Supporting Information

D–A Conjugated Polymers Based on Thieno[3,2-b]indole (TI) and 2,1,3-benzodiathiazole (BT) Derivatives: Synthesis, Characterization and Side-Chain Influence on Photovoltaic Properties

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Section 1. TGA plot.

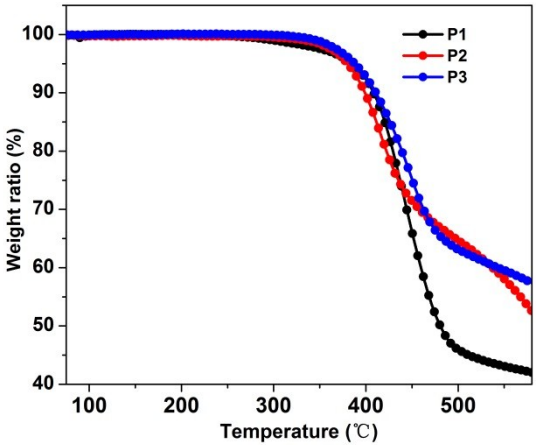


Fig S1. TGA polts of **P1**, **P2** and **P3** at a heating rate of 10 ^{o}C min^{-1} under nitrogen atmosphere.

Section 2. SCLC Mobility plot.

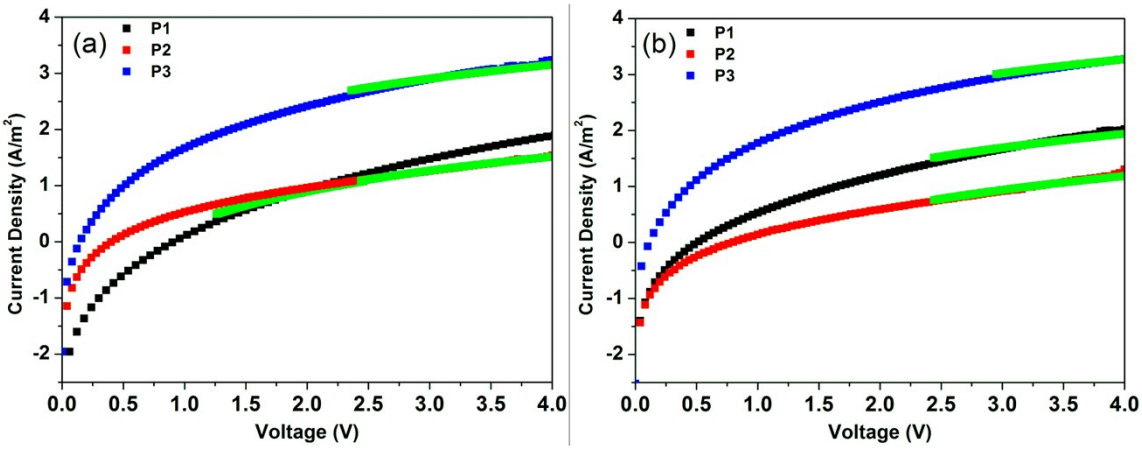


Fig S2. Current density (*J*)–voltage (*V*) profiles of Polymer/$PC_{71}BM$ based devices with a weight ratio of (a) 1:3 and (b) 1:4 for the measurement of the hole mobilities under the optimized conditions. (symbols are experimental data for transport of hole, and the green line were fitted according to the space-charge-limited-current model).

Table S1. Charge transport properties for the Polymer:$PC_{71}BM$ blend estimated by the SCLC model.

Blend	D/A ratio (w/w)	Mobility cm^2 V^{-1} s^{-1}
P1:$PC_{71}BM$	1:3	4.76×10^{-7}
	1:4	1.31×10^{-6}

P2:$PC_{71}BM$	1:3	4.98×10^{-7}
	1:4	2.38×10^{-7}
P3:$PC_{71}BM$	1:3	2.17×10^{-5}
	1:4	2.84×10^{-5}

Section 3. Device optimization.

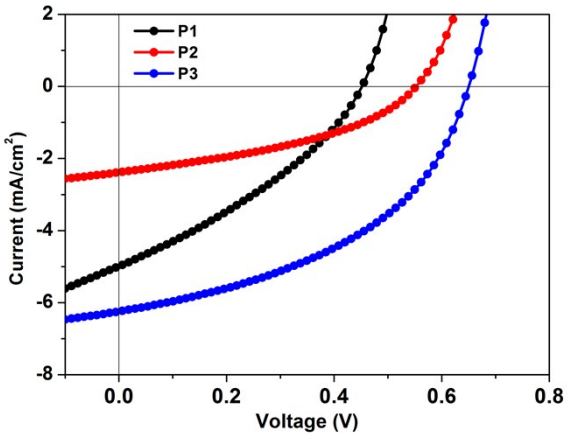


Fig S3. *J–V* characteristics of Polymers:$PC_{71}BM$ (1:4) with cosolvents of DCB:CF (9:1, *v/v*) under thermal annealing 150 °C.

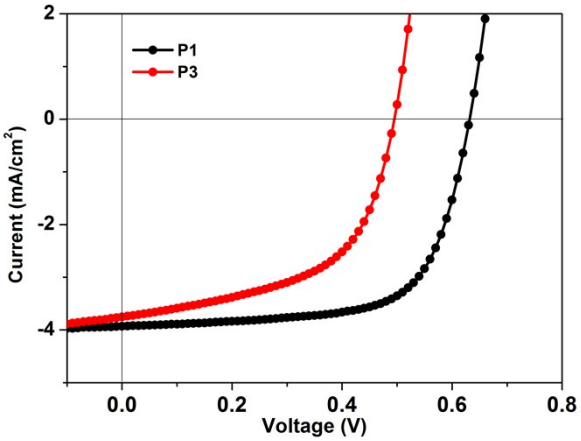


Fig S4. *J–V* characteristics of P1:PCBM (1:3), P2:PCBM (1:4) with addictive (DIO) as additive under thermal annealing at 150 °C.

