

Supporting Information

S. 1. Spectral data

S.1.1. FT-IR (KBr): $\nu_{\max}/\text{cm}^{-1}$

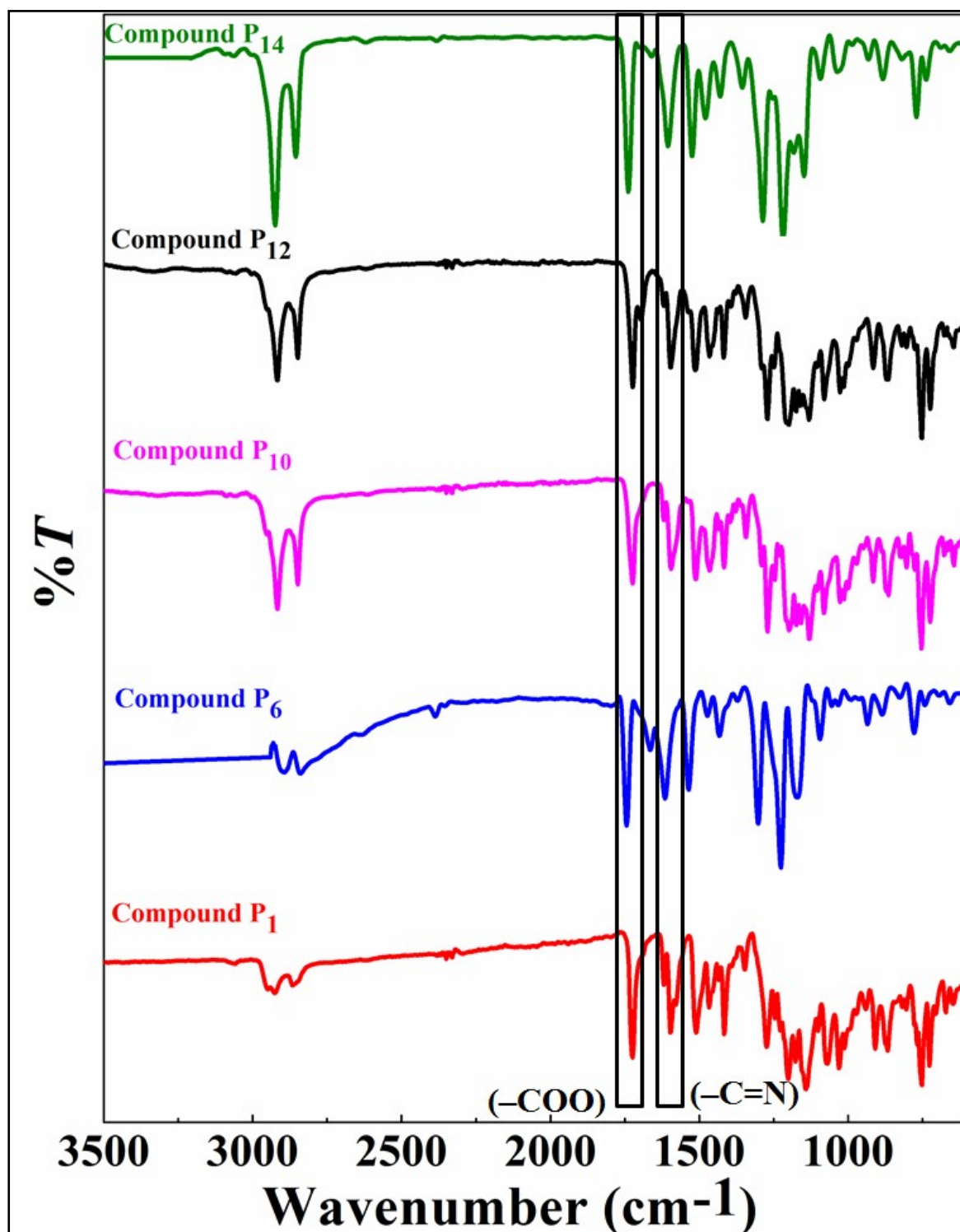


Figure S.1. FT-IR spectra of samples P₁, P₆, P₁₀, P₁₂ and P₁₄

The recorded FT-IR spectra of the prepared samples (P₁, P₆, P₁₀, P₁₂ and P₁₆) have been illustrated in **Figure S1** and interpreted as follows:

Compound P₁: ~3059 (=C–H str. multiple), ~2866 and ~2925 (–C–H str.), ~1597 (–C=N), ~1724 (–COO, ester linkage), ~1509 & ~1619, 1644 (–C=C– aromatic ring), ~1466 & ~1415 (C–H bending of alkene), ~1204 (C–O str. of ether linkage), ~1276 (C–N of thiophene ring), ~1029 & ~1141 (C–H hydrocarbon), ~726 & (C–S of thiophene ring), ~645 and ~752 (*p*-substituted phenyl ring), and ~866 poly(–CH₂–)*n*.

Compound P₆: ~3086 (=C–H str. multiple), ~2848 and ~2917 (–C–H str.), ~1598 (–C=N), ~1728 (–COO, ester linkage), ~1514 & ~1648 (–C=C– aromatic ring), ~1275 & ~1345 (C–H bending of alkene), ~1206 (C–O str. of ether linkage), ~1242 (C–N of thiophene ring), ~1031 & ~1125 (C–H hydrocarbon), ~724 & (C–S of thiophene ring), ~645 and ~752 (*p*-substituted phenyl ring), and ~865 poly(–CH₂–)*n*.

Compound P₁₀: ~3052 & ~3086 (=C–H str. multiple), ~2848 and ~2916 (–C–H str.), ~1594 (–C=N), ~1723 (–COO, ester linkage), ~1514 & ~1650 (–C=C– aromatic ring), ~1270 & ~1343 (C–H bending of alkene), ~1197 (C–O str. of ether linkage), ~1270 (C–N of thiophene ring), ~1026 & ~1129 (C–H hydrocarbon), ~723 & (C–S of thiophene ring), ~644 and ~752 (*p*-substituted phenyl ring), and ~864 poly(–CH₂–)*n*.

Compound P₁₂: ~3086 (=C–H str. multiple), ~2848 and ~2917 (–C–H str.), ~1596 (–C=N), ~1728 (–COO, ester linkage), ~1514 & ~1645 (–C=C– aromatic ring), ~1275 & ~1345 (C–H bending of alkene), ~1206 (C–O str. of ether linkage), ~1242 (C–N of thiophene ring), ~1031 & ~1125 (C–H hydrocarbon), ~724 & (C–S of thiophene ring), ~645 and ~752 (*p*-substituted phenyl ring), and ~865 poly(–CH₂–)*n*.

Compound P₁₄: ~3000 (=C–H str. multiple), ~2851 and ~2920 (–C–H str.), ~1594 (–C=N), ~1728 (–COO, ester linkage), ~1513 & ~1650 (aromatic ring), ~1275 & ~1344 (C–H bending of alkene), ~1206 (C–O str. of ether linkage), ~1241 (C–N), ~1080 & ~1135 (–C–H

hydrocarbon), ~724 & (C–S of thiophene ring), ~644 and ~724 (*p*-substituted phenyl ring), and ~805 and ~869 poly(–CH₂–)*n*.

S.1.2. Proton NMR Spectra (¹H-NMR) (CDCl₃) (δ value):

Compound P₁: ¹H NMR (400 MHz, CDCl₃) δ 9.13 (s, 2H), 8.18 – 8.10 (m, 4H), 8.05 – 7.96 (m, 3H), 7.89 (s, 1H), 7.89 – 7.78 (m, 4H), 7.69 (dd, *J* = 6.1, 2.1 Hz, 3H), 7.51 (ddd, *J* = 8.4, 7.3, 1.3 Hz, 3H), 7.47 – 7.34 (m, 8H), 6.98 (dd, *J* = 8.5, 2.3 Hz, 3H), 4.14 (td, *J* = 7.0, 1.8 Hz, 5H), 3.98 (d, *J* = 2.6 Hz, 8H), 1.92 (p, *J* = 7.0 Hz, 6H), 1.55 – 1.48 (m, 6H), 1.39 (hept, *J* = 3.1, 2.5 Hz, 11H), 0.99 – 0.90 (m, 8H).

