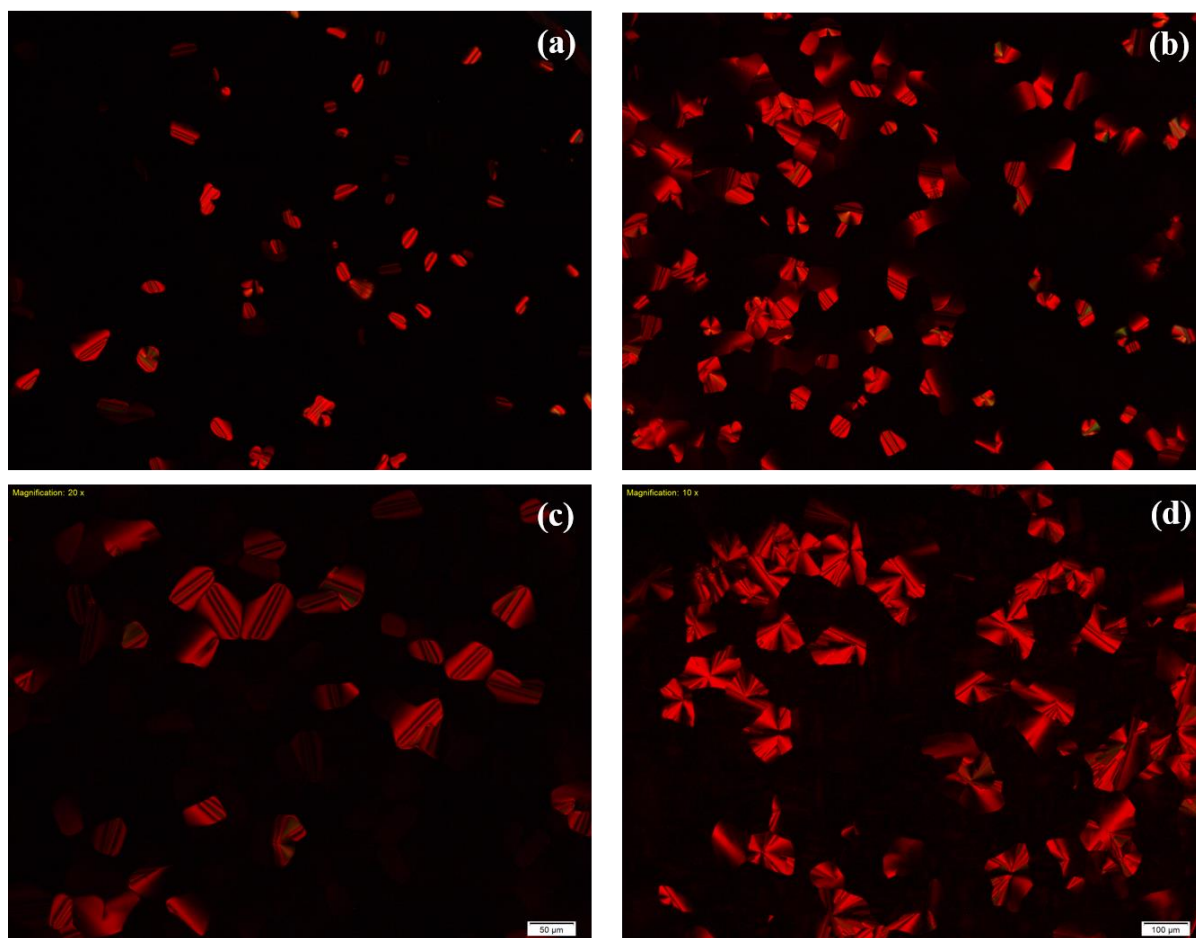


Figure S1. POM images. (a) Compound **7a** at 194 °C, viewed at viewed at 100× magnification. (b) Compound **7b** at 190 °C, viewed at viewed at 100× magnification. (c) Compound **7c** at 136 °C, viewed at viewed at 50× magnification. (d) Compound **7e** at 110 °C, viewed at viewed at 100× magnification