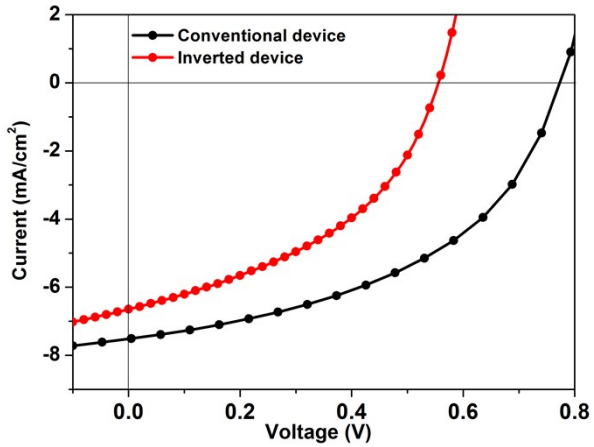
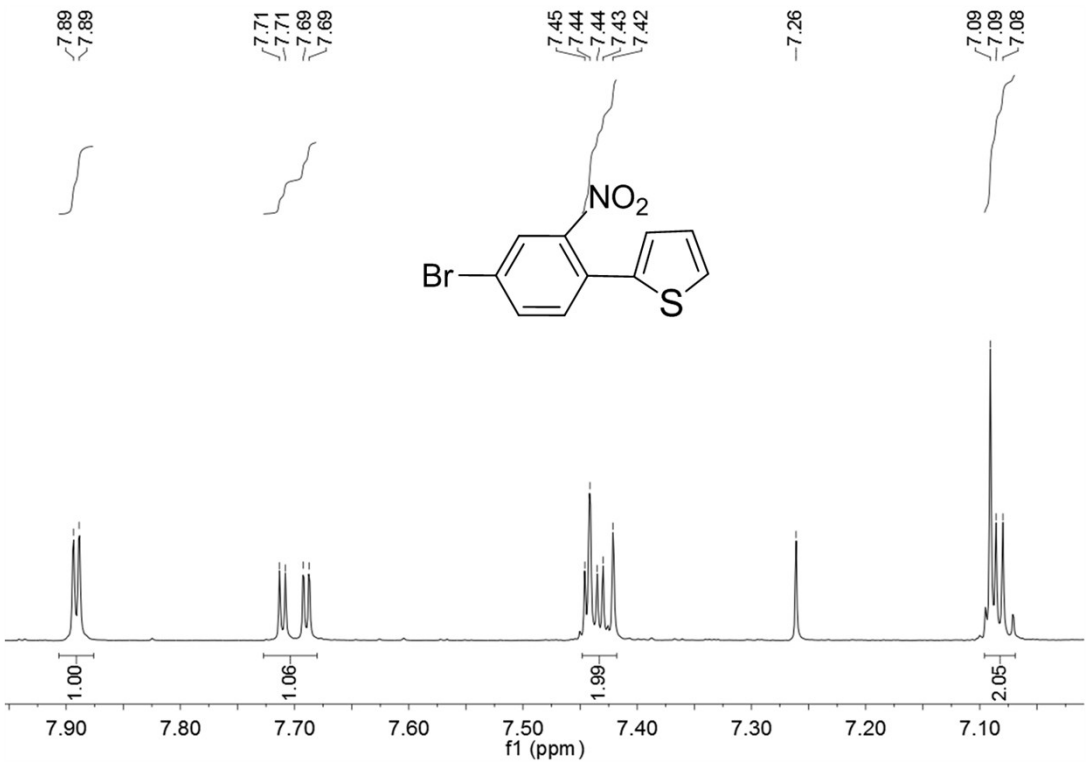


Fig S5. *J–V* characteristics of P3 : $PC_{71}BM$ (1 : 4) with inverted configuration.

Section 4. NMR spectra.



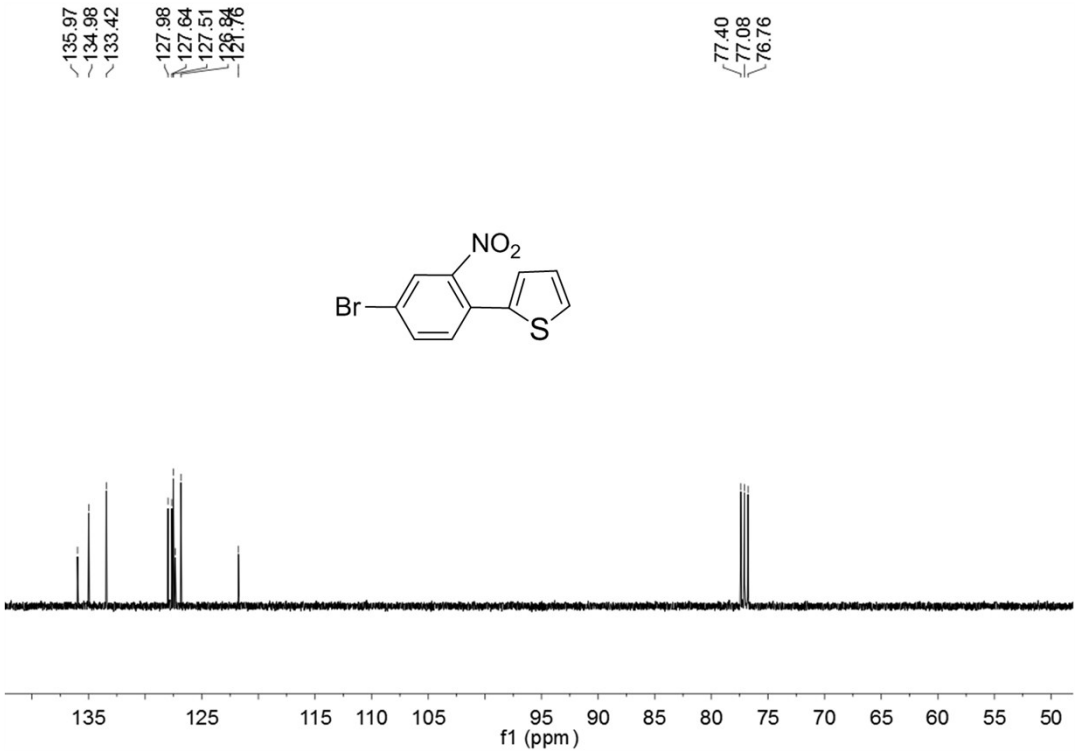
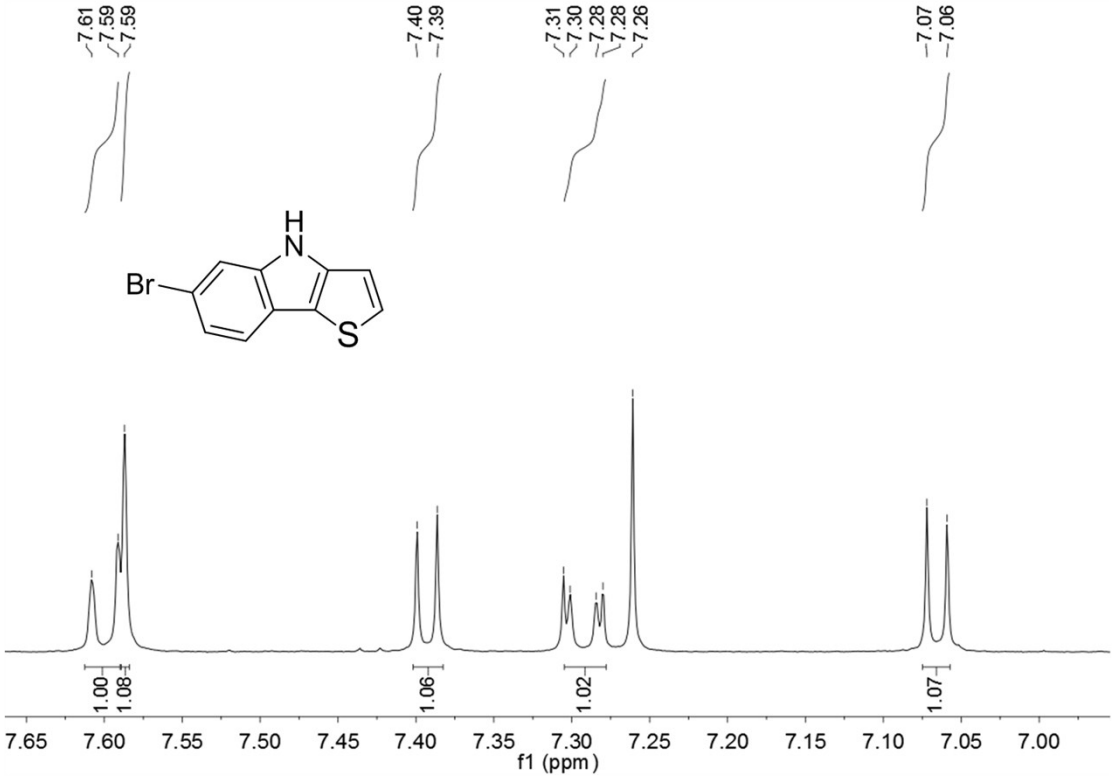


Fig S6. ^{1}H and ^{13}C NMR spectra of 2-(4-bromo-2-nitrophenyl)thiophene (2) in $CDCl_3$



