

Supporting Information

Iodine and Nickel Ions Adsorption by Conjugated Copolymers Bearing Repeating Units of Dicyclopentapyrenyl and Various Thiophene Derivatives

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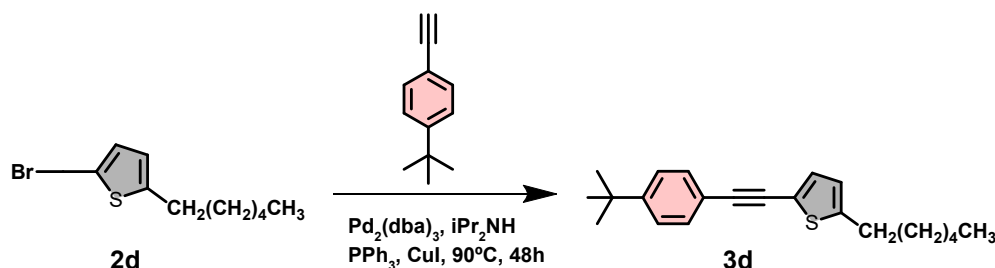
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(i). Synthesis of 2-((4-(tert-butyl)phenyl)ethynyl)-5-hexylthiophene (**3d**)



3d was prepared following procedure A with 2-bromo-5-hexylthiophene **2d** (0.3 g, 1.2 mmol, 1 eq.), 1-(tert-butyl)-4-ethynylbenzene **1a** (0.46 g, 2.9 mmol, 2.4 eq.) $\text{Pd}_2(\text{dba})_3$ (6.7 mg, 0.0073 mmol, 0.6 mol%), PPh_3 (28 mg, 0.1 mmol), and CuI (4.6 mg, 0.02 mmol) in 10 mL of degassed diisopropylamine (iPr_2NH) at 90°C for 2 days. pale pink solid (140 mg, 93%). $^1\text{H-NMR}$ (600 MHz, CD_2Cl_2 , ppm): δ 7.76 (d, 2H, $J = 7.8$ Hz, ArH), 7.66 (s, 2H, ArH), 7.56 (dd, 2H, $J = 7.8, 6.6$ Hz, ArH), 7.52 (m, 4H, $J = 3.6$ Hz, ArH), 7.45 (m, 4H, ArH), 1.55 (s, 6H, $-\text{CH}_3$), 1.37 (s, 18H, $-\text{CH}_3$). $^{13}\text{C-NMR}$ (150 MHz, CD_2Cl_2 , ppm): δ 154.66, 152.35, 139.20, 131.80, 131.30, 126.50, 126.09, 122.94, 120.84, 90.44, 89.98, 47.47, 35.29, 31.50, 27.32. EI-HRMS: m/z calculated for M^{+} $\text{C}_{39}\text{H}_{38}$ 506.2974 found 506.2975.

(ii). CO_2 gas uptake studies

The CO_2 gas adsorption properties of **TPP1-3** were investigated by recording their CO_2 sorption isotherms with a pressure up to one atmosphere at temperatures of 273 K and 298 K (Figures S31-S33). The CO_2 uptake capacity of **TPP1** is 12.72 mg g^{-1} and 17.86 mg g^{-1} at 273 K and 298 K respectively. Furthermore, the conjugated polymers **TPP2** and **TPP3** display CO_2 uptake efficiency up to 17.53 mg g^{-1} and 18.20 mg g^{-1} at 273 K and 16.99 mg g^{-1} and 18.82 mg g^{-1} at 298 K, respectively