3. Differential scanning calorimetry (DSC)

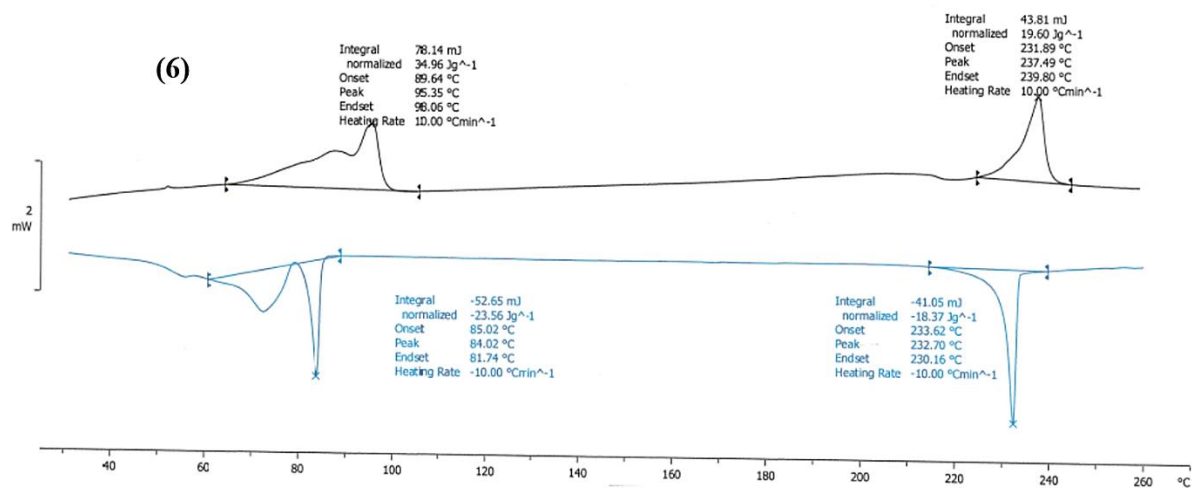


Figure S2. DSC thermogram of compound 6.

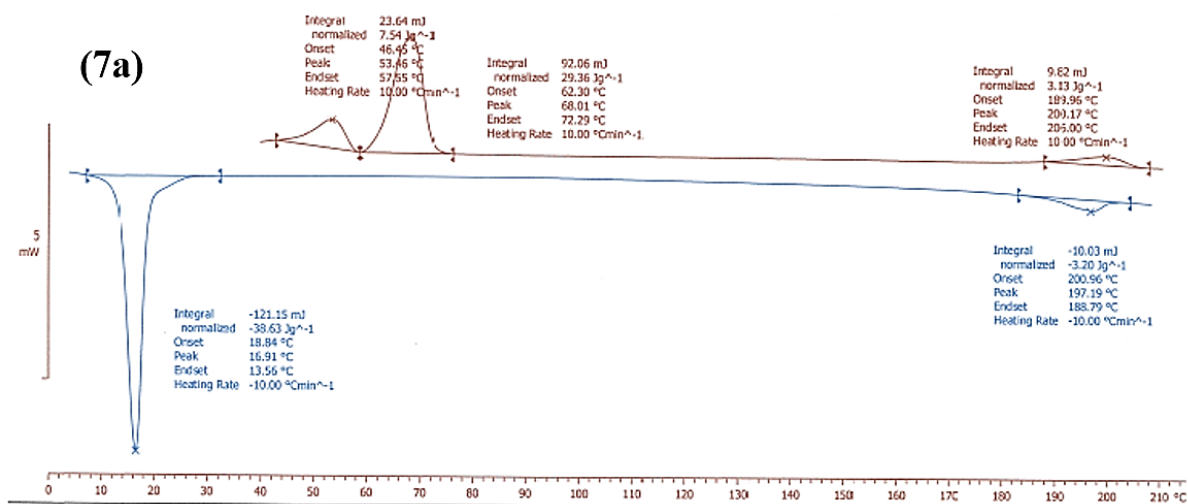


Figure S3. DSC thermogram of compound 7a.

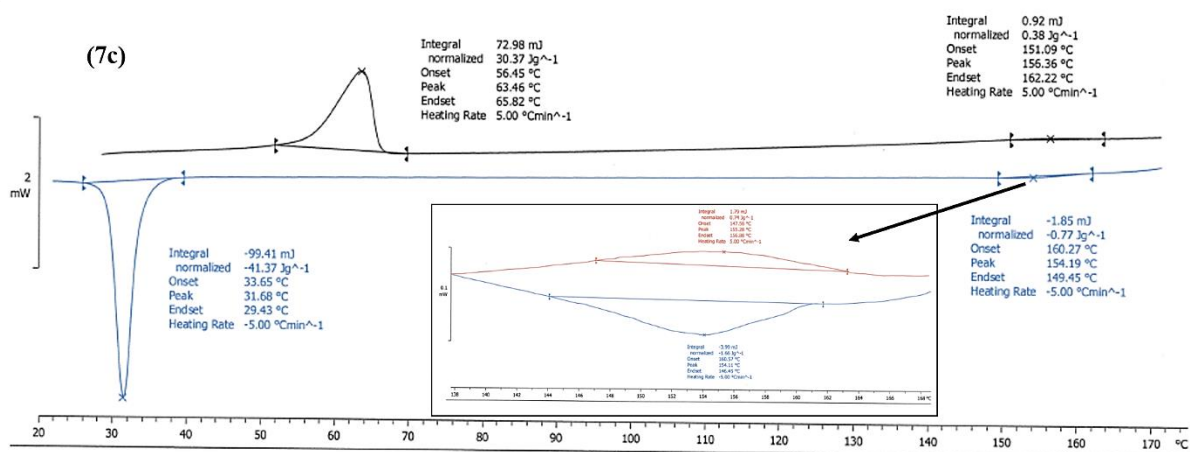


Figure S4. DSC thermogram of compound 7c.