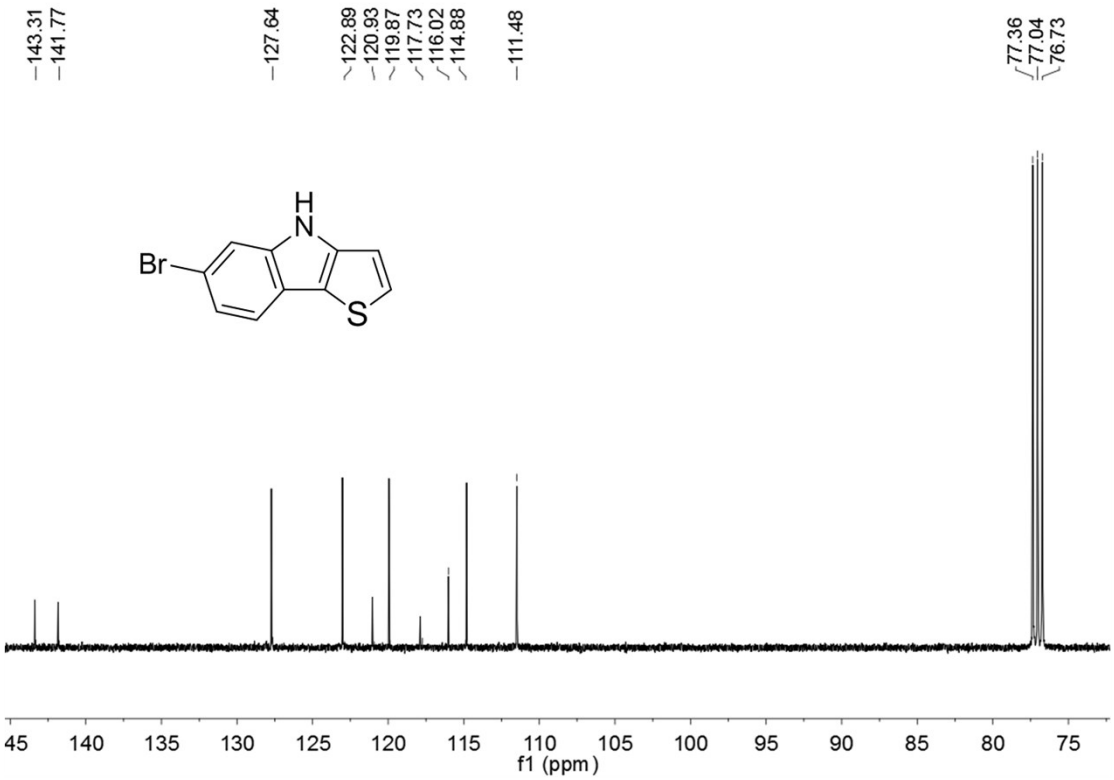
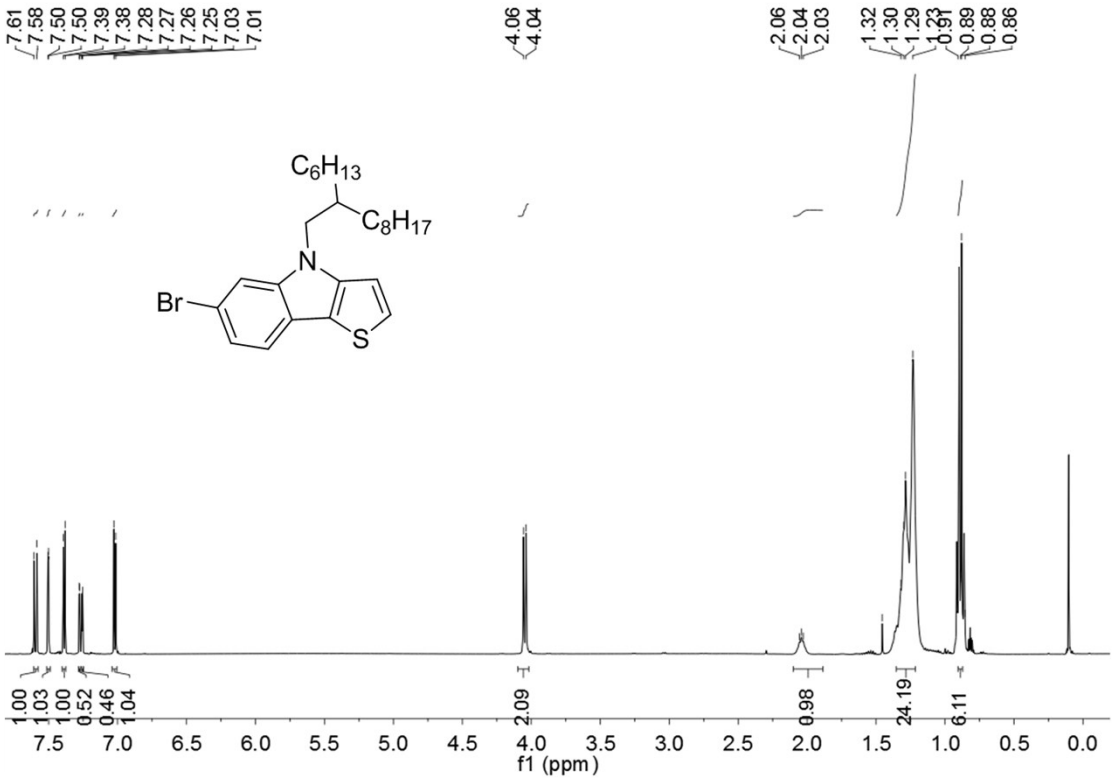


Fig S7. ^{1}H and ^{13}C NMR spectra of 6-bromo-4H-thieno[3,2-b]indole (3) in $CDCl_3$