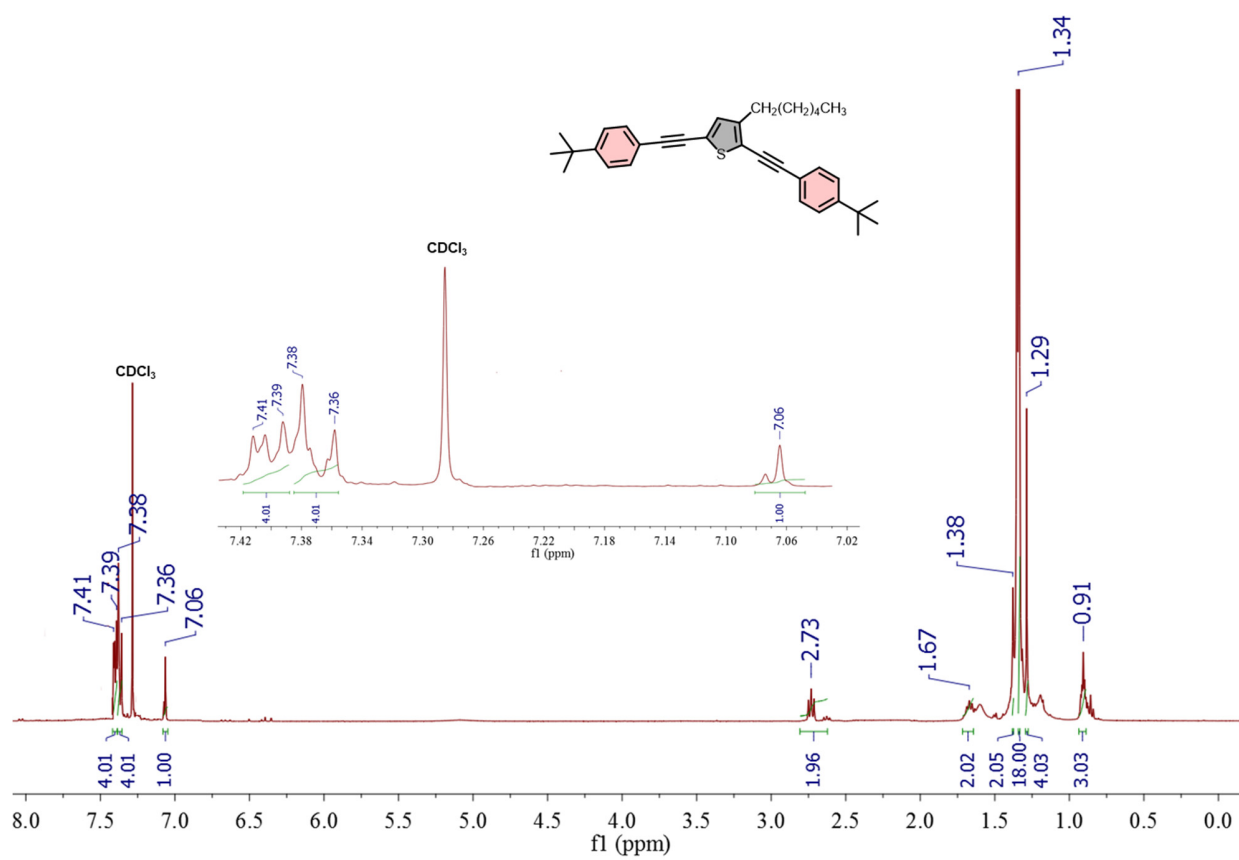


Figure S1 ¹H NMR spectrum of **3a**

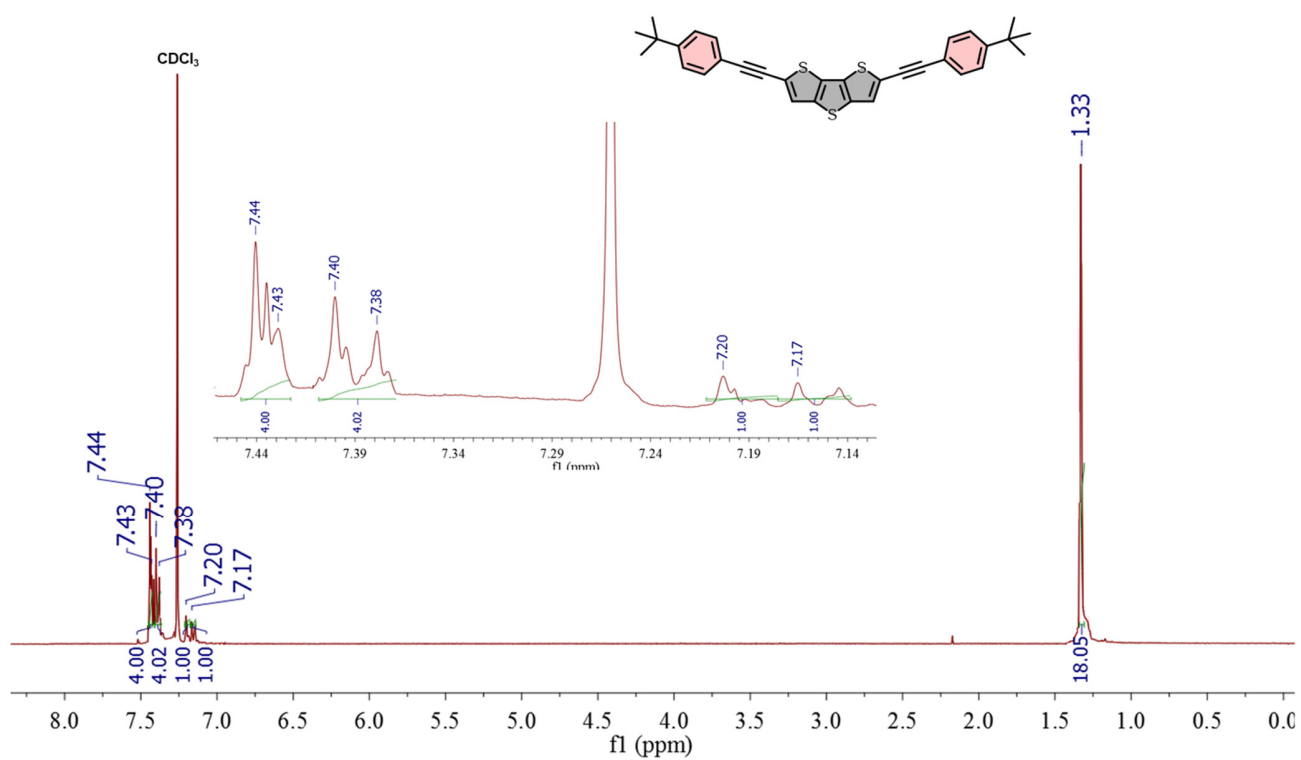


Figure S2 ¹H NMR spectrum of **3b**

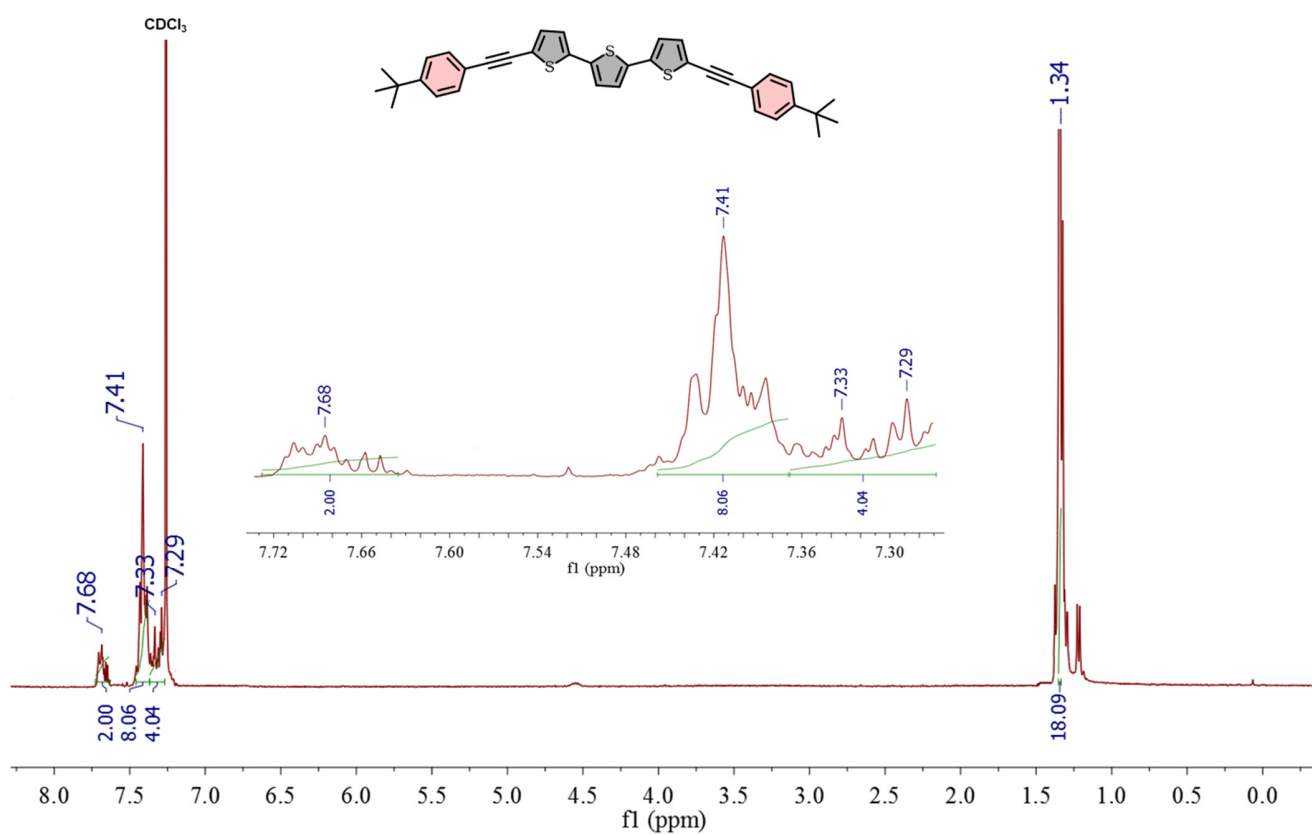


Figure S3 ^1H NMR spectrum of **3c**

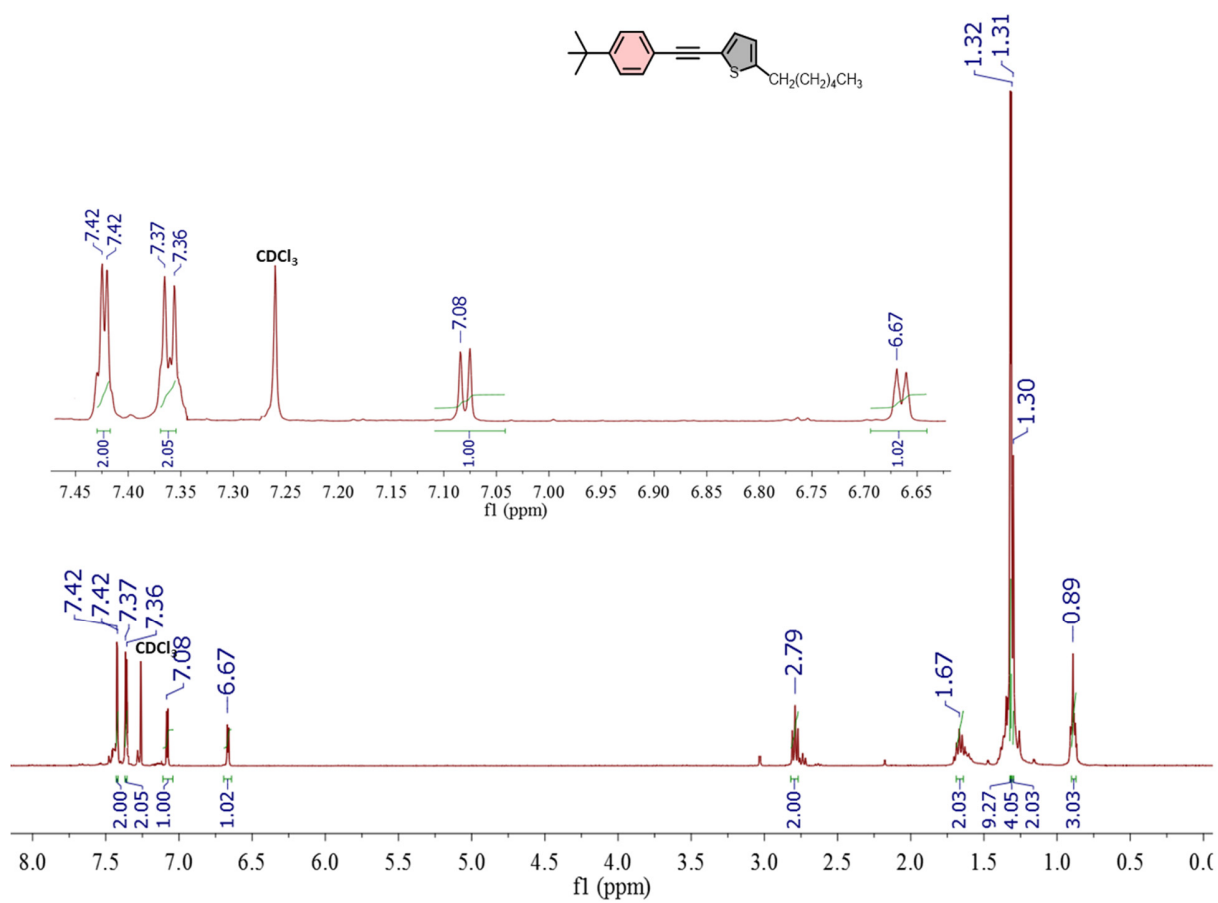


Figure S4 ^1H NMR spectrum of **3d**

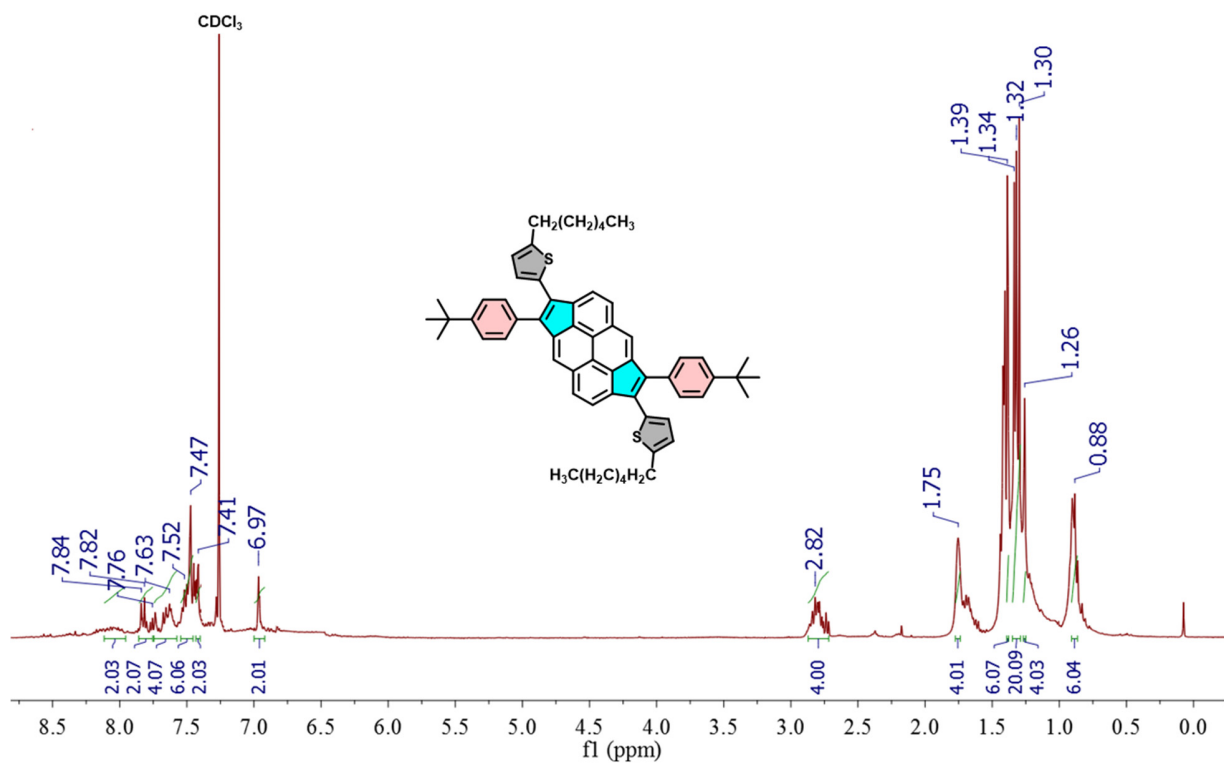


Figure S5 ^1H NMR spectrum of TPM

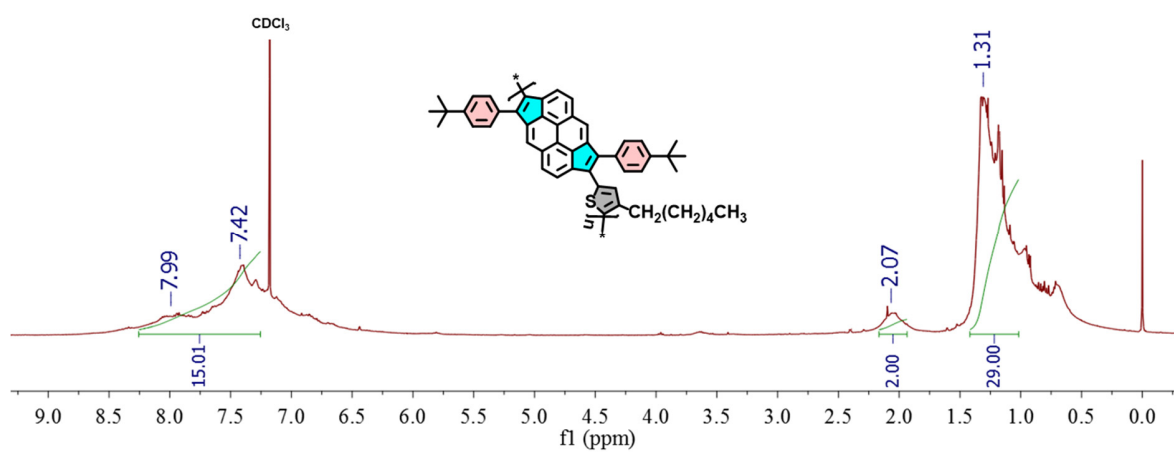