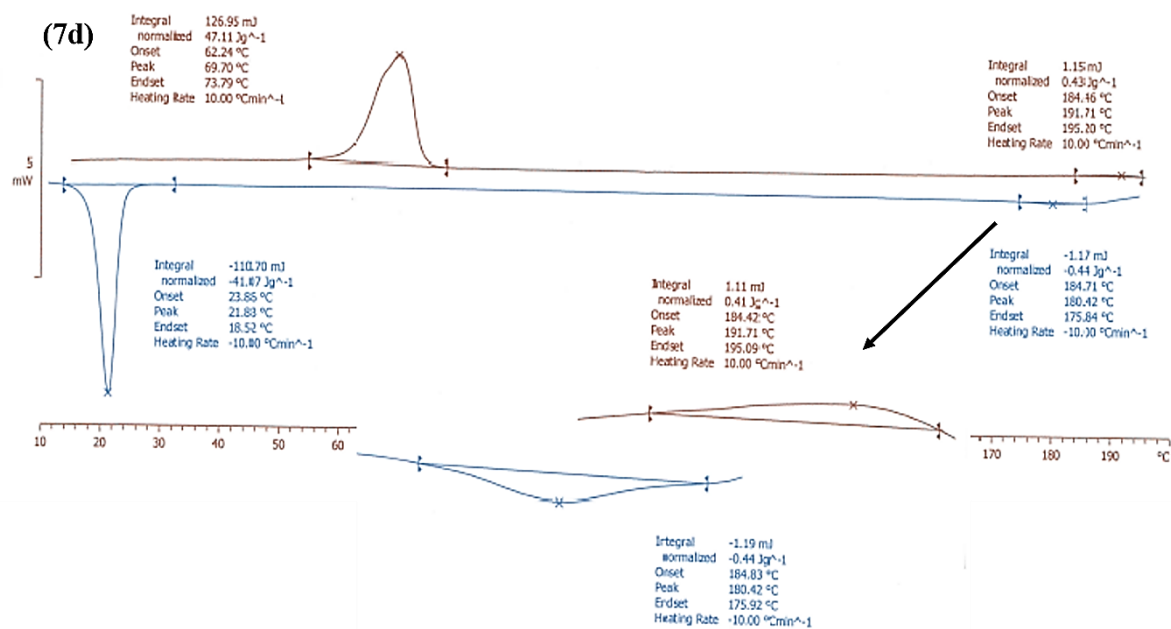


Figure S5. DSC thermogram of compound 7d.

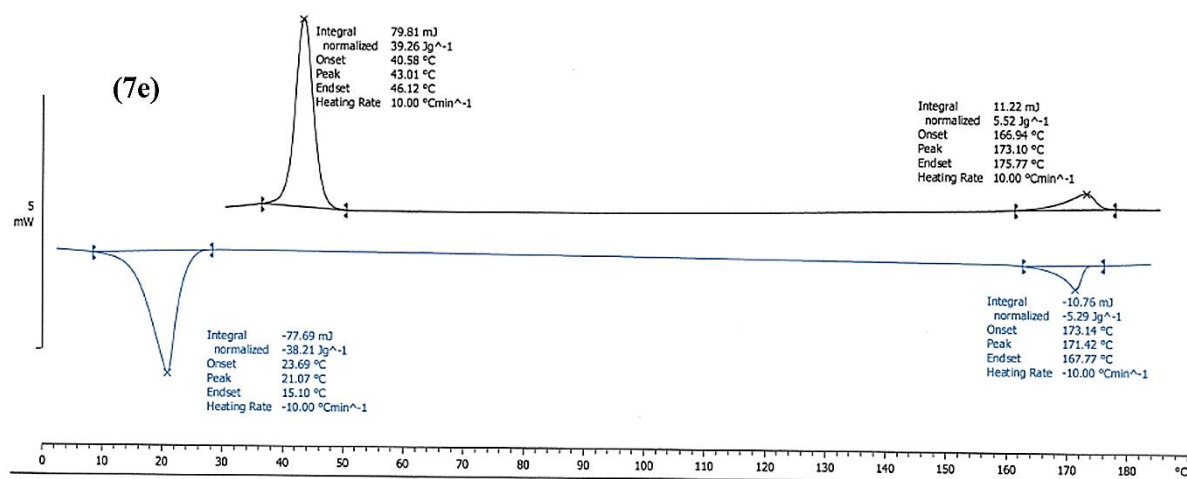


Figure S6. DSC thermogram of compound **7e**.