Compound P₆: ¹H NMR (400 MHz, CDCl₃) δ 8.23 (d, *J* = 8.3 Hz, 2H), 8.07 (d, *J* = 8.7 Hz, 2H), 7.98 (d, *J* = 8.3 Hz, 2H), 7.89 (d, *J* = 8.8 Hz, 1H), 7.71 (s, 1H), 7.42 (d, *J* = 8.7 Hz, 2H), 4.45 (d, *J* = 7.0 Hz, 2H), 4.14 (t, *J* = 6.9 Hz, 2H), 3.99 (s, 3H), 1.46 (t, *J* = 7.1 Hz, 4H), 1.30 (d, *J* = 17.5 Hz, 6H), 0.91 (d, *J* = 6.9 Hz, 3H).

Compound P₁₀: ¹H NMR (400 MHz, CDCl₃) δ 8.48 (s, 1H), 8.15 – 8.08 (m, 2H), 8.05 – 7.98 (m, 2H), 7.88 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.69 (d, *J* = 2.0 Hz, 1H), 7.41 – 7.34 (m, 2H), 7.28 – 7.20 (m, 2H), 6.98 (d, *J* = 8.5 Hz, 1H), 4.41 (q, *J* = 7.1 Hz, 2H), 4.14 (t, *J* = 6.9 Hz, 2H), 3.98 (s, 3H), 1.98 – 1.86 (m, 1H), 1.64 (s, 6H), 1.52 – 1.37 (m, 5H), 1.30 (s, 11H), 0.94 – 0.87 (m, 3H).

Compound P₁₂: ¹H NMR (400 MHz, CDCl₃) δ 8.26 – 8.20 (m, 2H), 7.28 (s, 1H), 6.54 – 6.48 (m, 2H), 4.17 (dd, *J* = 22.6, 7.5 Hz, 3H), 3.97 (s, 1H), 3.02 (s, 6H), 1.71 (dt, *J* = 13.5, 3.9 Hz, 5H), 1.61 (s, 2H), 1.65 – 1.57 (m, 1H), 1.47 – 1.36 (m, 2H), 1.35 (s, 5H), 1.32 (d, *J* = 3.2 Hz, 0H), 1.29 (d, *J* = 10.1 Hz, 4H), 1.23 – 1.12 (m, 3H), 1.09 (dd, *J* = 12.7, 9.2 Hz, 5H), 0.94 – 0.86 (m, 1H).

Compound P₁₄: ¹H NMR (400 MHz, CDCl₃) δ 8.21 (d, *J* = 8.3 Hz, 2H), 8.05 (d, *J* = 8.7 Hz, 2H), 7.96 (d, *J* = 8.3 Hz, 2H), 7.86 (d, *J* = 8.8 Hz, 1H), 7.68 (s, 1H), 7.39 (d, *J* = 8.7 Hz, 2H),

4.42 (d, $J = 7.0$ Hz, 2H), 4.12 (t, $J = 6.9$ Hz, 2H), 3.96 (s, 3H), 1.43 (t, $J = 7.1$ Hz, 4H), 1.27 (d, $J = 17.5$ Hz, 6H), 0.88 (d, $J = 6.9$ Hz, 3H).

The obtained ^1H NMR data are reliable with the molecular structure of corresponding compound.