Figure S6 ^1H NMR spectrum of **TPP1**

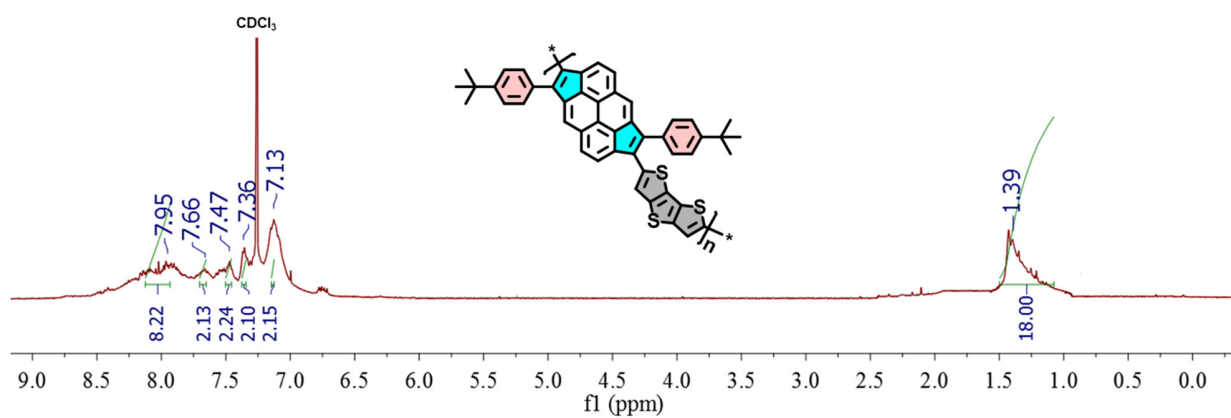


Figure S7 ¹H NMR spectrum of TPP2

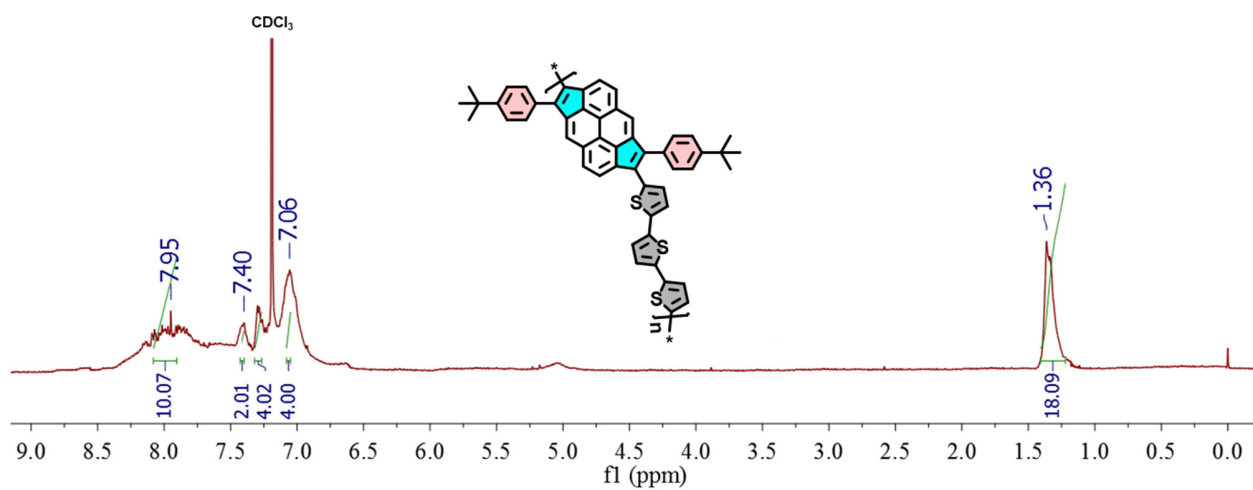


Figure S8 ¹H NMR spectrum of TPP3

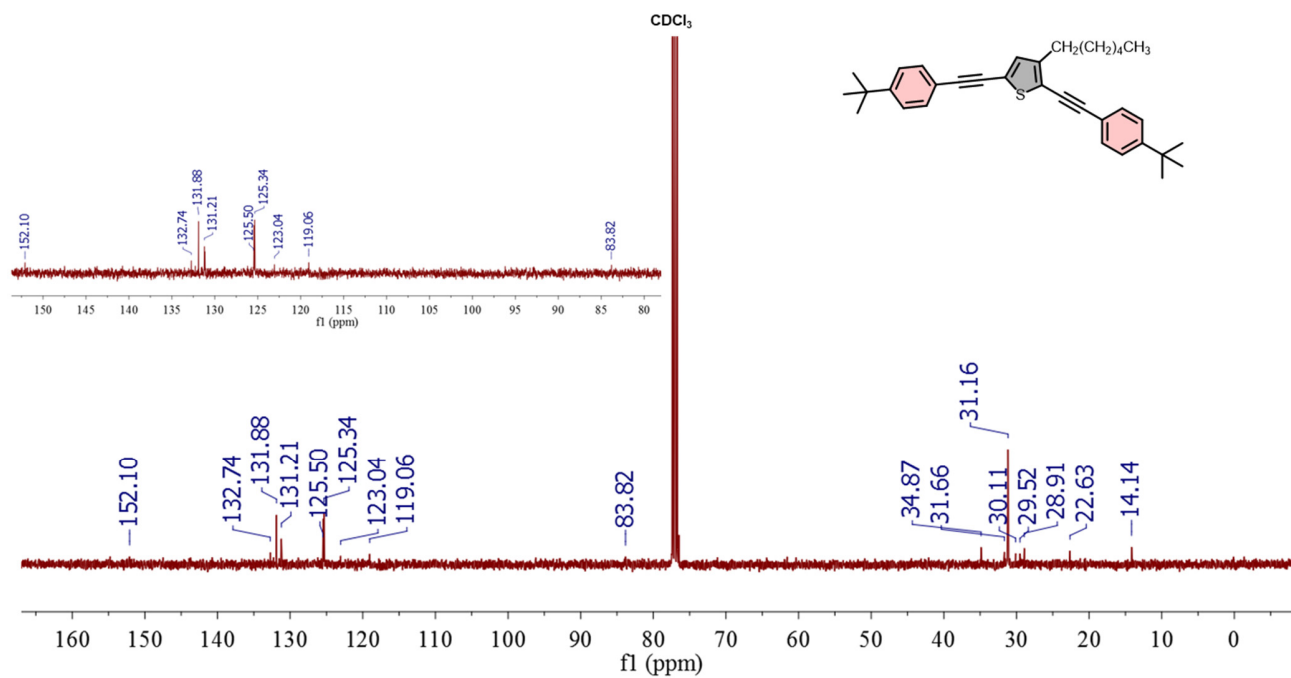


Figure S9 ^{13}C NMR spectrum of **3a**

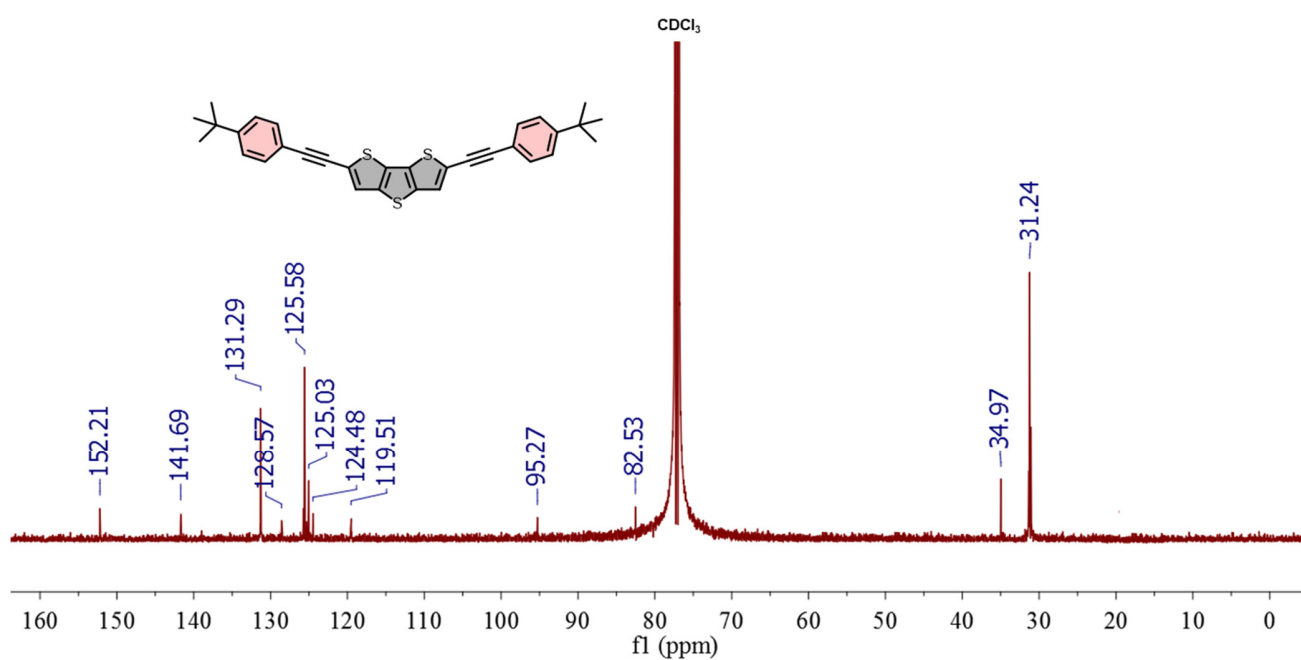


Figure S10 ^{13}C NMR spectrum of **3b**

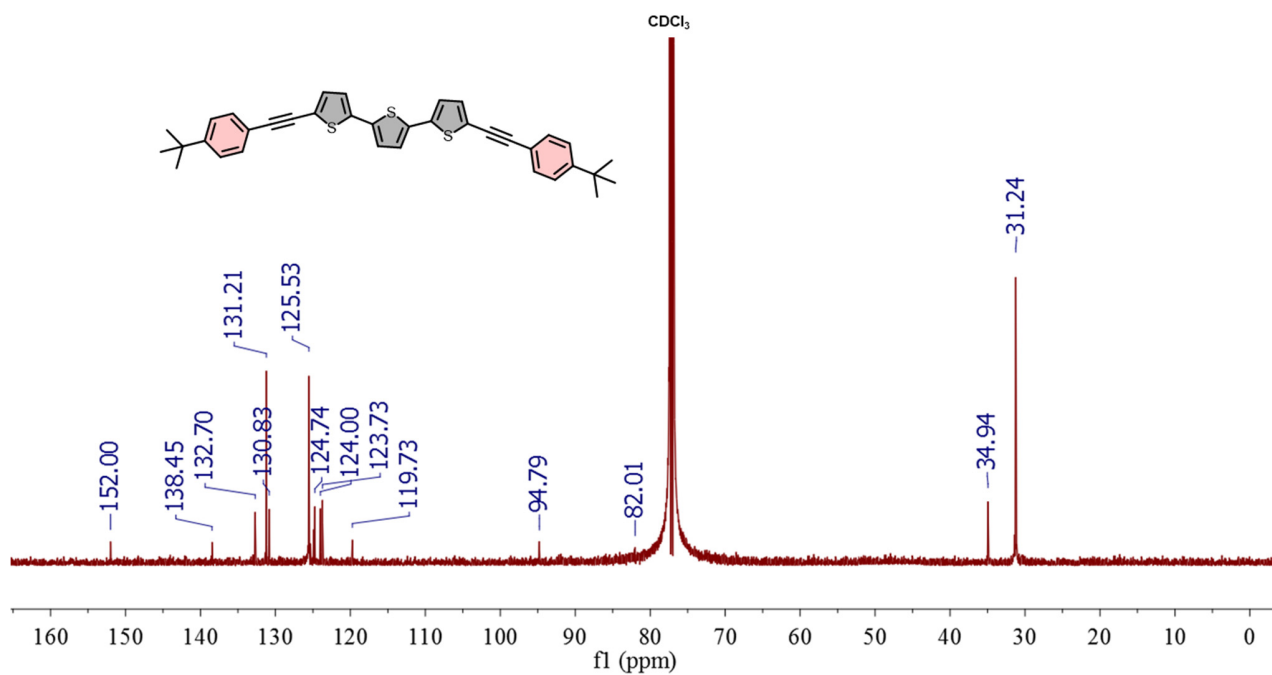