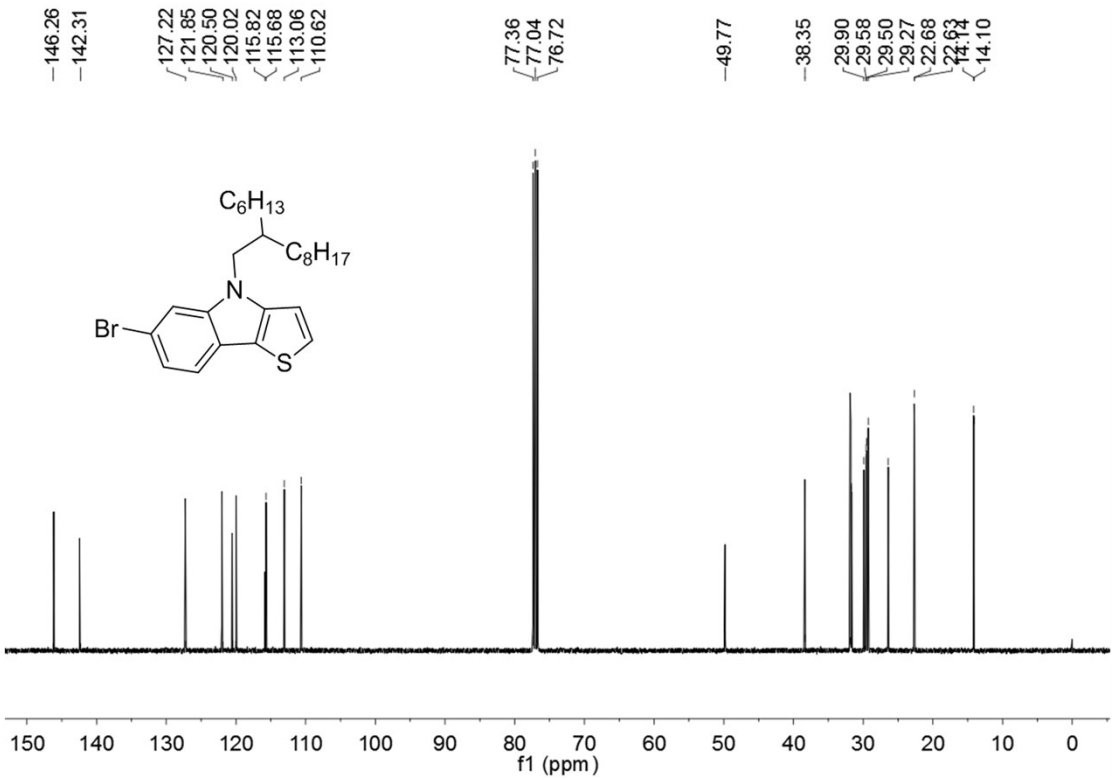
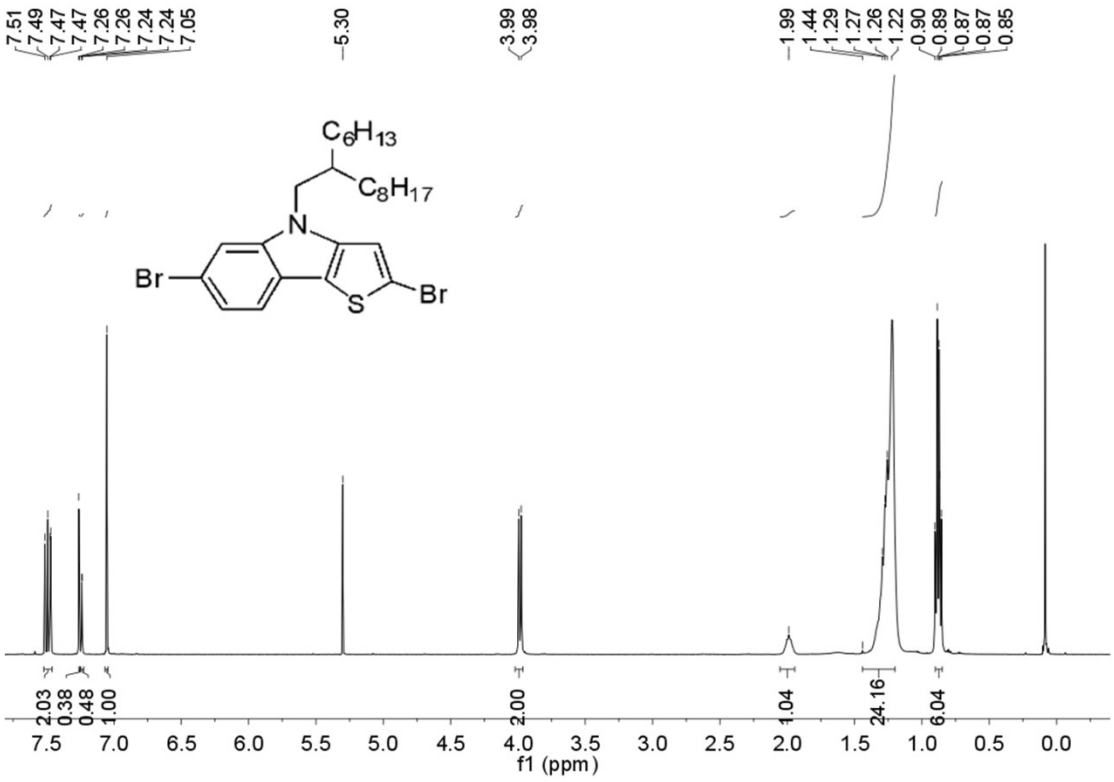


Fig S8. ^{1}H and ^{13}C NMR spectra of 6-bromo-4-(2-hexyldecyl)-4H-thieno[3,2-b]indole (4) in $CDCl_3$



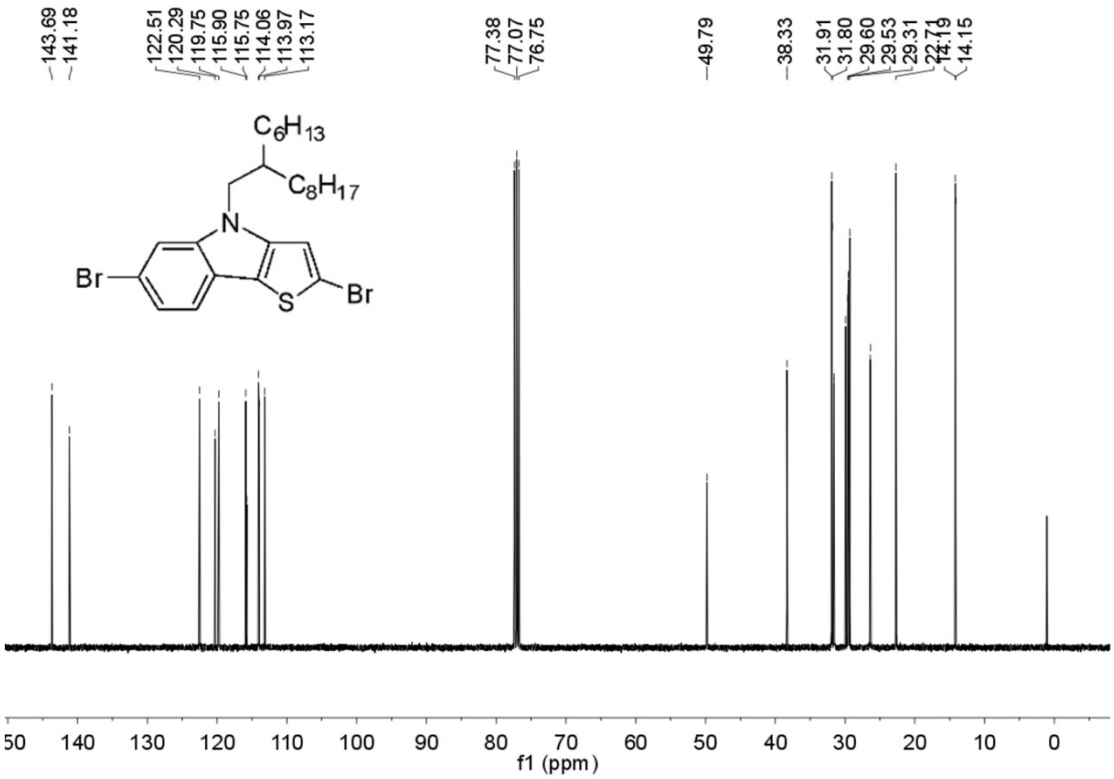
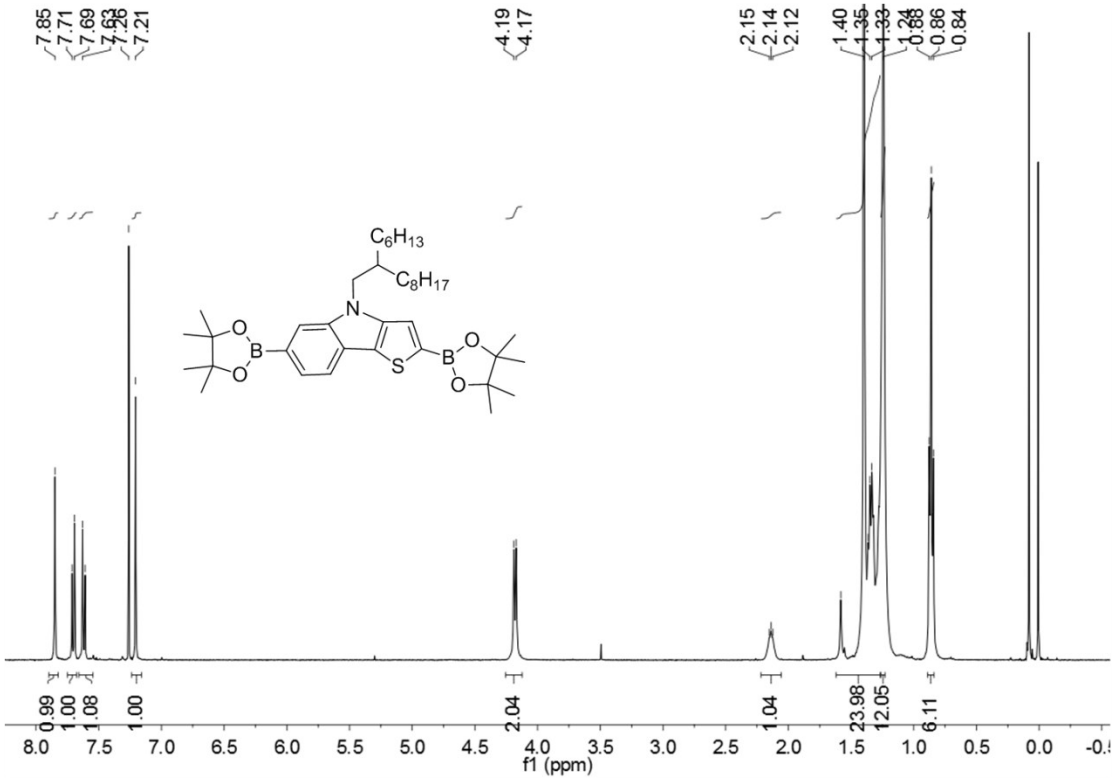