4. X-ray diffraction studies (XRD)

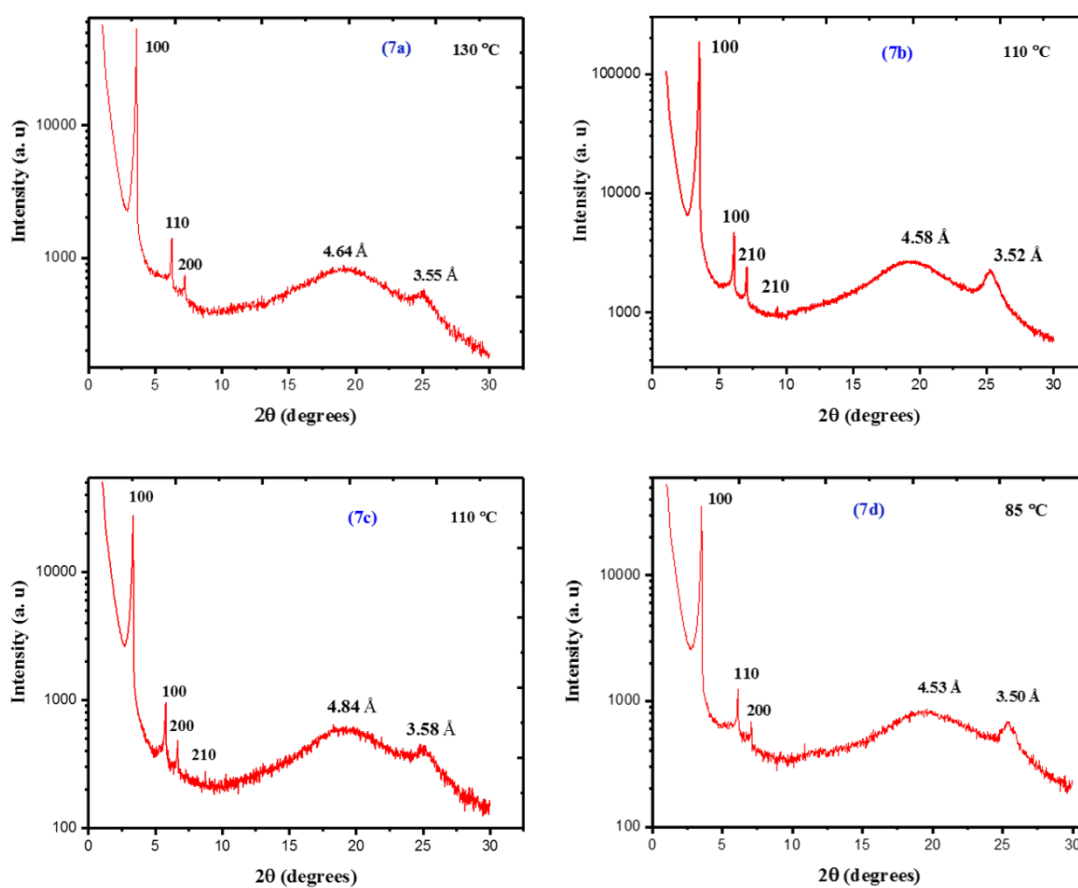


Figure S7. XRD of monomeric ester derivatives obtained on cooling from isotropic melt. (a) Compound **7c**, (b) compound **7b**, (c) compound **7c** and compound **7d** respectively.

5. NMR spectra (^1H and ^{13}C NMR)

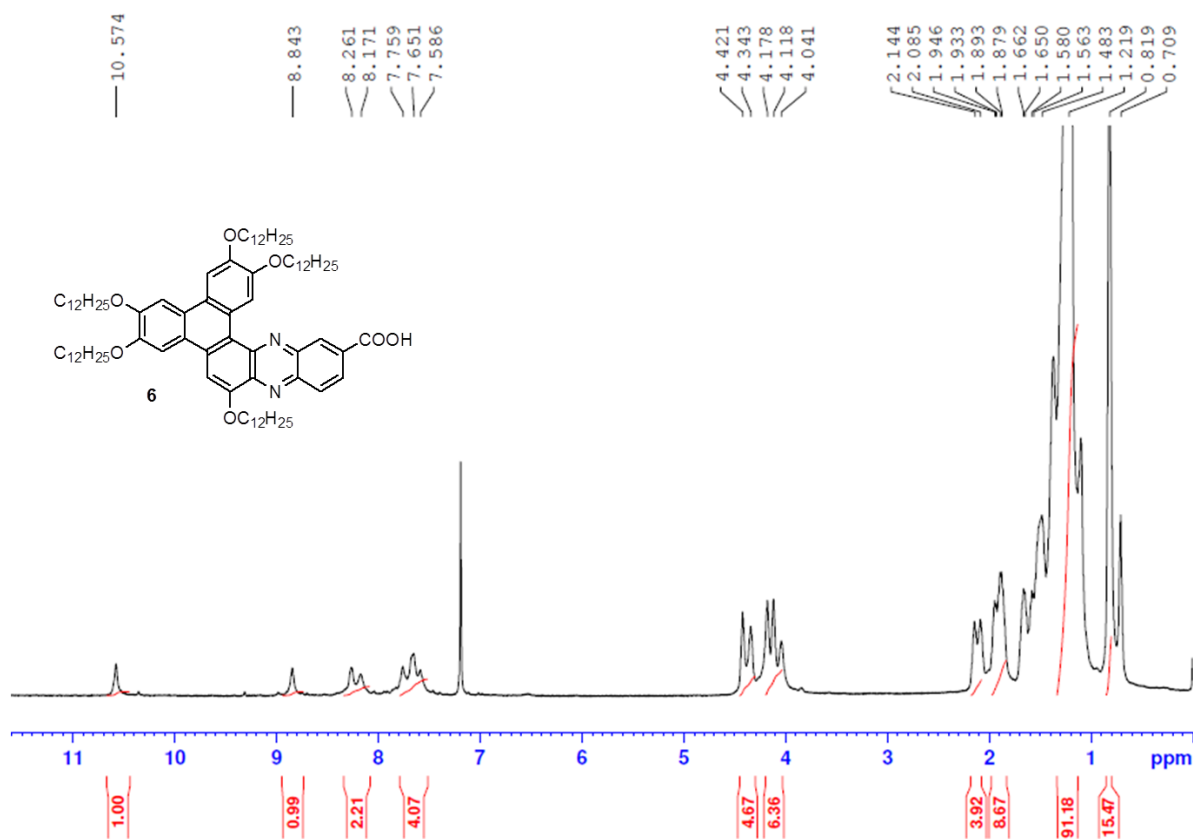


Figure S8. ^1H NMR spectra of compound 6.