Figure S11 ¹³C NMR spectrum of **3c**

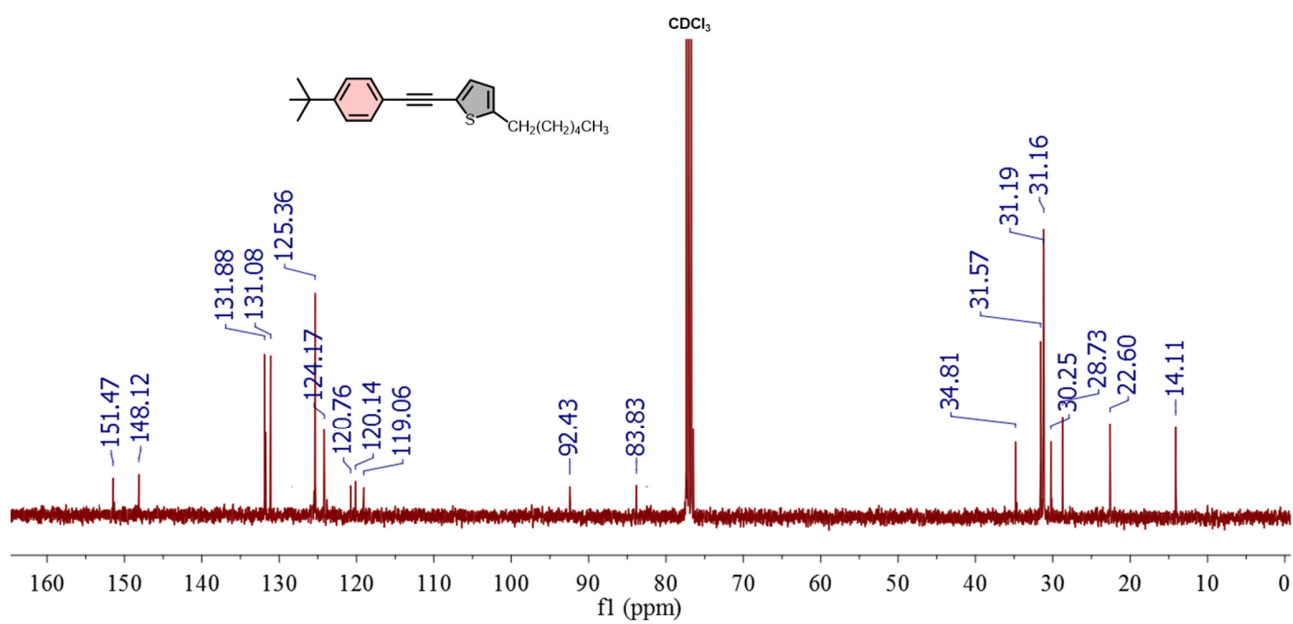


Figure S12 ¹³C NMR spectrum of **3d**

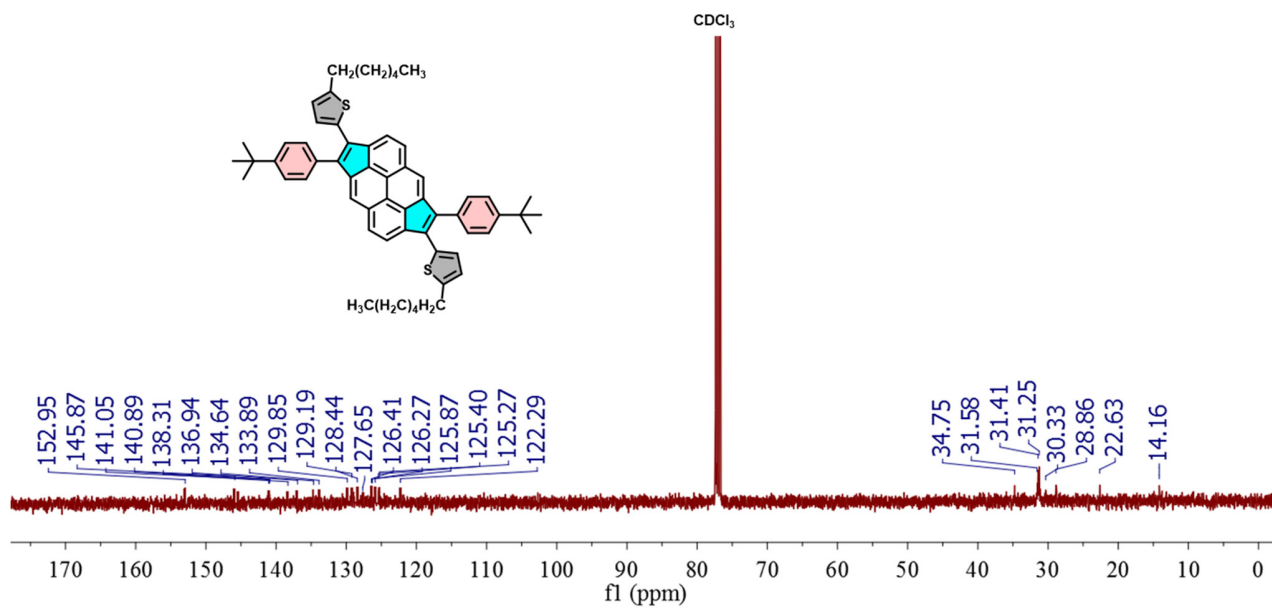


Figure S13 ^{13}C NMR spectrum of TPM

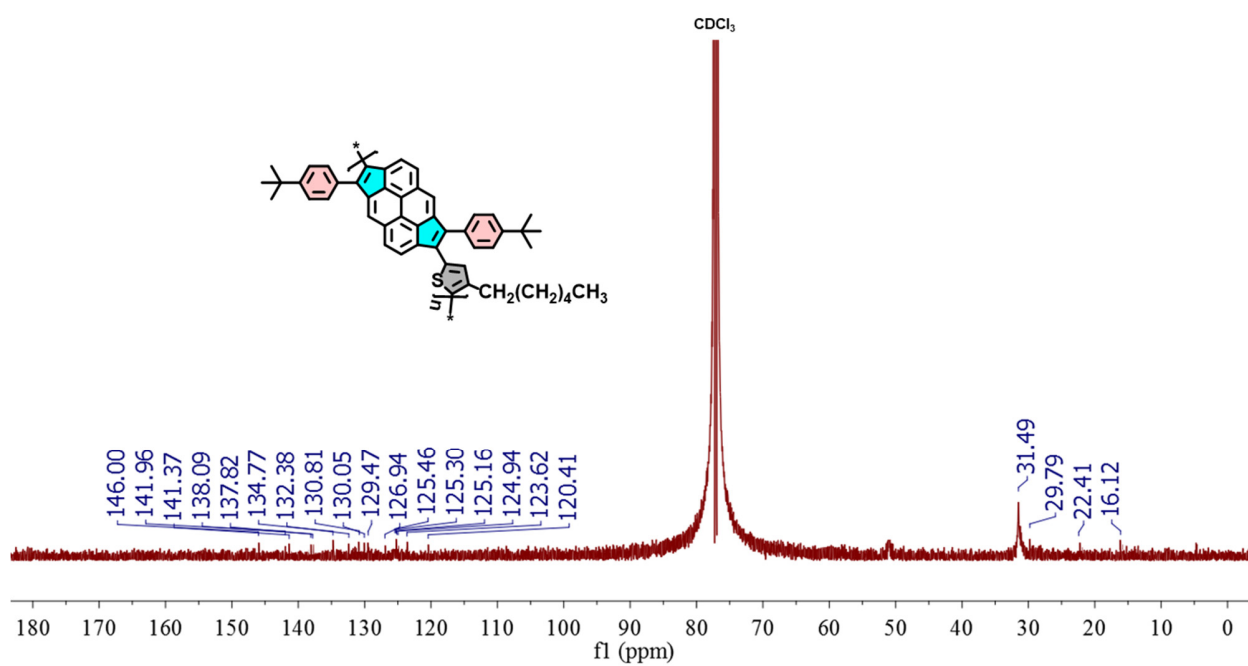


Figure S14 ^{13}C NMR spectrum of TPP1

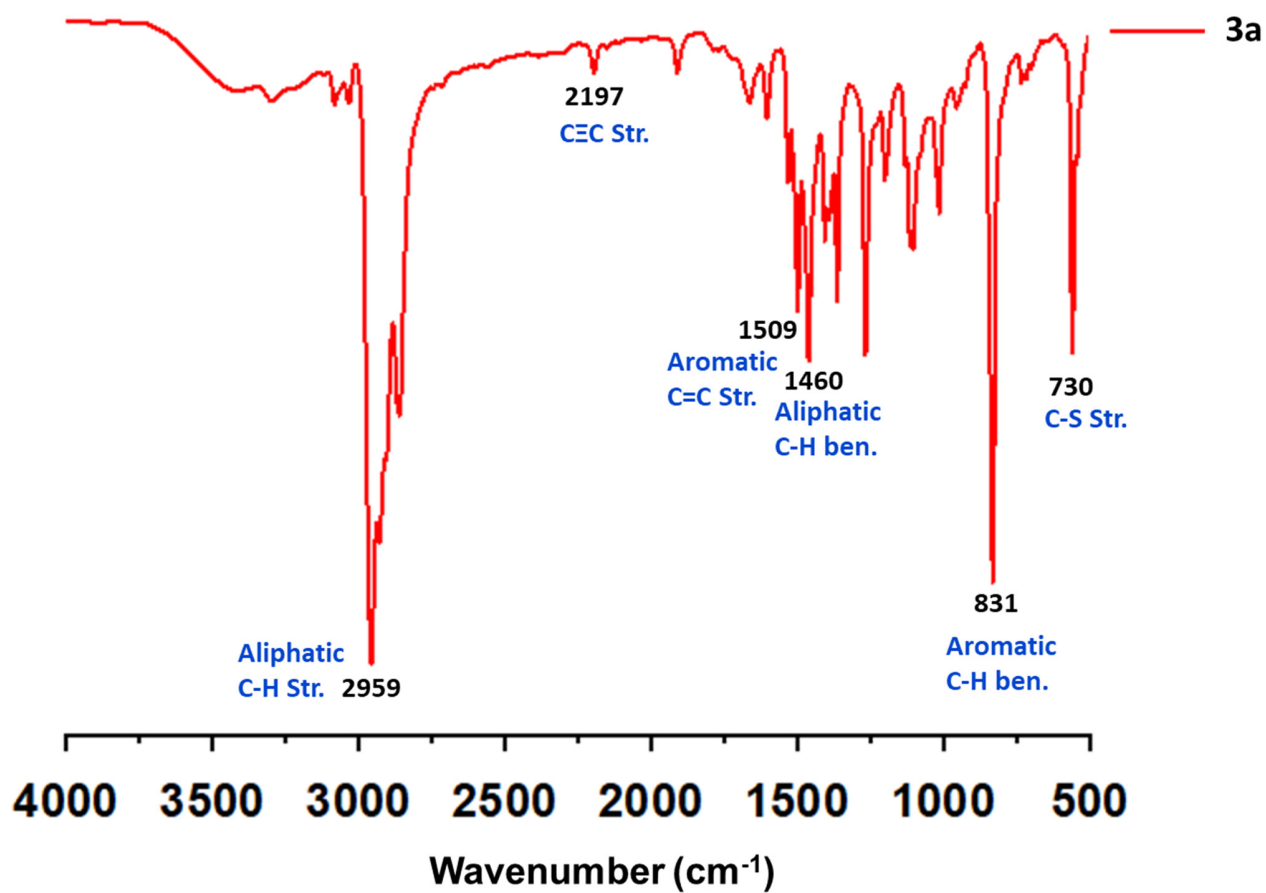


Figure S15 FTIR spectrum of 3a

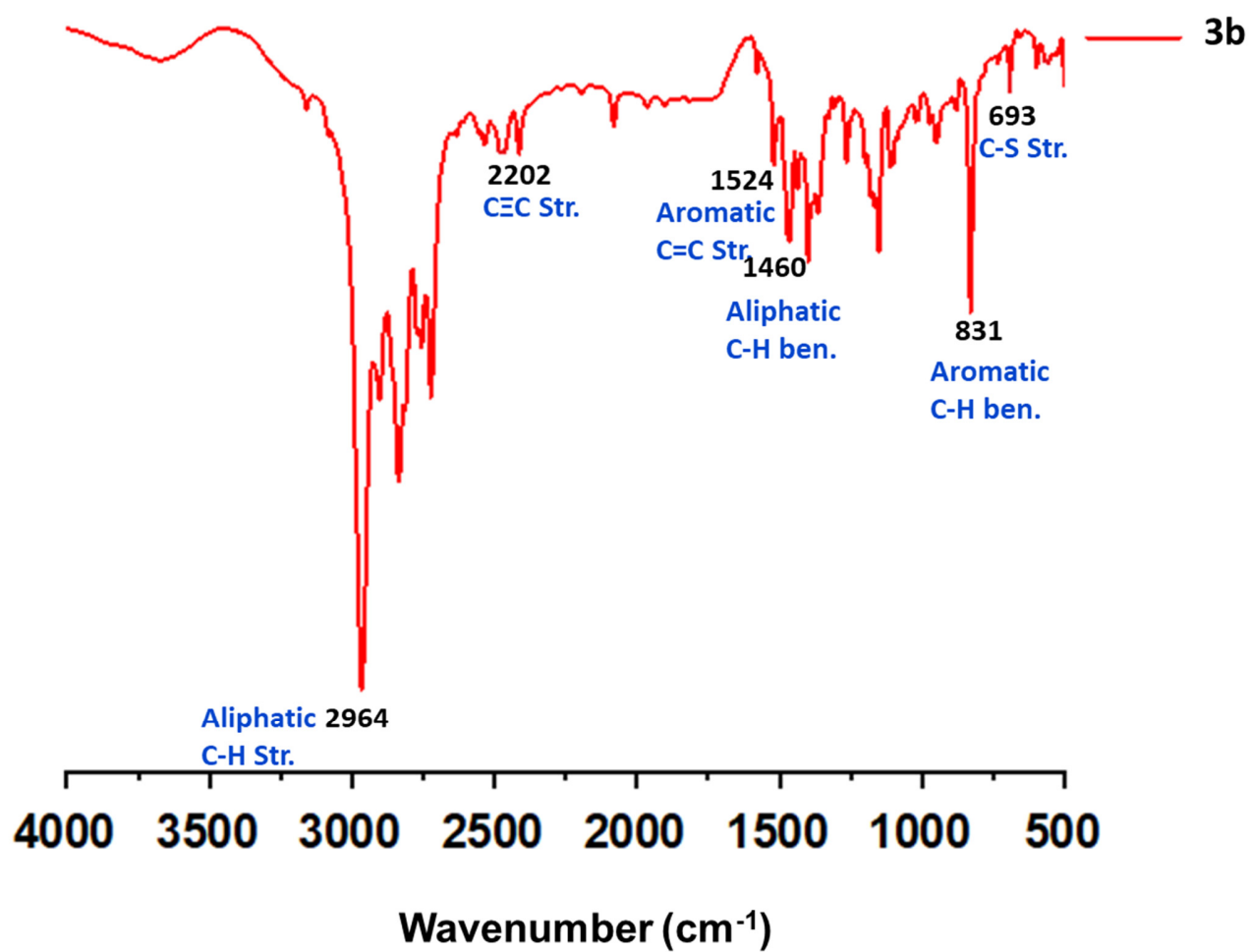


Figure S16 FTIR spectrum of 3b