Fig S9. ^{1}H and ^{13}C NMR spectra of 2,6-dibromo-4-(2-hexyldecyl) -4H- thieno[3,2-b]indole (5) in $CDCl_3$.



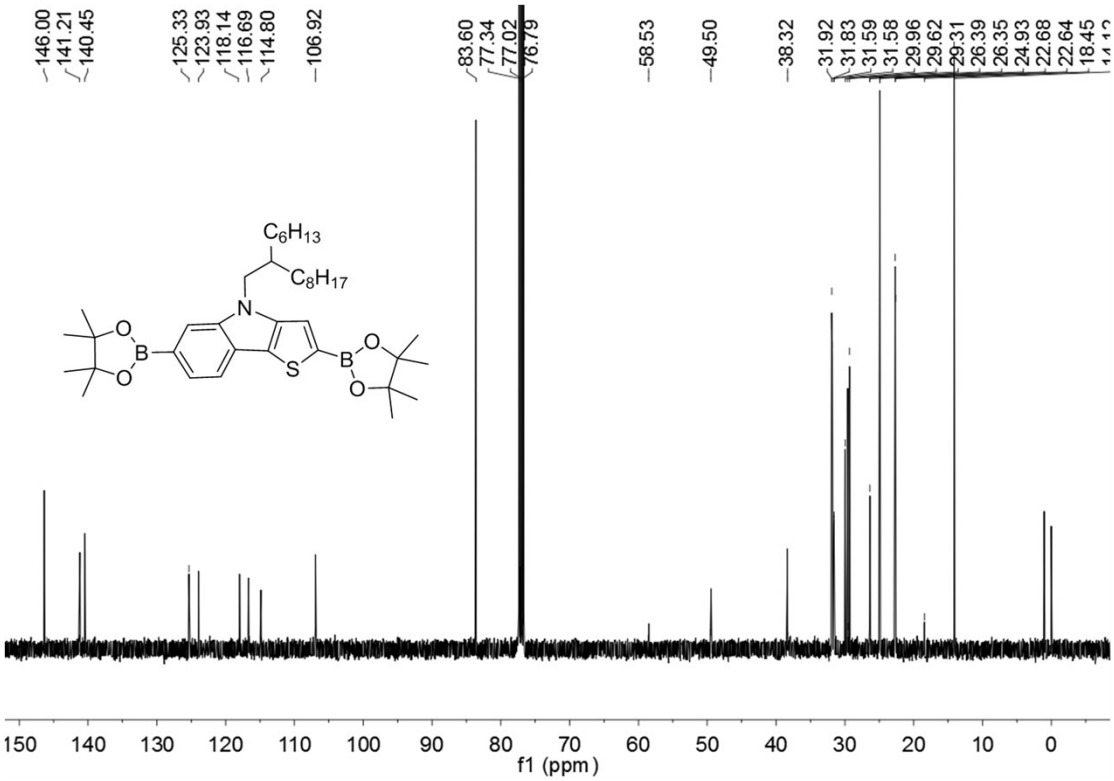
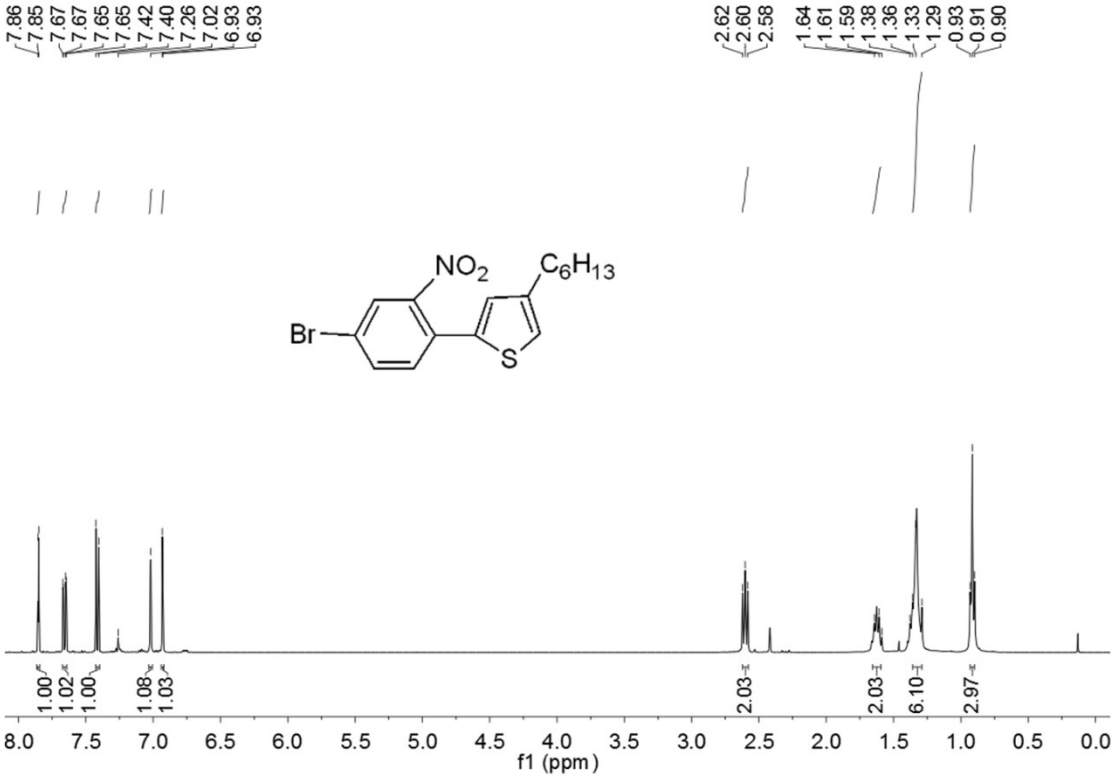


Fig S10. ^{1}H and ^{13}C NMR spectra of 4-(2-hexyldecyl)-2,6-bis(4,4,5,5- tetramethyl-1,3,2-dioxaborolan-2-yl)-4H-thieno[3,2-b]indole (M1) in $CDCl_3$