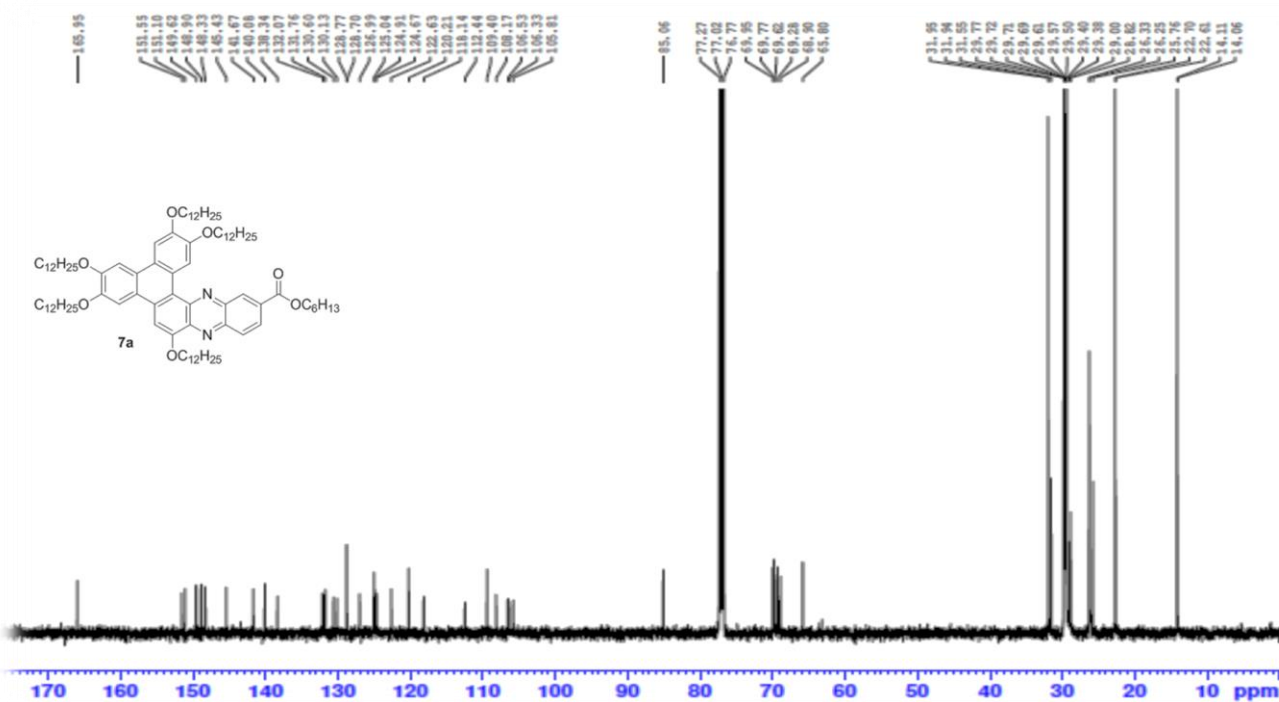
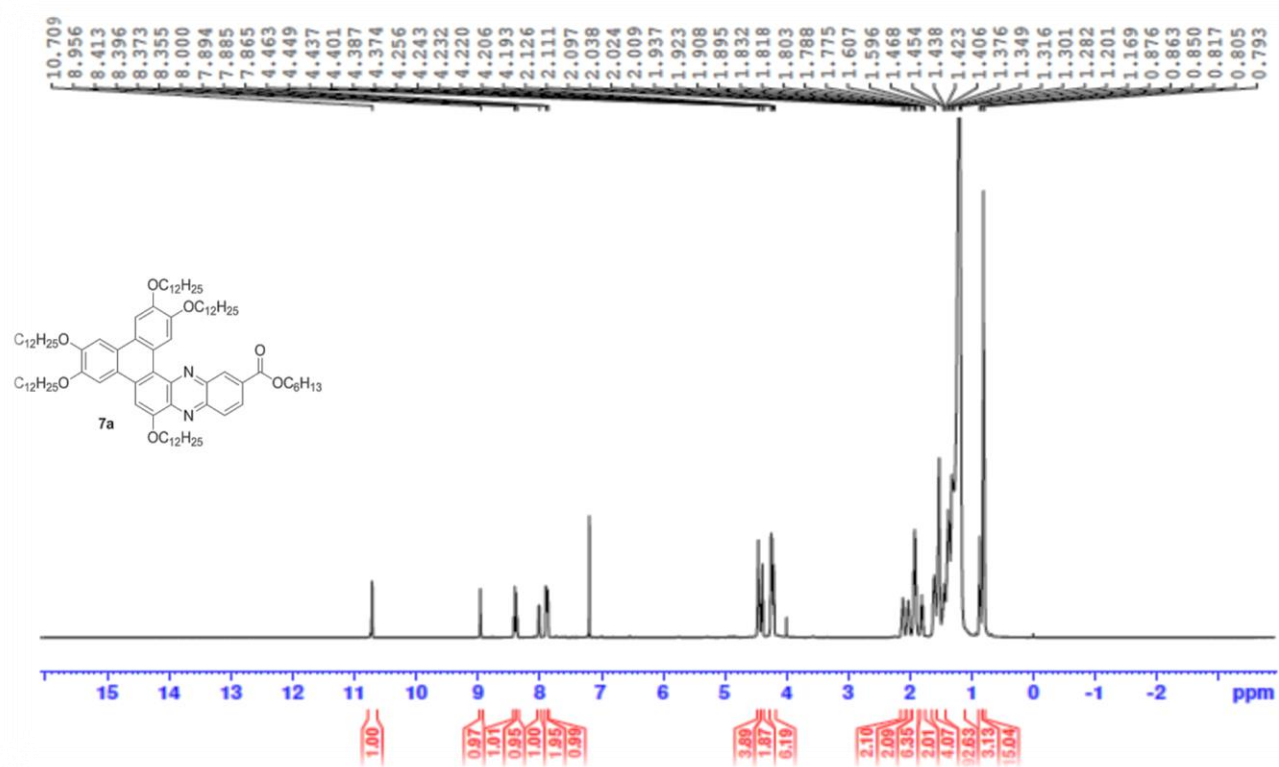