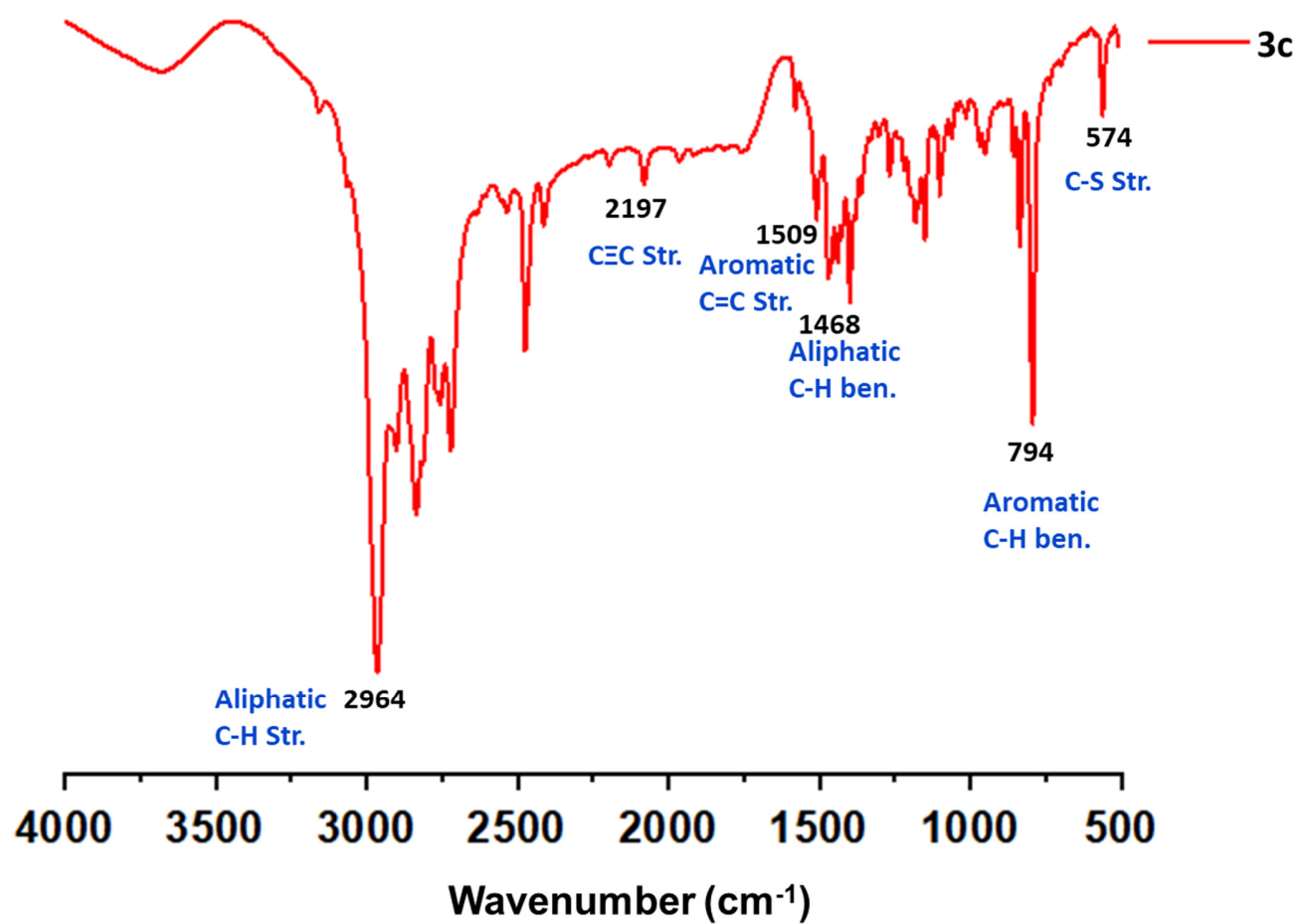


Figure S17 FTIR spectrum of 3c

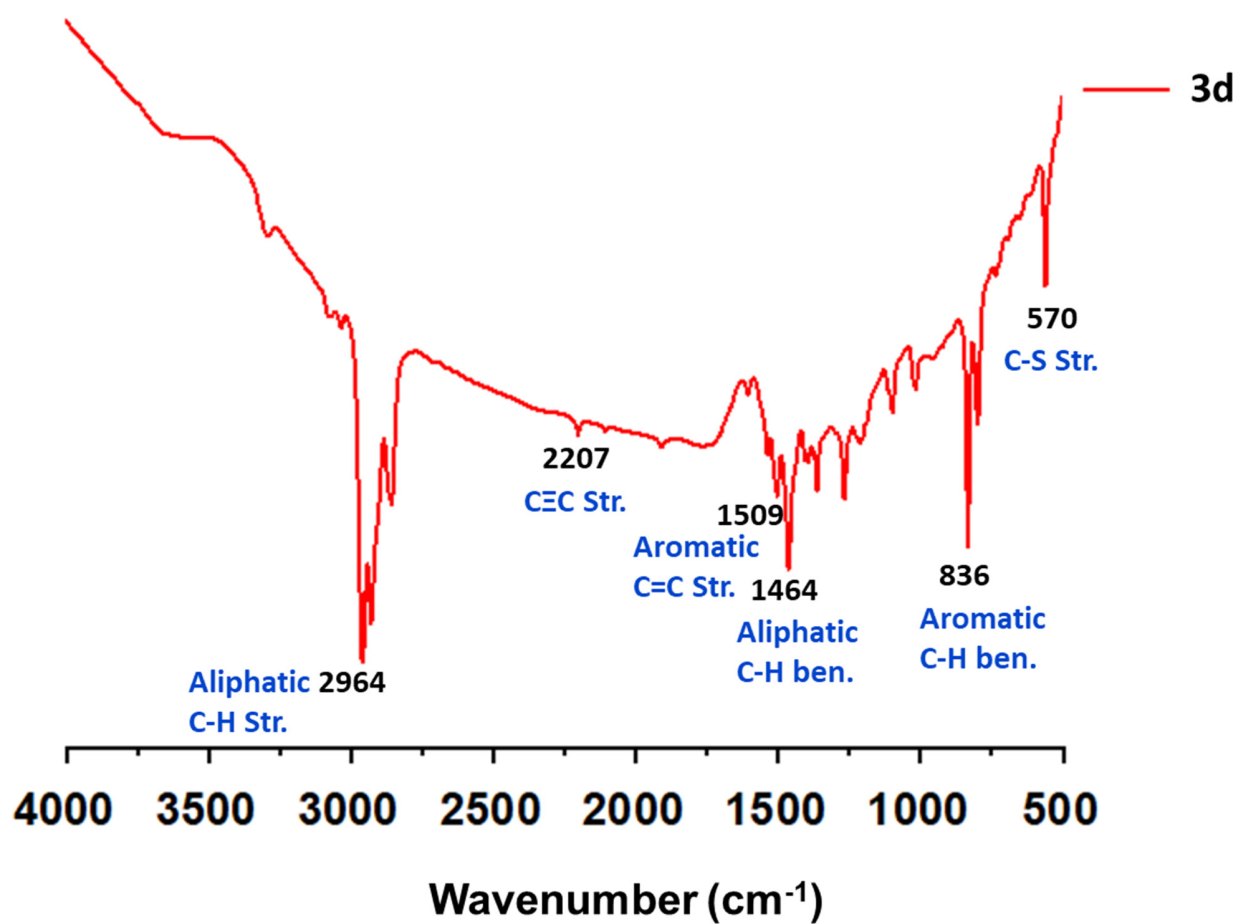


Figure S18 FTIR spectrum of 3d

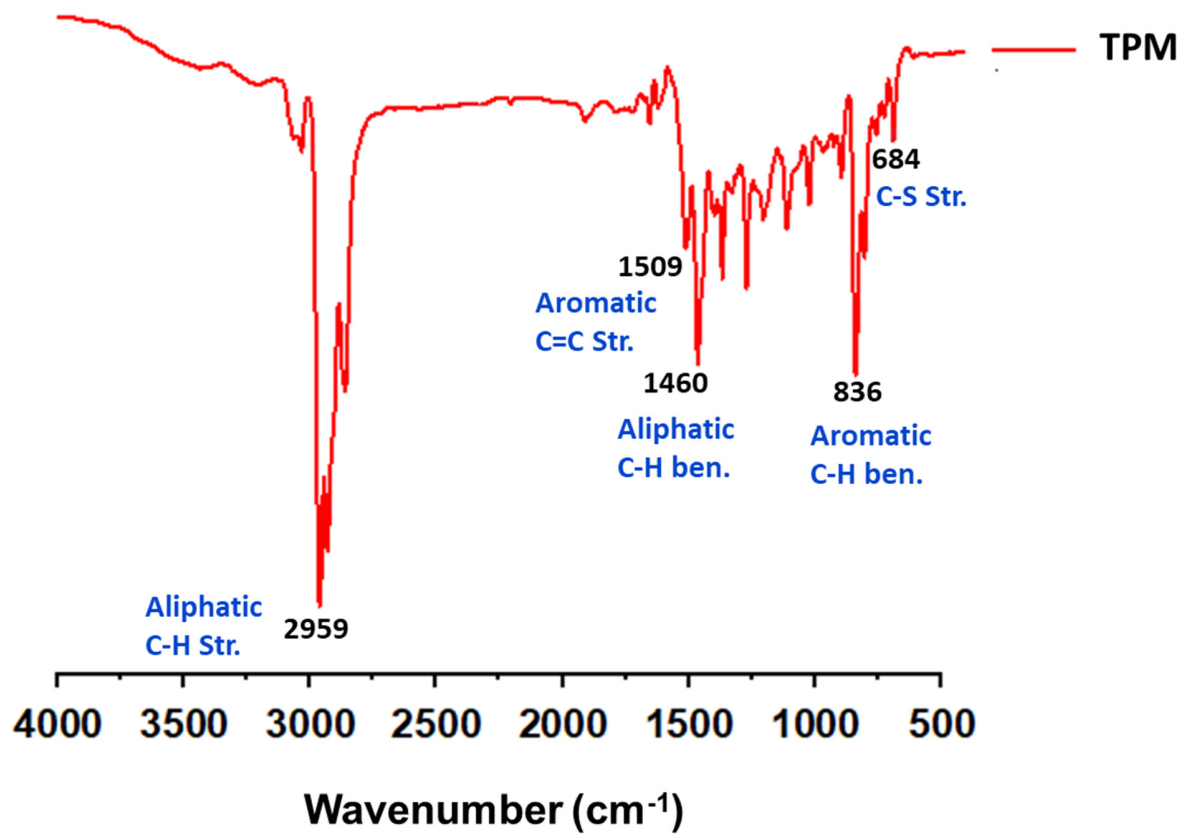


Figure S19 FTIR spectrum of TPM

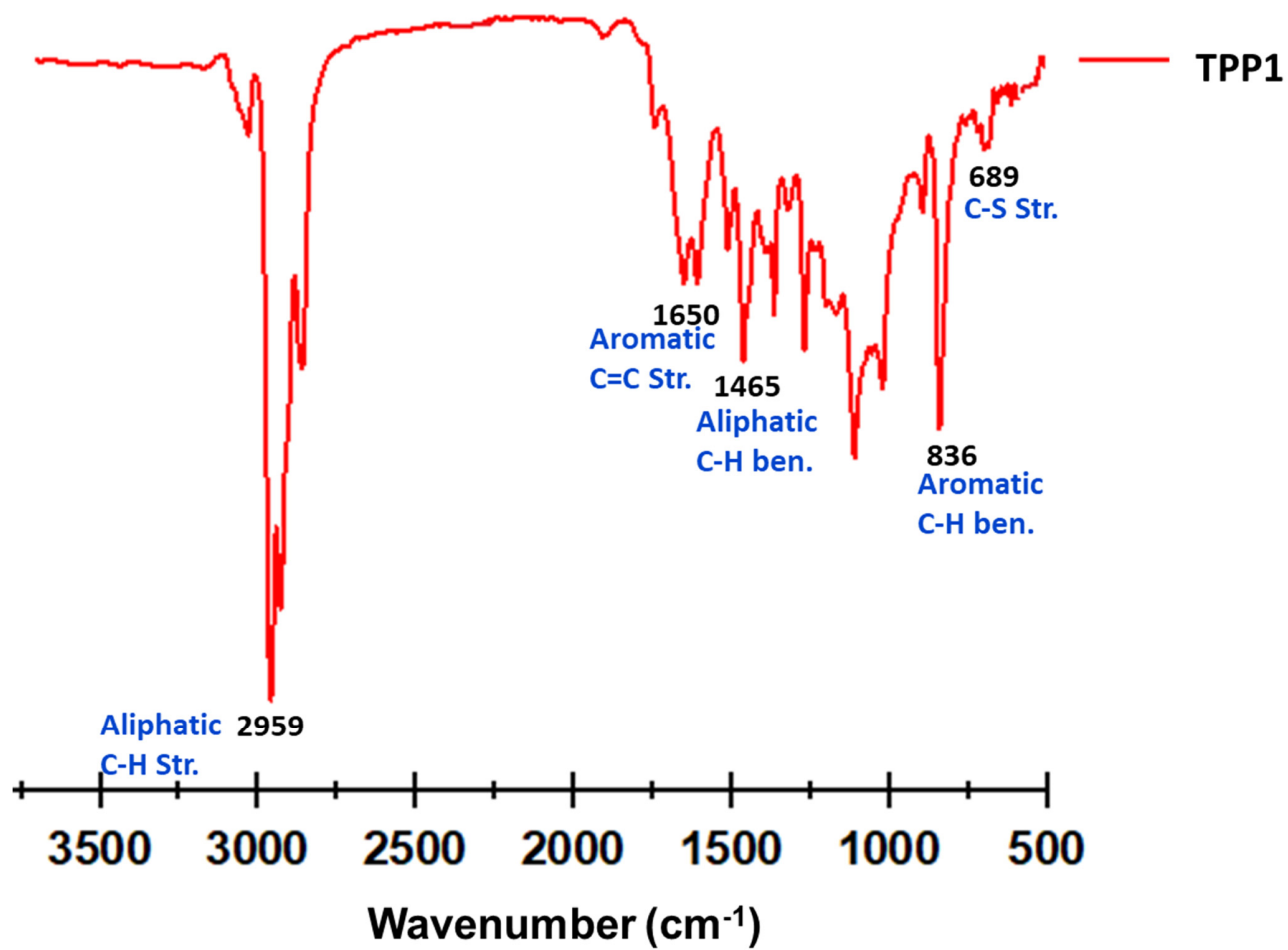


Figure S20 FTIR spectrum of TPP1

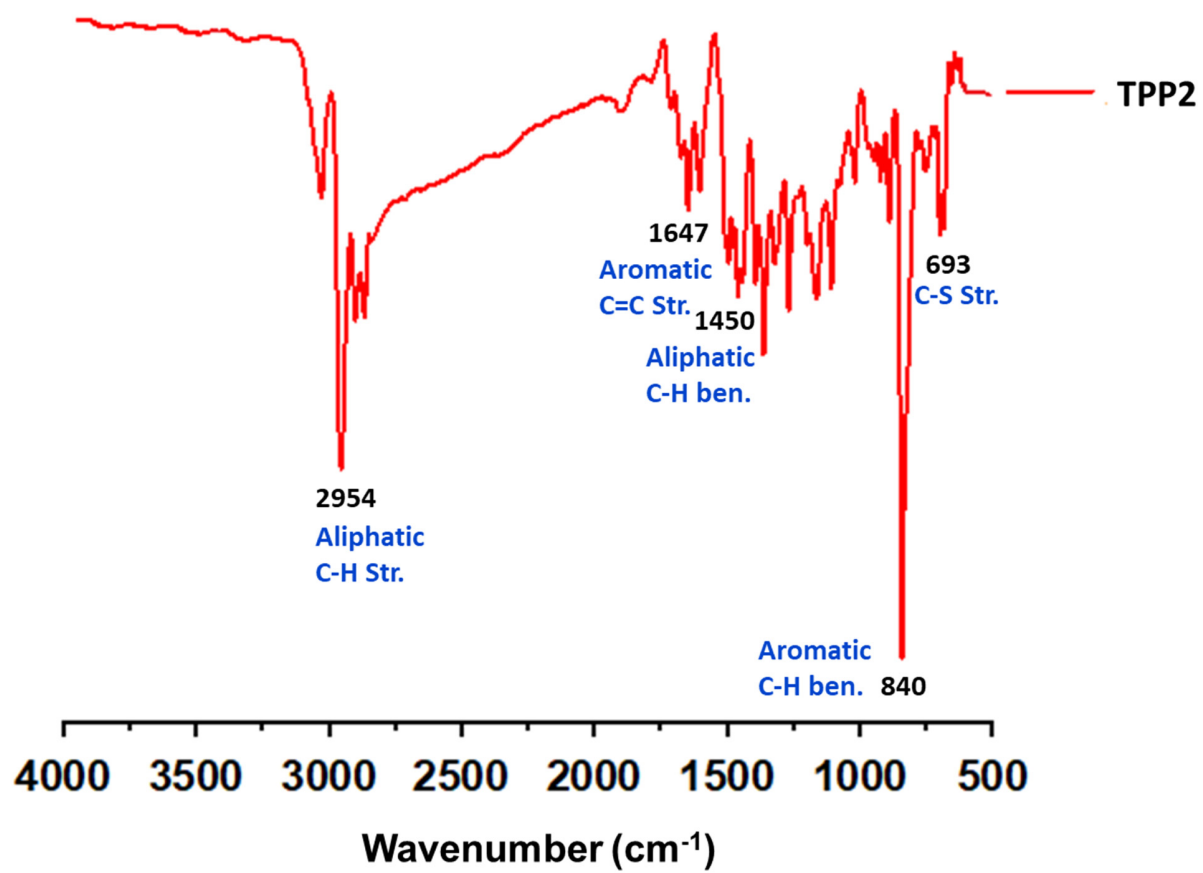


Figure S21 FTIR spectrum of **TPP2**

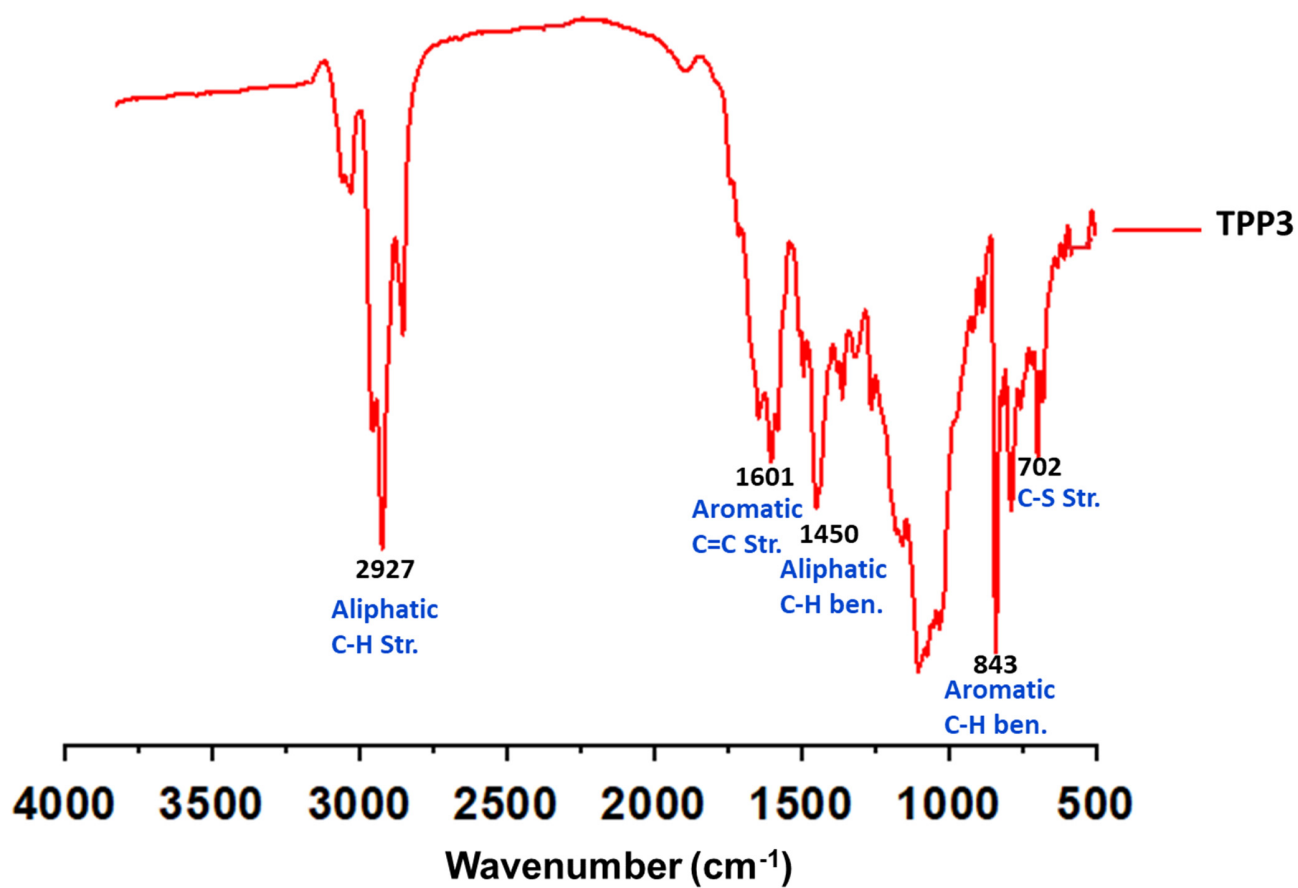