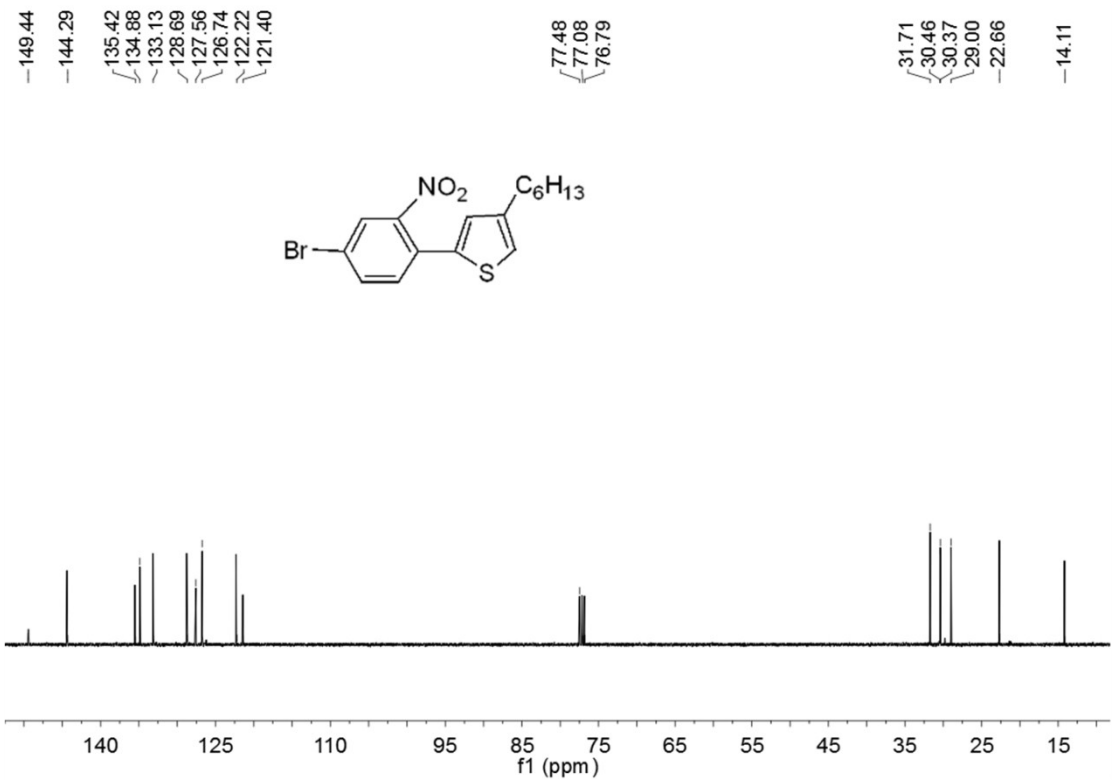
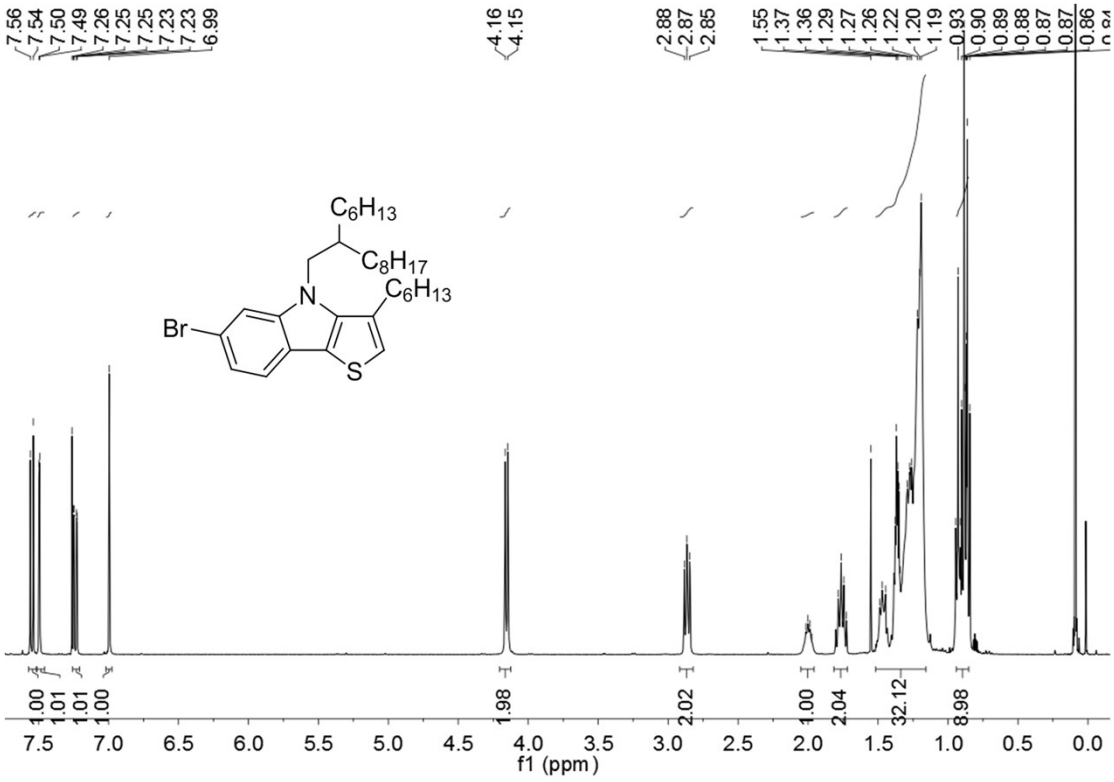


Fig S11. ^{1}H and ^{13}C NMR spectra of 2-(4-bromo-2-nitrophenyl)-4-hexylthiophene (6) in $CDCl_3$