Figure S9. ¹H NMR and ¹³C NMR spectra of compound 7a.

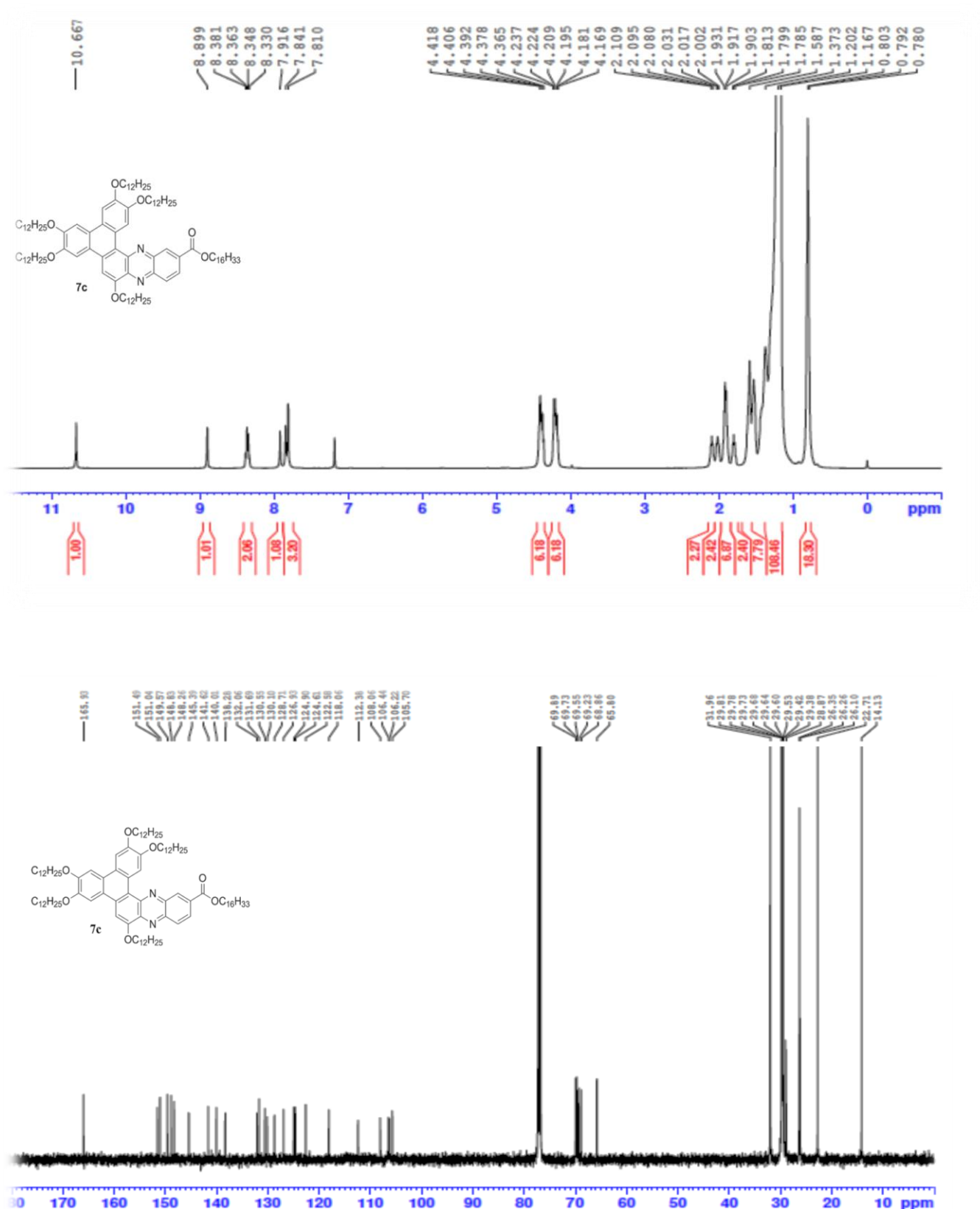


Figure S11. ¹H NMR and ¹³C NMR spectra of compound **7c**.