Figure S22 FTIR spectrum of TPP3

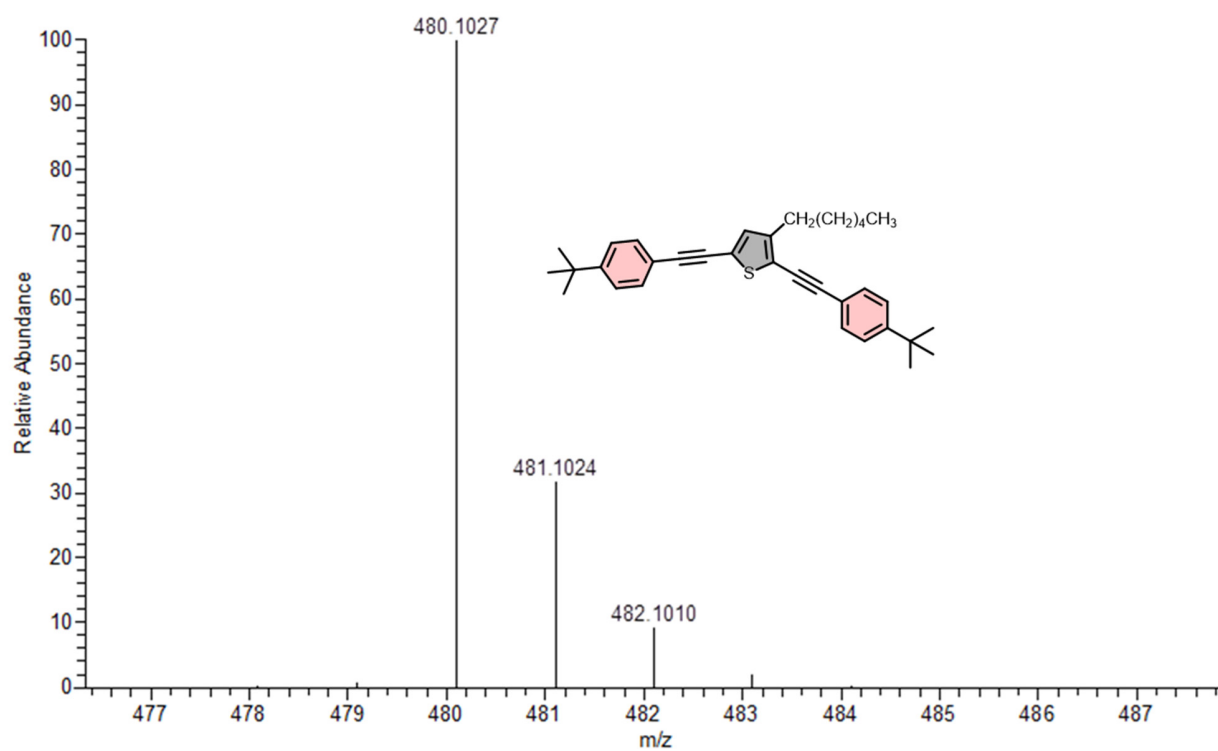


Figure S23 EI-HRMS spectrum of **3a**

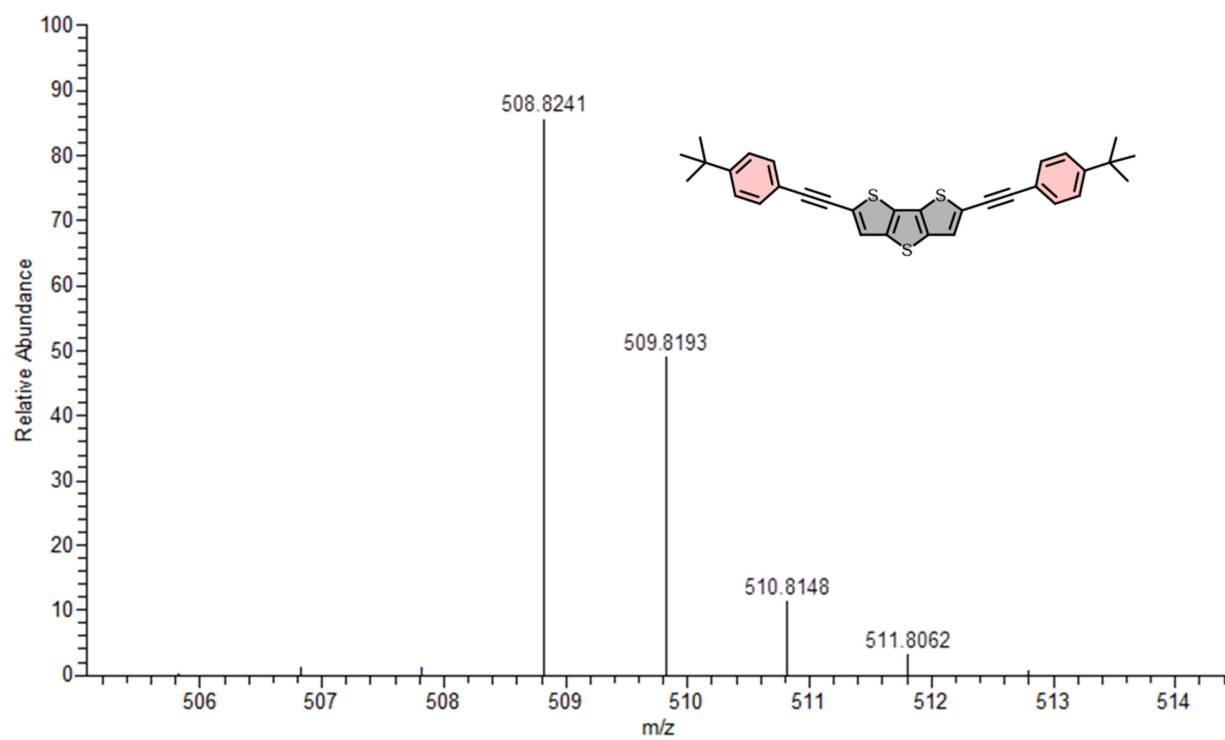


Figure S24 ESI-HRMS spectrum of **3b**

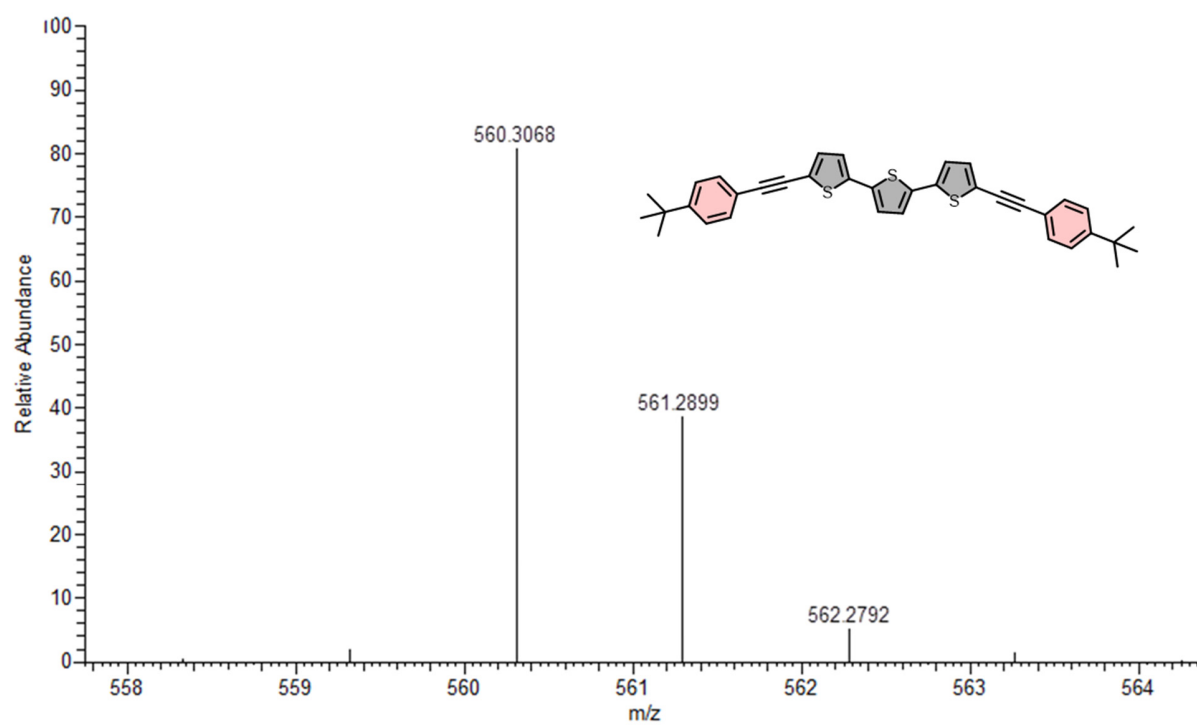


Figure S25 ESI-HRMS spectrum of **3c**

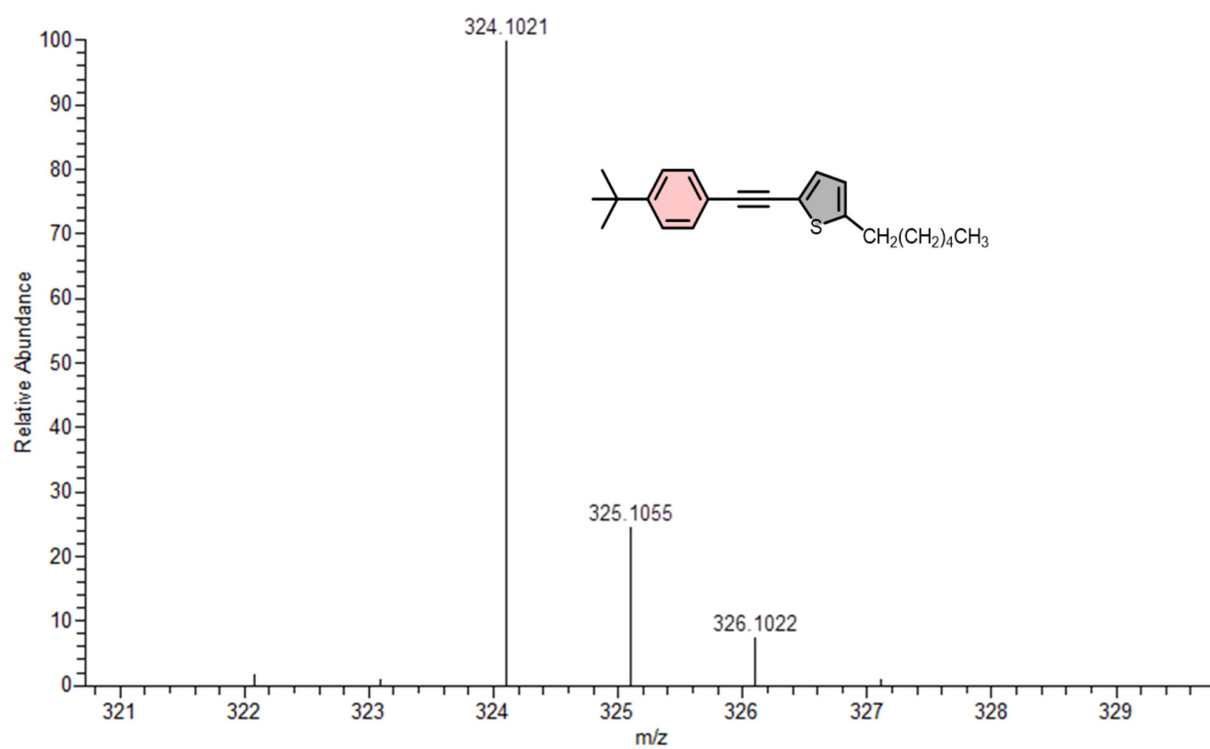


Figure S26 ESI-HRMS spectrum of **3d**

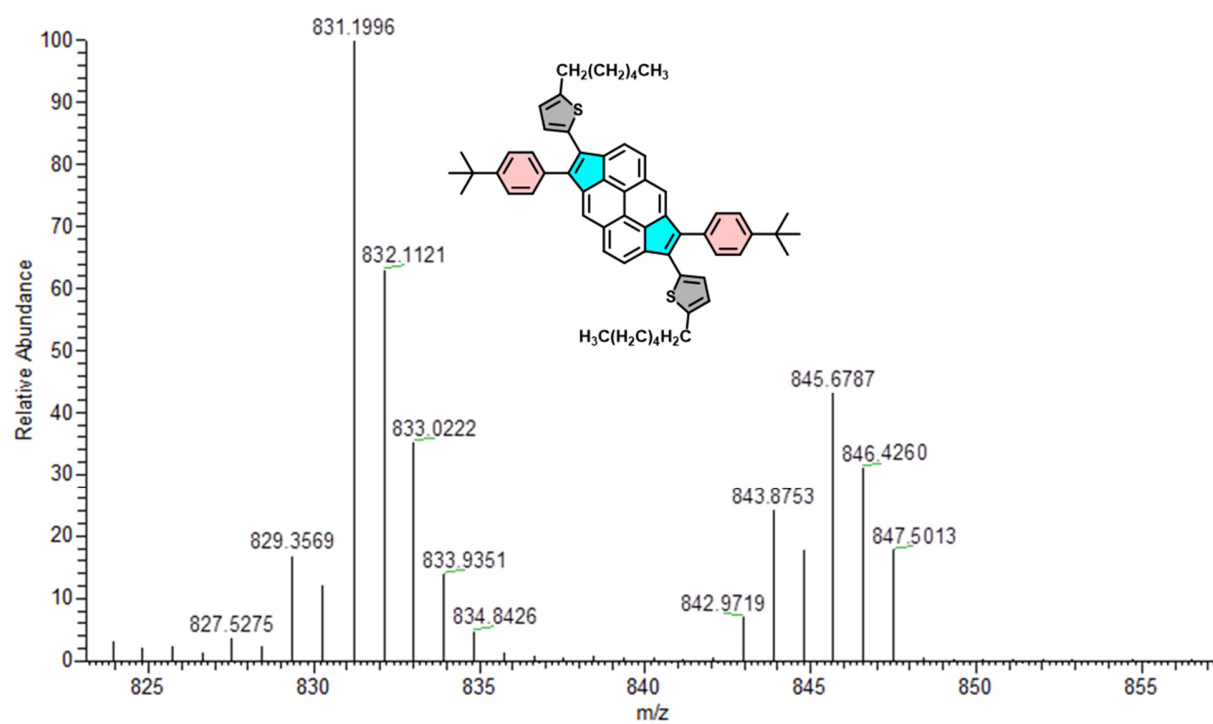


Figure S27 ESI-HRMS spectrum of **TPM**