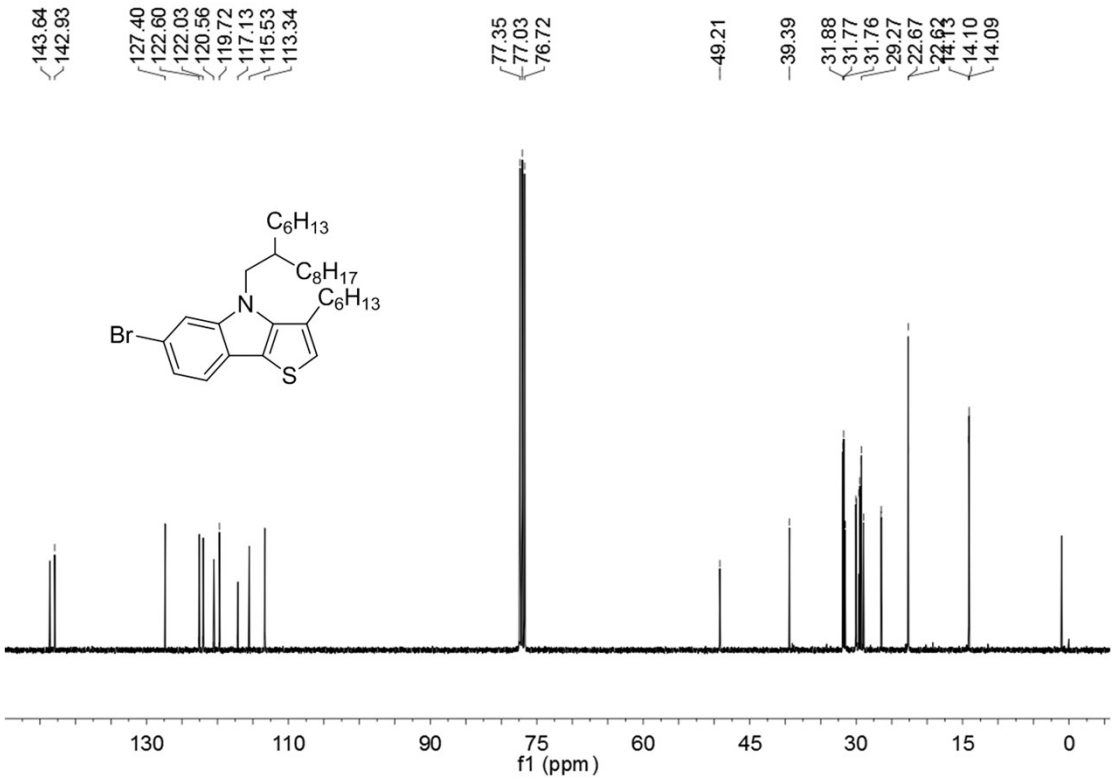
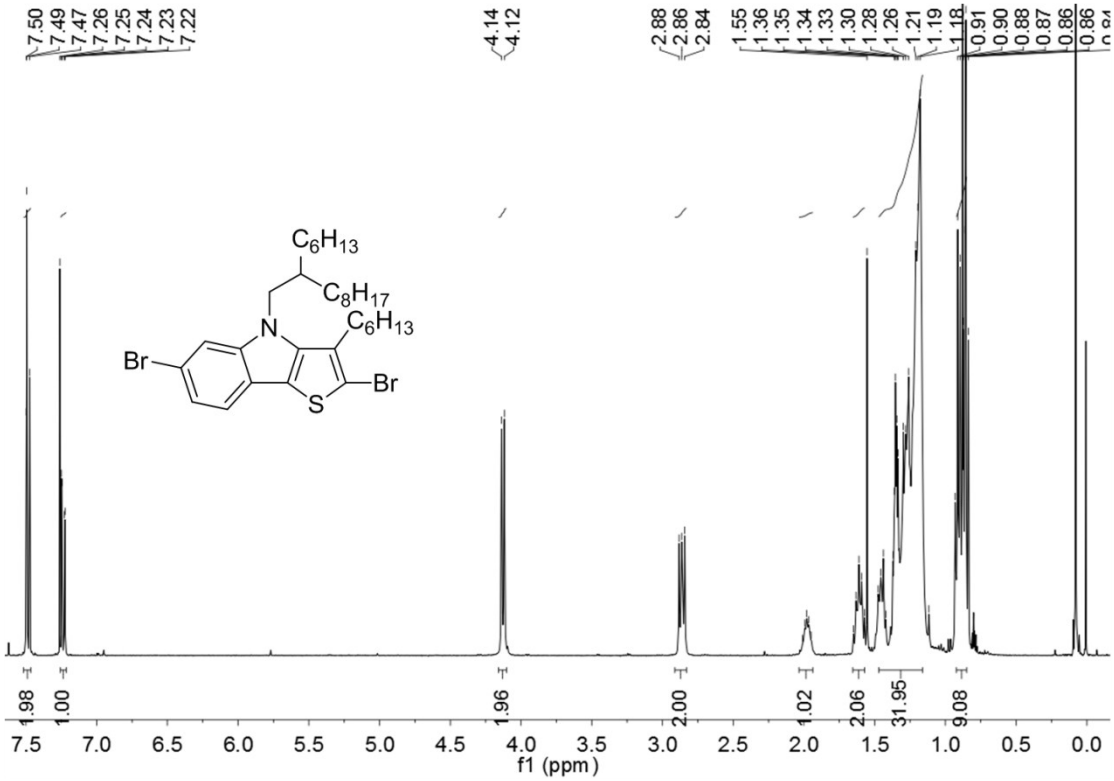


Fig S12. ^{1}H and ^{13}C NMR spectra of 6-bromo-3-hexyl-4-(2-hexyldecyl)-4H-thieno[3,2-b]indole (8) in $CDCl_3$



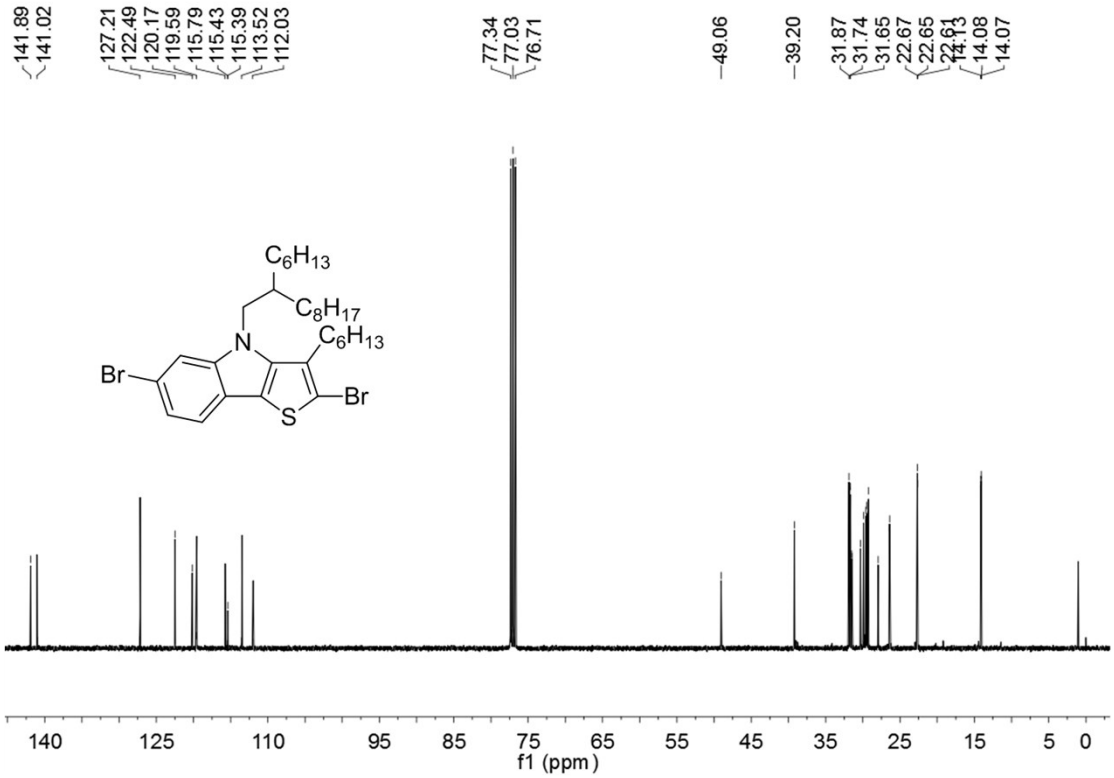


Fig S13. ^{1}H and ^{13}C NMR spectra of 2,6-dibromo-3-hexyl-4-(2-hexyldecyl)-4H-thieno[3,2-b]indole (M2) in $CDCl_3$