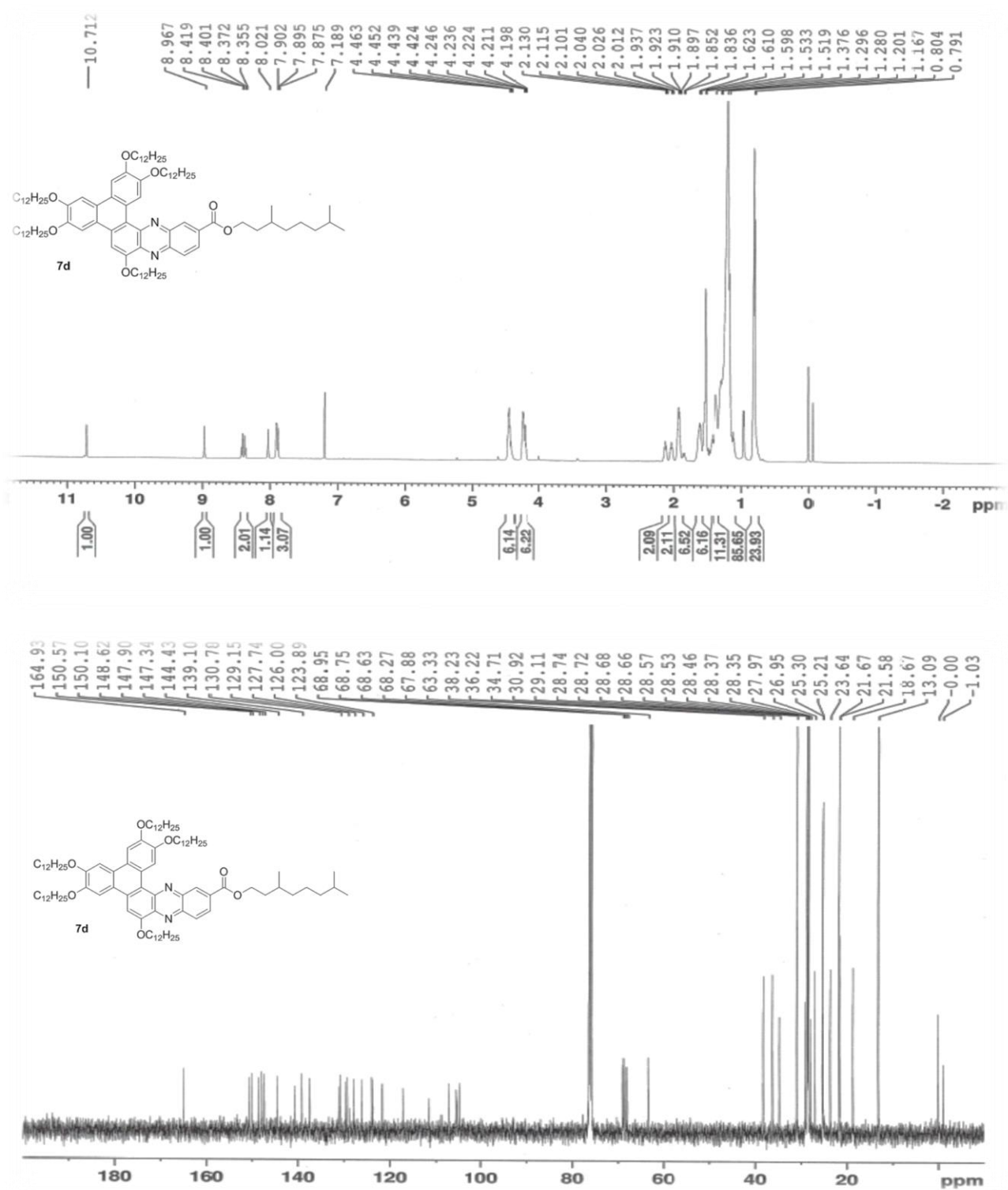


Figure S12. ¹H NMR and ¹³C NMR spectra of compound **7d**.

