Supporting Information

New Benzotriazole-Containing Wide Bandgap D1-D'A-D2 Conjugated Polymer for Air-Processed Ternary Organic Solar Cells with Efficiency Approaching 17 %

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1. Instruments

^{1}H NMR spectra were obtained on Agilent 600 MHz DD2 nuclear magnetic resonance (NMR) spectrometer, using $CDCl_3$ as solvent at a resonance frequency of 600 MHz at room temperature. UV-vis absorption spectra were recorded on a Shimadzu UV-2600 spectrophotometer. The molecular weight of polymers determined by waters 1515 gel permeation chromatography using 1,2,4-trichlorobenzene as eluent at 60 °C and polystyrene as a standard. The thermal characteristics of the polymers were investigated using thermogravimetric analysis (TGA) on a Perkin Elmerand differential scanning calorimetry (DSC) at a rapid heating rate of 10°C/min in argon. Oxidation and reduction potentials of the compounds were determined by cyclic voltammetry (CV) experiments on a computer-controlled potentiostat Auto Lab type III" at a scan rate of 100mVs^{-1}. A platinum working electrode, Ag/Ag+ (0.1 M in anhydrous acetonitrile), and a platinum wire were used as the working electrode, reference electrode, and counter electrode, respectively, in a nitrogen-saturated tetrabutylammoniumhexafluorophosphate (Bu_4NPF_6) solution (0.1 M in anhydrous acetonitrile). Assuming the absolute energy level of Fc/Fc^+ to be - 4.44 eV versus vacuum level, thus the HOMO and LUMO energy levels were obtained from the equation of $E_{HOMO}/E_{LUMO} = -(E_{ox}/E_{red} + 4.44)$ (eV), where oxidation/reduction onset potential (E_{ox}/E_{red}) were determined from the position at which the current raised initially from the baseline.

2.0 Device fabrication and characterization

The binary and ternary devices were fabricated with a conventional structure of ITO/PEDOT:PSS/active layer/PFN-Br/Ag as the following procedures. The ITO-coated glasses were cleaned using a detergent scrub, and subsequently subjected to ultrasonic treatment in

deionized water, acetone and isopropyl alcohol for 20 min in each step. After that, the ITO substrates were treated with ultraviolet-ozone for 15 min and spin-coated with PEDOT:PSS solution at 4000 rpm for 30 s and subsequently annealed at 120° C for 20 min under ambient conditions. We have used **P154** as a donor and NFA-4 as an acceptor for the fabrication of OSCs. The **P154 :**NFA-4 (with different weight ratios) was dissolved in solution using chloroform containing 0.5 % 1,8-diiodooctane additive with a total concentration of 16 mg/mL, and thin films were prepared via spin coating on top of PEDOT:PSS. For further optimization, the thin film of P154:NFA-4 (1:1.2) was subjected to solvent vapor annealing via exposing the film to THF environment for 40 s. The devices were also fabricated with PBDB-T:NFA-4, under identical conditions. For the ternary active layer, the weight ratio between two donors (P154 and PBDB-T) is varied, keeping the concentration of NFA-4 constant. The total concentration for each blend was kept 16 mg/mL. Afterward, PFN-Br with a concentration of 1.0 mg/mL of methanol containing 0.3 % (v/v) glacial acetic acid was spin-coated on the active layer at 3000 rpm for 20 s. Finally, the Ag (thickness 150 nm) was deposited under high vacuum onto PFN-Br layer. The effective area of the device is 0.04 cm^2, defined by the masks for all the OSCs.

The current-voltage characteristics of the OSCs were measured under illumination intensity of 100 mW/cm^2 (AM1.5 G) using a solar simulator (AAA model) and a Keithley 2400 source meter unit. The Solar simulator calibration is done using a calibrated reference solar cell, which outputs a standard value of 1Sun. The External quantum efficiency (EQE) measurements were performed using Bentham EQE system.