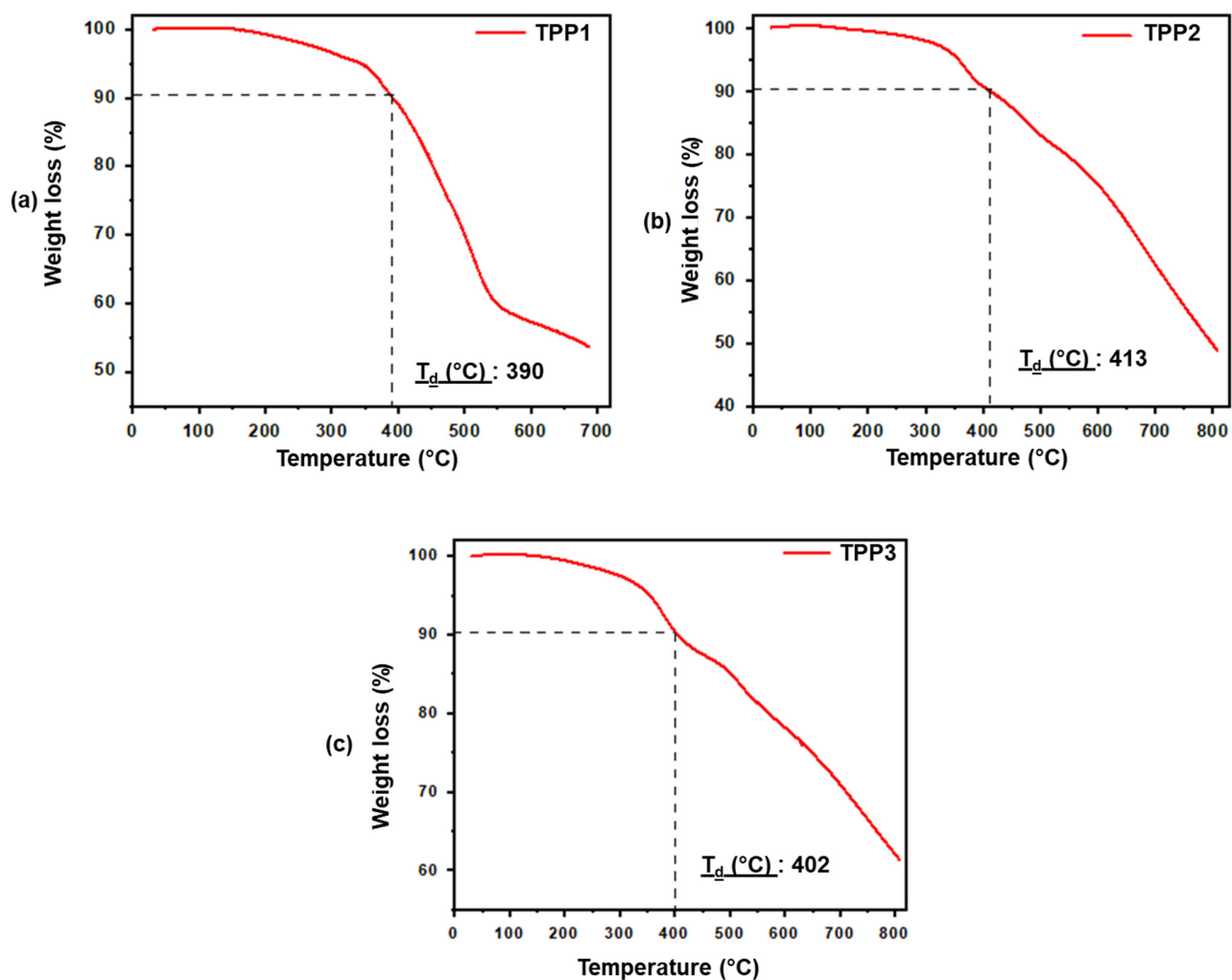


Figure S28 TGA thermograms of (a) TPP1, (b) TPP2 and (c) TPP3, T_d represents the temperature of 10% weight loss

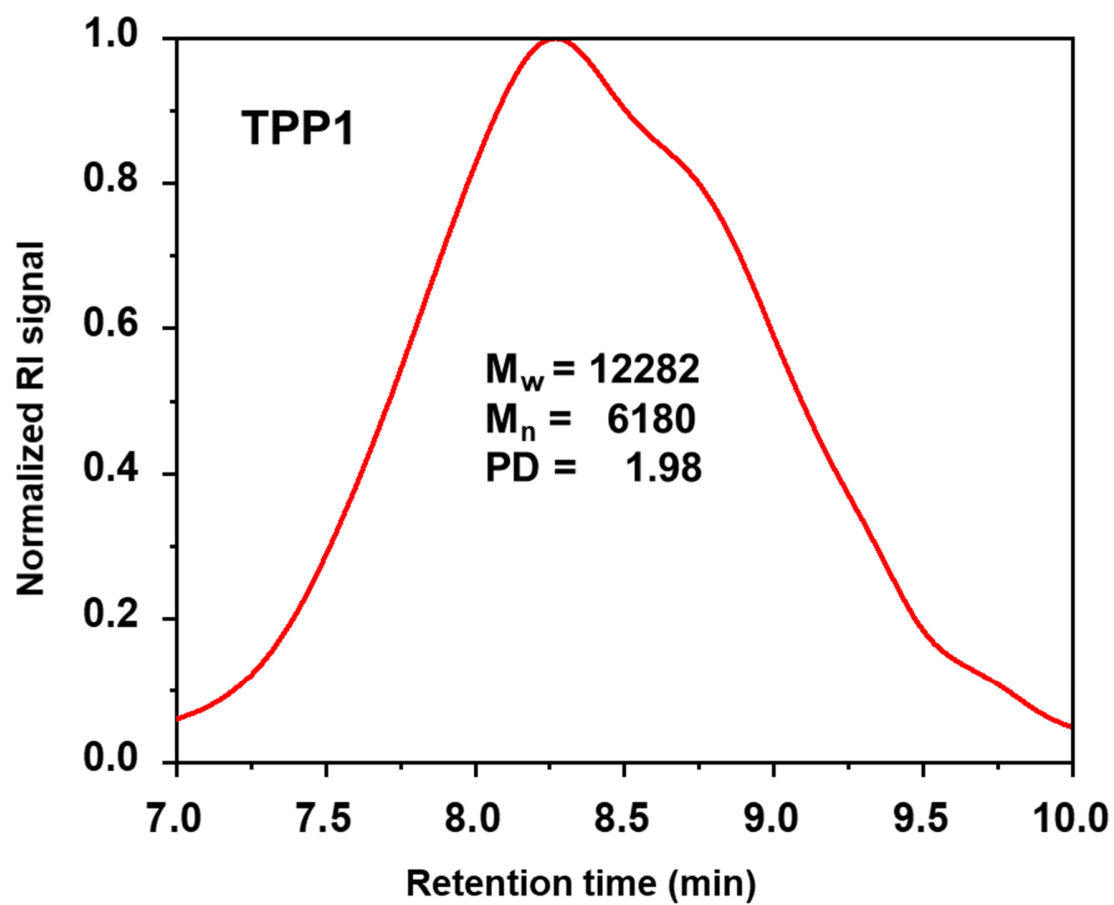


Figure S29 Normalized GPC chromatogram TPP1

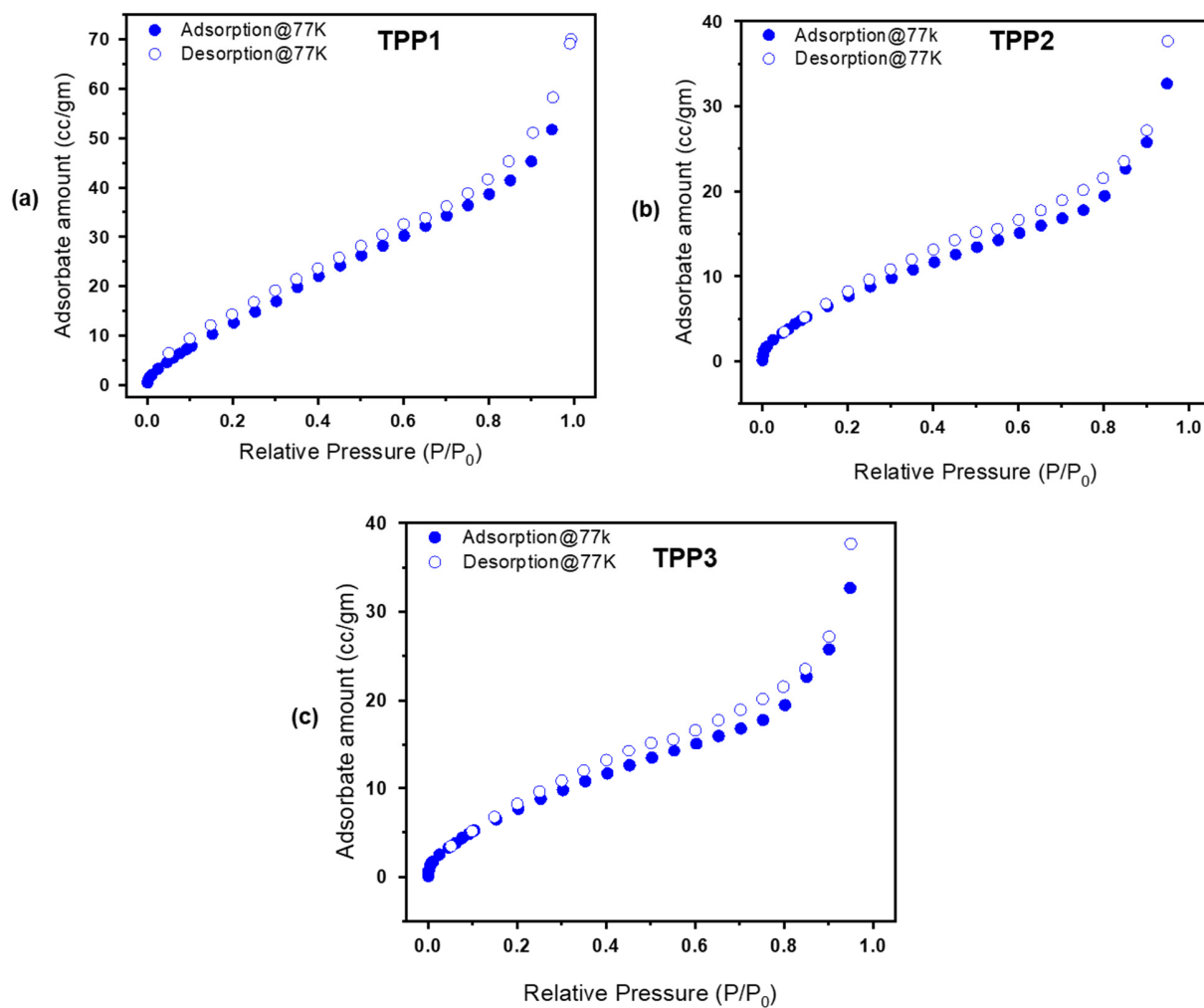


Figure S30 Nitrogen adsorption and desorption isotherms of (a) **TPP1**, (b) **TPP2** and (c) **TPP3** measured at 77 K.