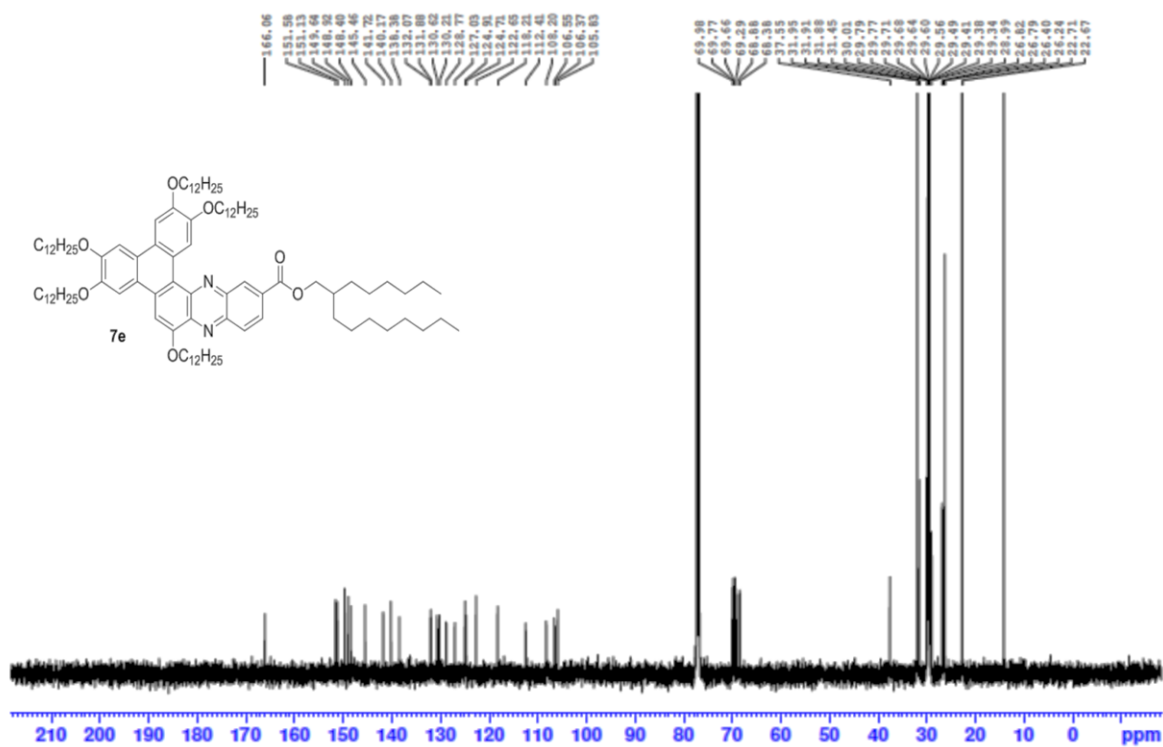
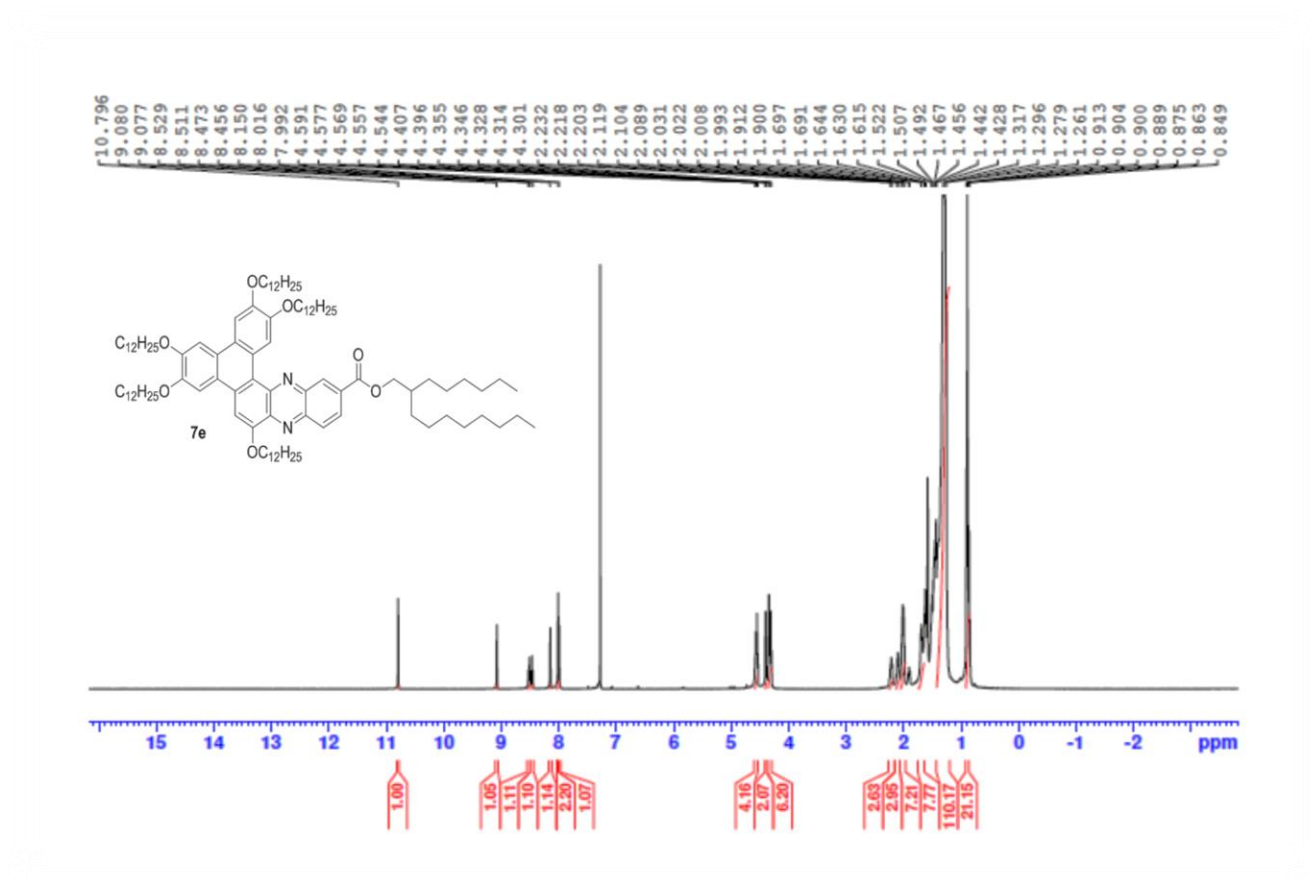


Figure S13. ¹H NMR and ¹³C NMR spectra of compound **7e**.