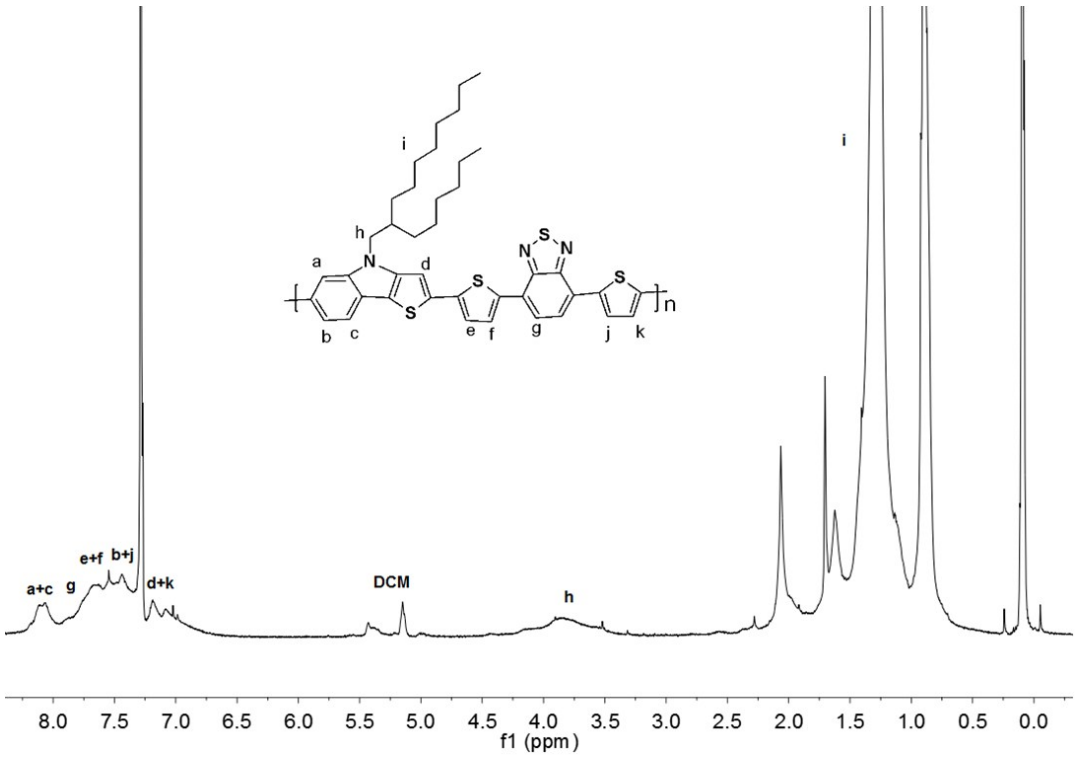


Fig S14. ^{1}H NMR spectra of the copolymer P1 in $CDCl_3$

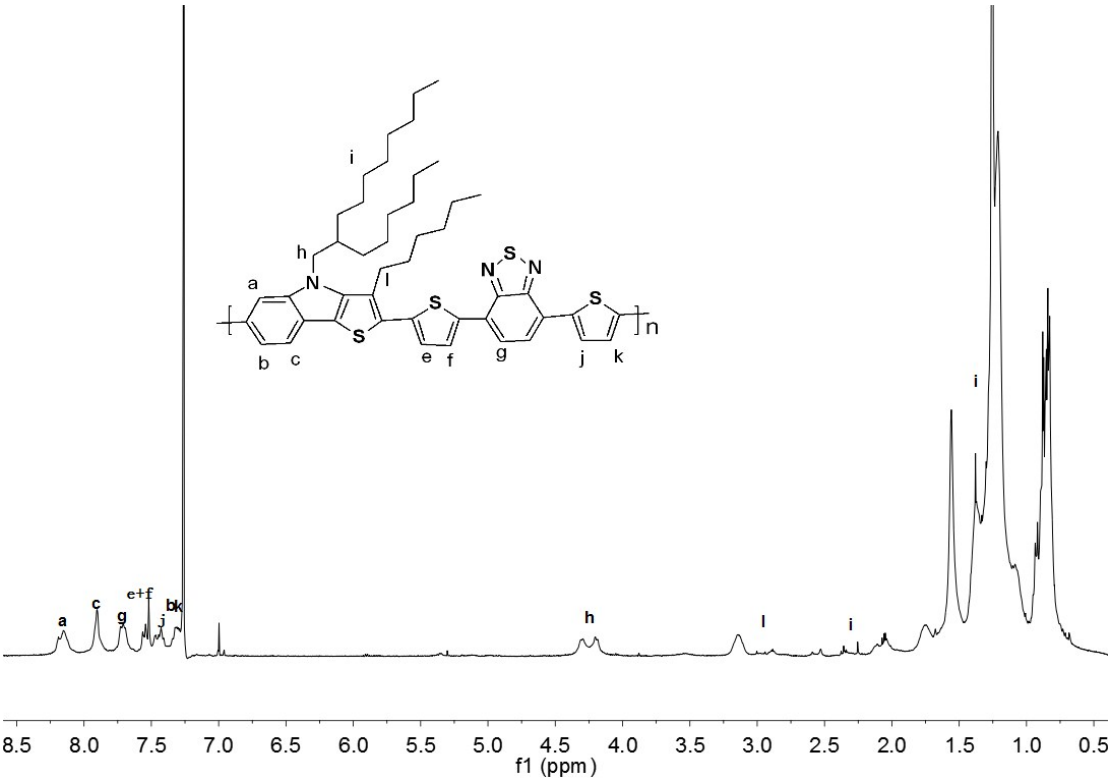


Fig S15. ^{1}H NMR spectra of the copolymer P2 in $CDCl_3$

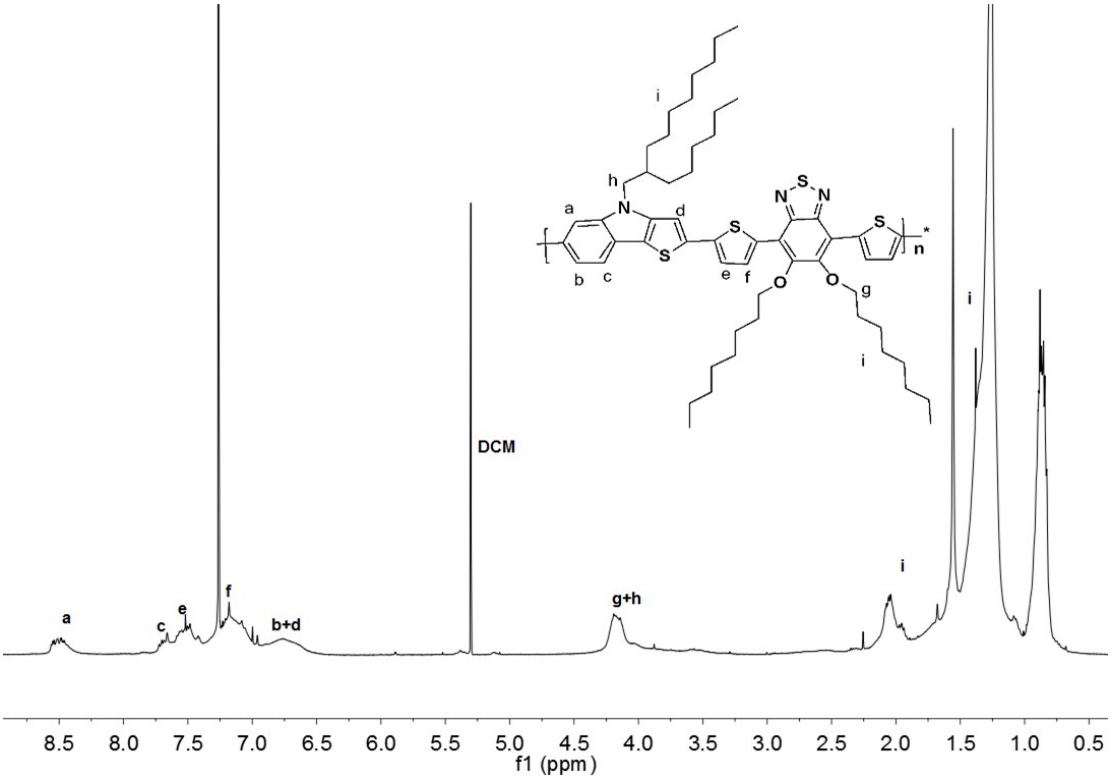


Fig S16. ^{1}H NMR spectra of the copolymer P3 in $CDCl_3$