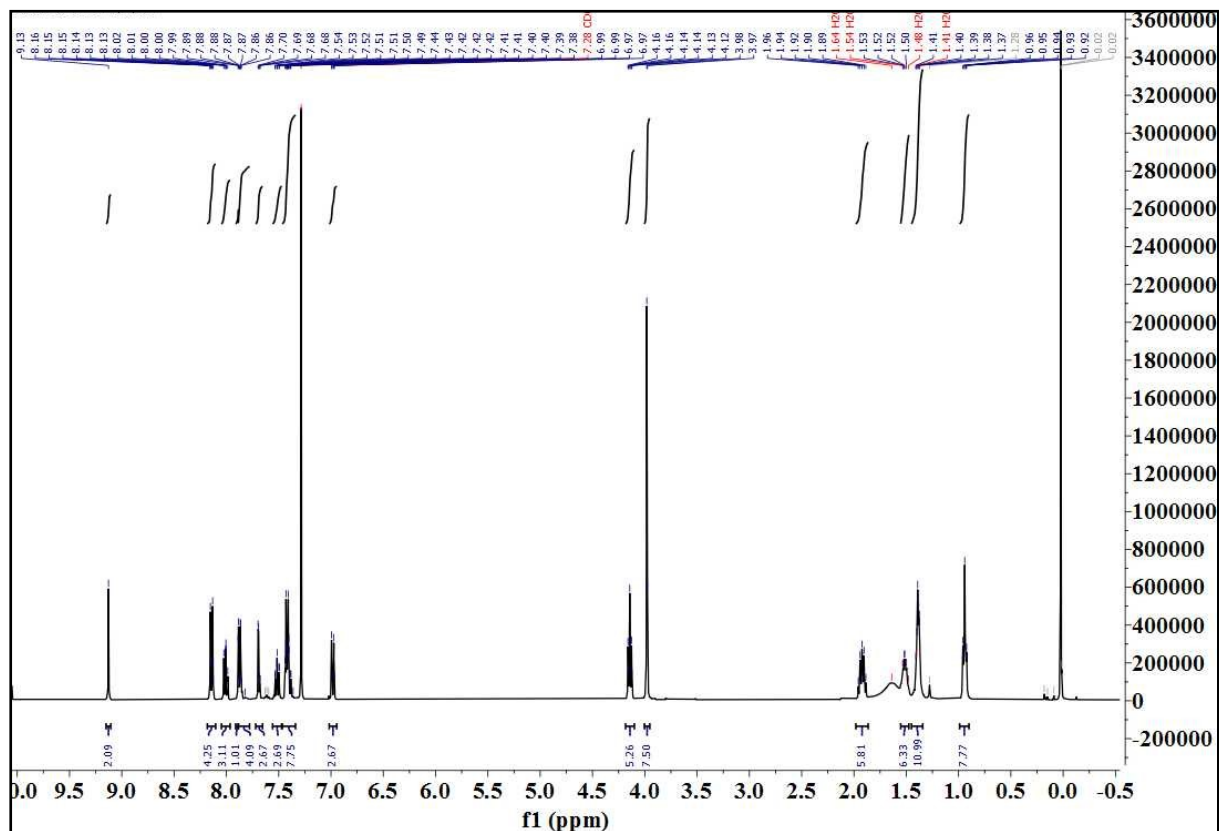


Figure S2. ^1H -NMR spectra of compound P₁

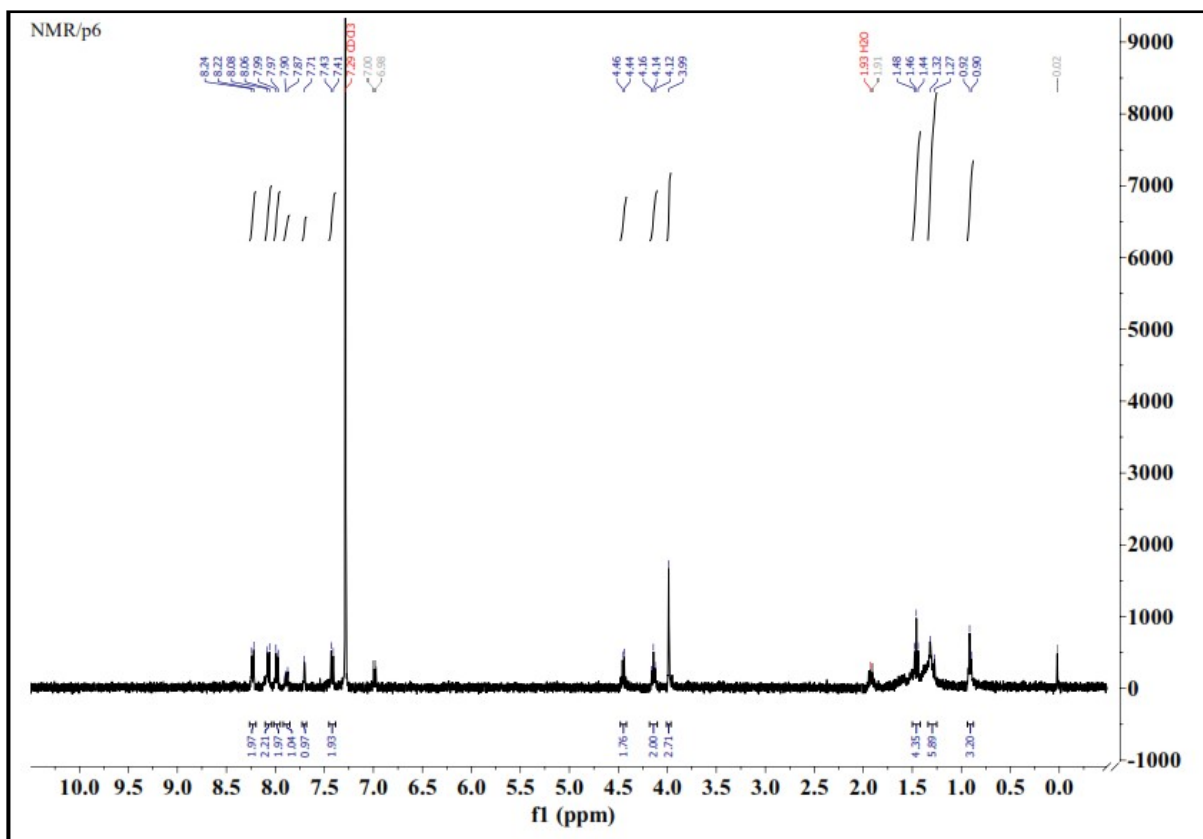


Figure S3. ¹H-NMR spectra of compound P₆