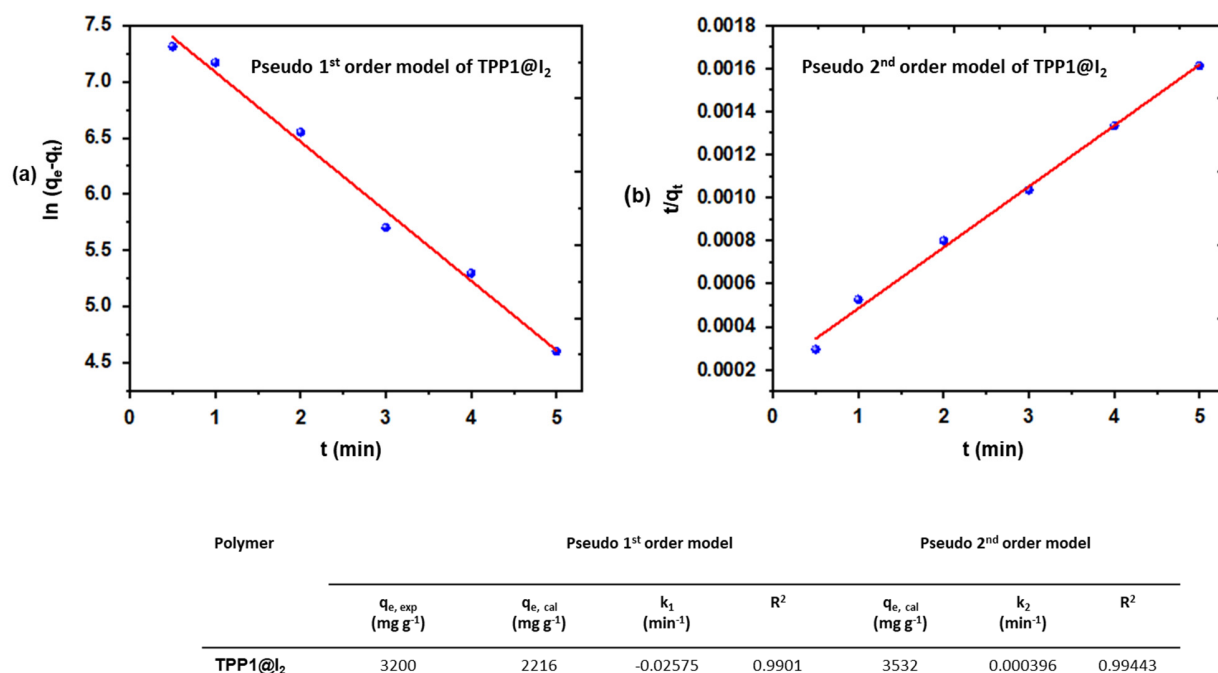


Figure S31 Pseudo-first-order (a) and pseudo-second-order (b) models of TPP1@I₂

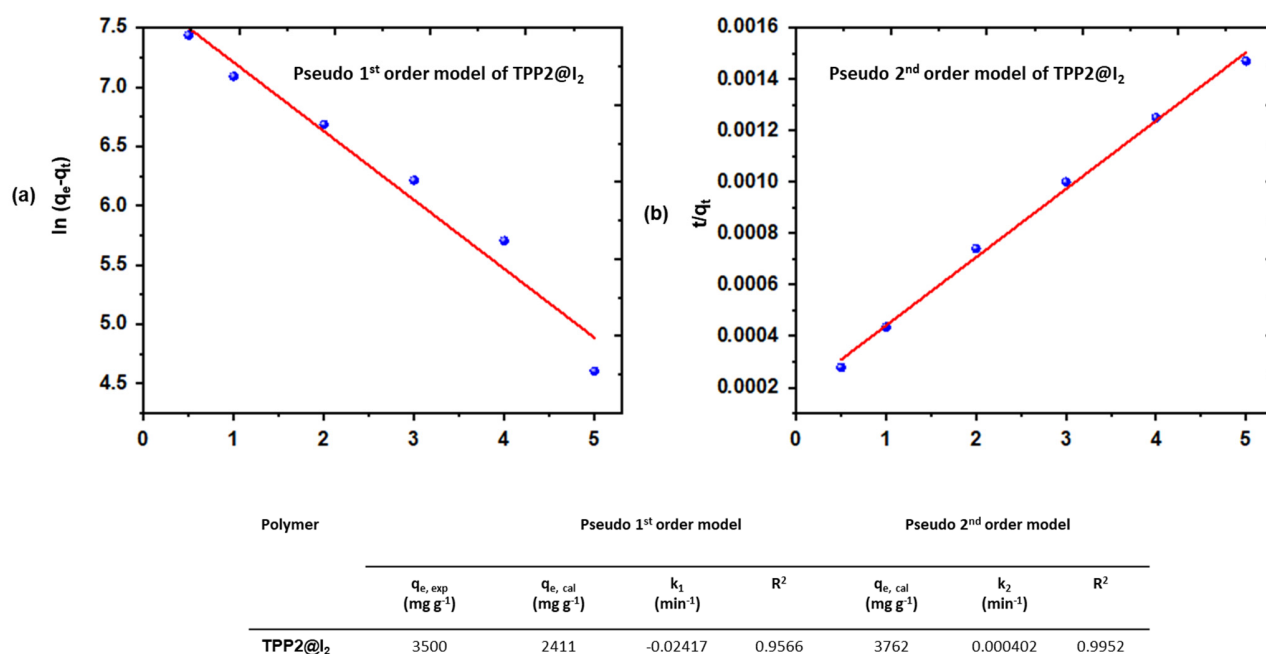


Figure S32 Pseudo-first-order (a) and pseudo-second-order (b) models of TPP2@I₂

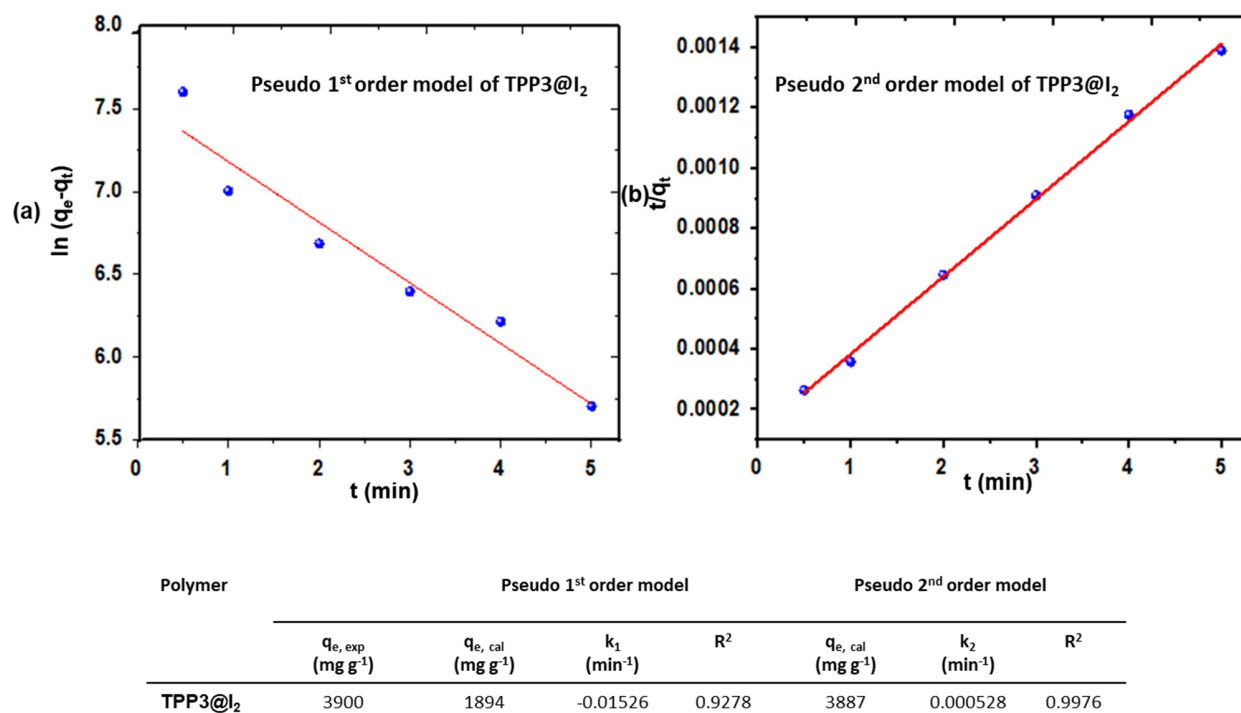


Figure S33 Pseudo-first-order (a) and pseudo-second-order (b) models of TPP3@I₂

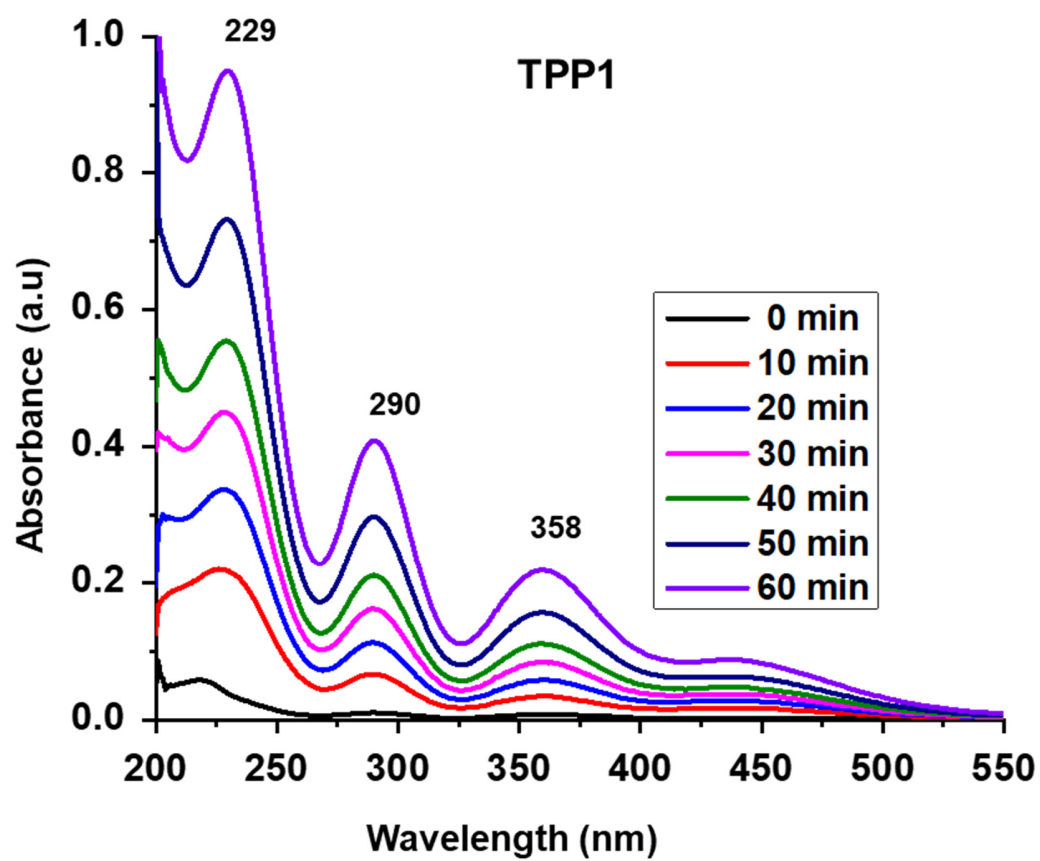


Figure S34 UV-Vis absorption spectra upon immersion of **TPP1@I₂** in ethanol

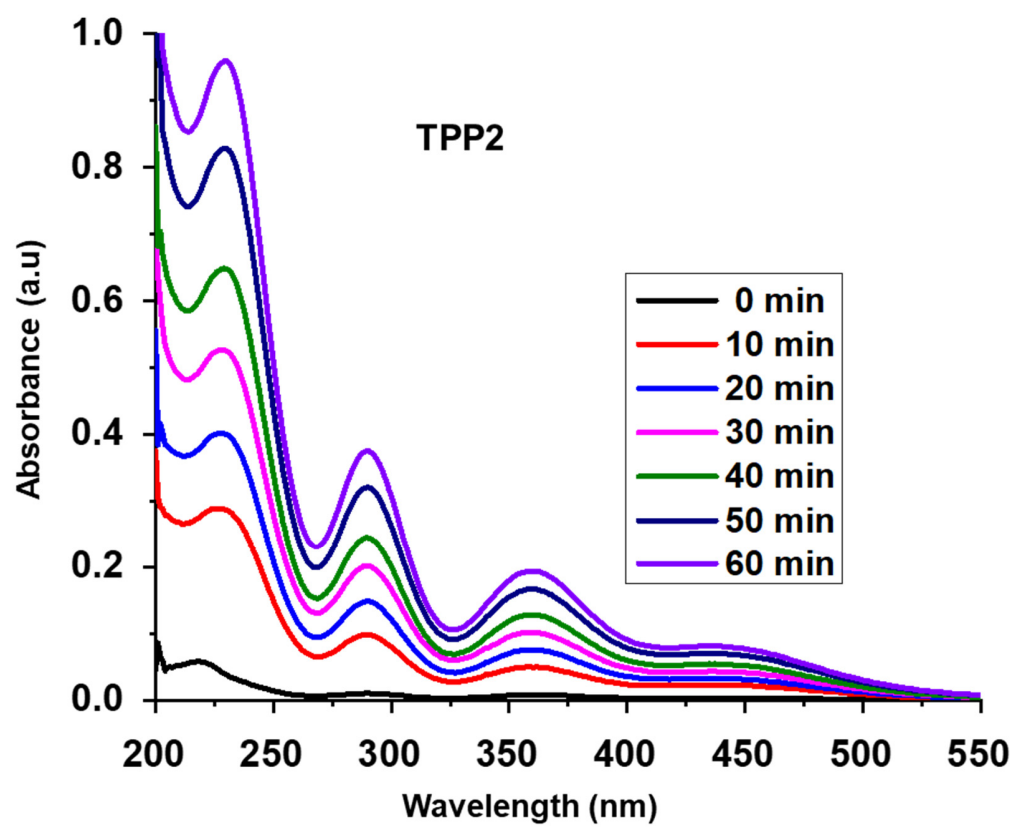


Figure S35 UV-Vis absorption spectra upon immersion of **TPP2@I₂** in ethanol

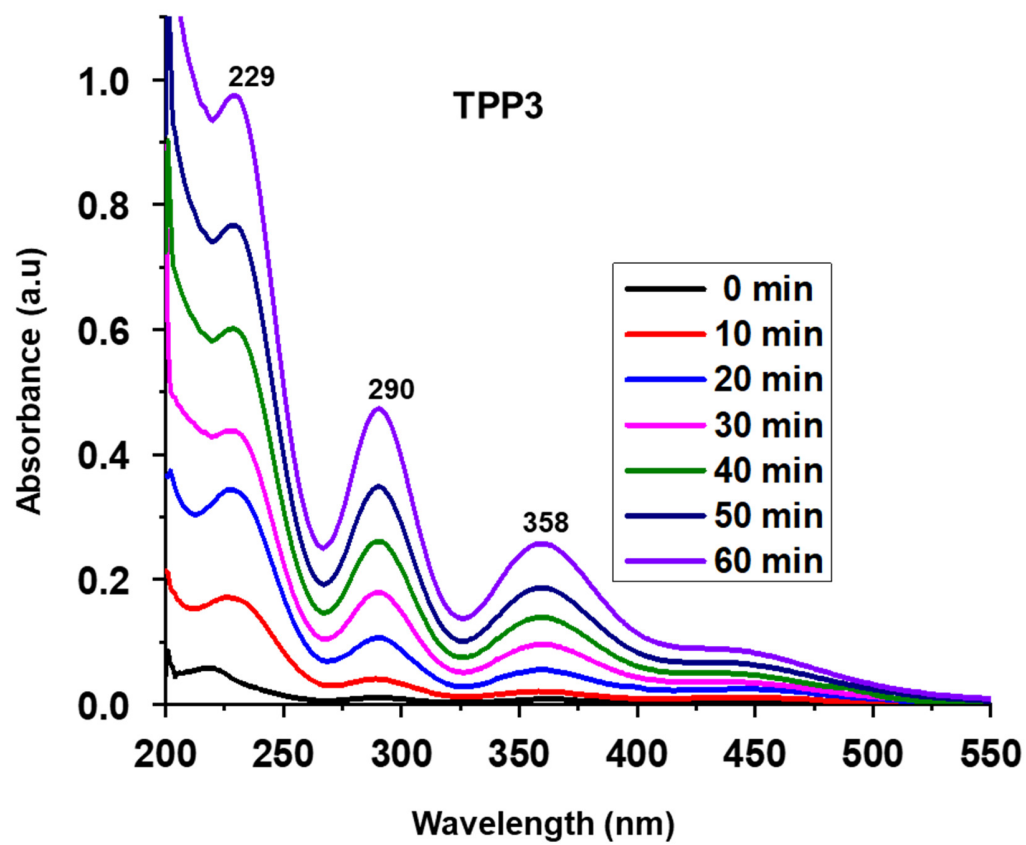


Figure S36 UV-Vis absorption spectra upon immersion of **TPP3@I₂** in ethanol