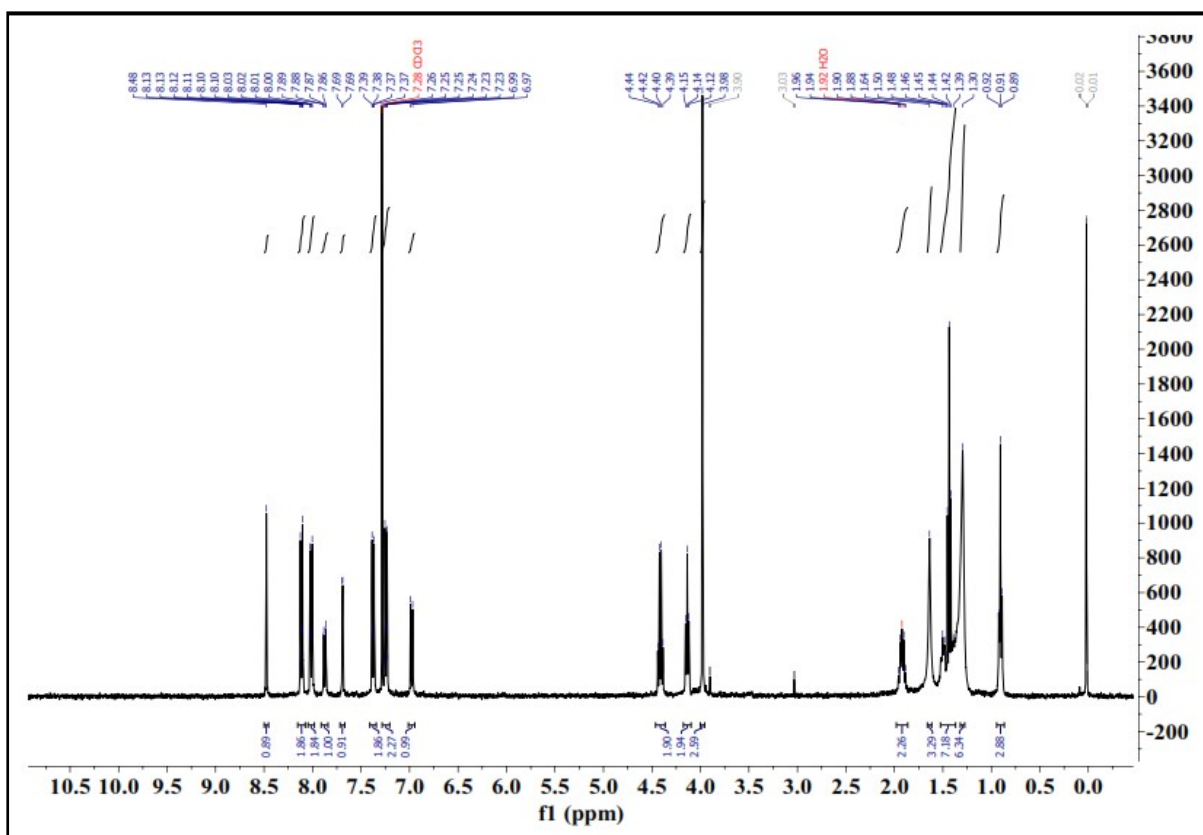


Figure S4. ¹H-NMR spectra of compound P₁₀

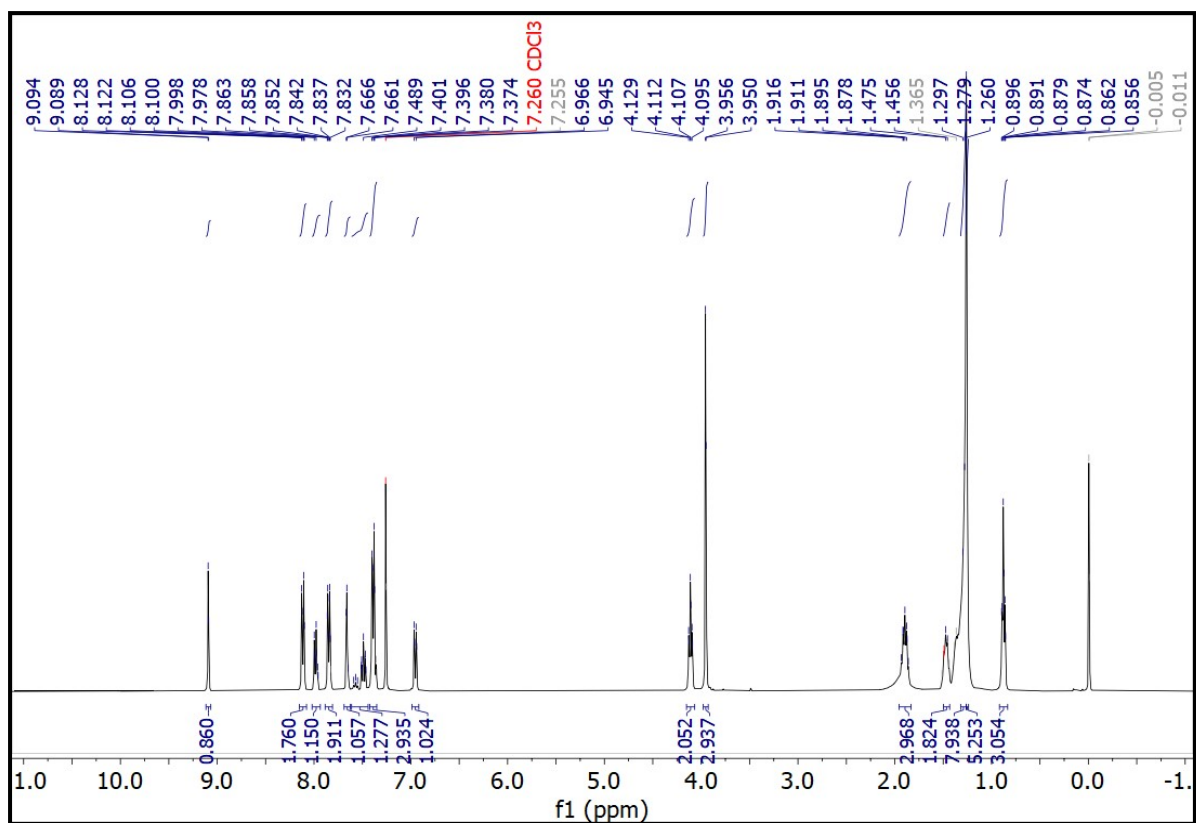


Figure S5. ¹H-NMR spectra of compound P₁₂

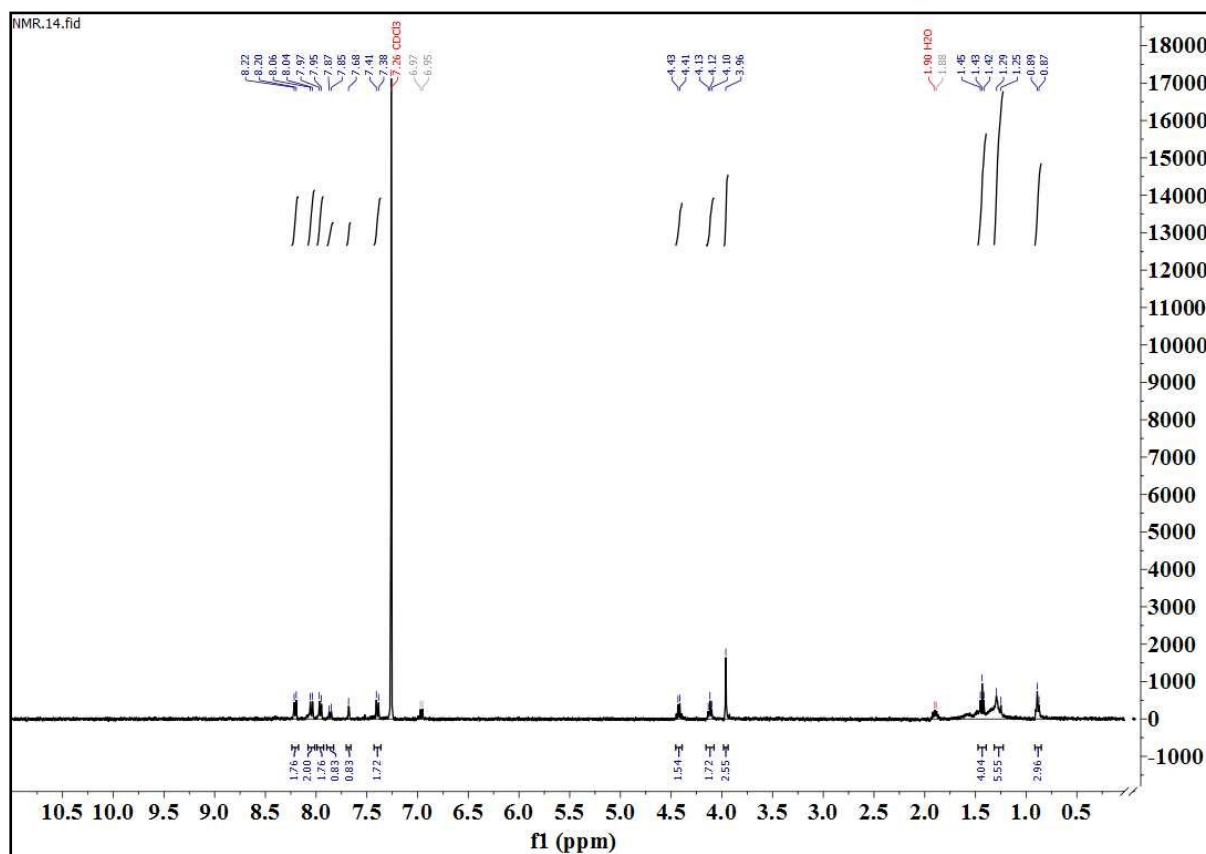


Figure S6. ¹H-NMR spectra of compound P₁₄

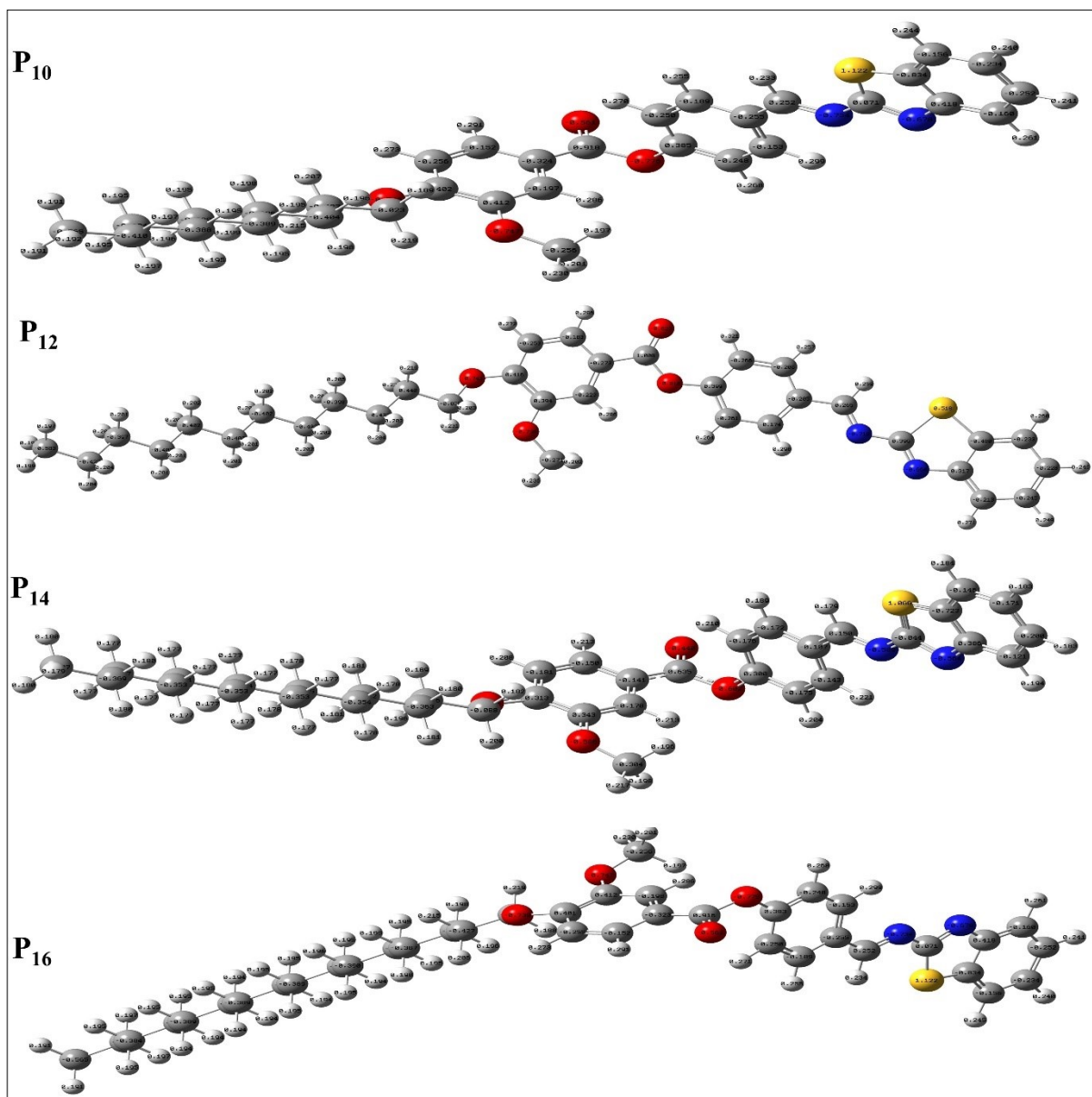


Figure S7. Mulliken charges for the optimized structures of Sample P₁₀, P₁₂, P₁₄ and P₁₆ samples

Table S1. Melting point and transition temperature (°C)

Samples	Melting point	Liquid crystal to isotropic
P₁	122	126
P₂	143	178
P₃	141	168
P₄	121	159
P₆	111	150
P₈	104	137
P₁₀	82	108
P₁₂	78	104
P₁₄	89	101
P₁₆	85	108