The hole-only and electron-only devices with ITO/PEDOT:PSS/active layer /Au and ITO/Al/ active layer/Al architectures were also fabricated in a similar way, to measure the hole and electron mobility. We have measured the dark J-V characteristics and fitted with the space charge limited current model using the following expression:

$J_{SCLC} = (9/8)\varepsilon\varepsilon_0\mu[(V-V_{bi})^2/L^3]$, where ε, ε_0 is the permeability of active layer and vacuum, respectively, V and Vbi are the applied voltage and built-in potential, respectively, μ is the charge carrier mobility, and L is the thickness of the active layer.

The photocurrent density (J_{ph}) and effective voltage (V_{eff}) were estimated as:

$J_{ph}= J_L-J_D$, where J_L and J_D are the photocurrent densities under illumination and in dark conditions, respectively.

$V_{eff}= V_o-V_a$, where V_o is the voltage when $J_{ph}=0$ and V_a is the applied bias voltage.

For the transient photocurrent (TPC) and transient photovoltage (TPV) decay, the device was mounted on a conductive clip under steady state illumination from the focused quartz-tungsten

halogen lamp light source. An optical perturbation is applied to the device with a 1kHz femtosecond pulse laser under 500 nm excitation. The TPV signal was acquired by a digital oscilloscope at open circuit conditions (1MΩ). The TPC signal was measured under short circuit by applying a 50 resistor. The carrier lifetime and charge carrier extraction times were estimated via fitting the TPV and TPC decay with an exponential fitting.

Steady state PL spectra of the thin film were recorded on the Shimazu PL spectrophotometer.

The time-resolved photoluminescence (TPRL) in the films was recorded on HORIBA make.

3. Materials

All of the reagents and chemicals were purchased from Aldrich, Acros, TCI and used without further purification. THF was dried and purified by fractional distillation over sodium/ benzophenone under argon.

4. Synthesis and characterization of monomer and polymer P154

2,2'-(2,6-bis(trimethylstannyl)benzo[1,2-b:4,5-b']dithiophene-4,8-diyl)bis(4,5-diundecyl thiazole) **M2**[1] and [, 2,2'-((2Z,2'Z)-((6,6'-(5-dodecylbenzo[1,2-b:3,4-b':6,5-b"]trithiophene-2,8-diyl) bis(4-(2-hexyldecyl)-4H-dithieno[3,2-b:2',3'-d]pyrrole-6,2-diyl)) bis (methanylylidene))bis (3-oxo-2,3-dihydro-1H-indene-2,1-diylidene)) dimalononitrile [2] were synthesized according to the literature procedures.

2-(2-Ethylhexyl)-2H-benzo[d][1,2,3]triazole (1). 2,1,3-Benzotriazole (92.0 g, 772 mmol) and KOH (92.0 g, 818 mmol) were dissolved in 1L of DMSO under argon atmosphere. Then 2-ethylhexyl bromide (145.4 mL, 818 mmol) was added dropwise to the solution and heated to 75 °C for 24 h. The resulting solution was extracted with CH_2Cl_2 and washed three times with distilled water. The organic layer was dried over $MgSO_4$, and the solvent was evaporated under vacuum. The crude product was purified by column chromatography on silica gel with petroleum ether as eluent. Compound **1** was obtained as a yellow oil with a yield of 73.24g, (41%). ^{1}H NMR (500 MHz, $CDCl_3$), δ: 7.87 (dd, J = 6.6, 3.0 Hz, 2H), 7.36 (dd, J = 6.6, 3.0 Hz, 2H), 4.63 (d, J = 7.1 Hz, 2H), 2.24 (s, 1H), 1.35 (s, 8H), 0.93 (t, J = 7.5 Hz, 3H), 0.87 (t, J = 7.1 Hz, 3H).13C NMR (126 MHz, $CDCl_3$), δ: 144.23, 126.05, 117.96, 59.93, 40.49 , 30.50 , 28.47, 23.83, 22.85, 13.97, 10.45.

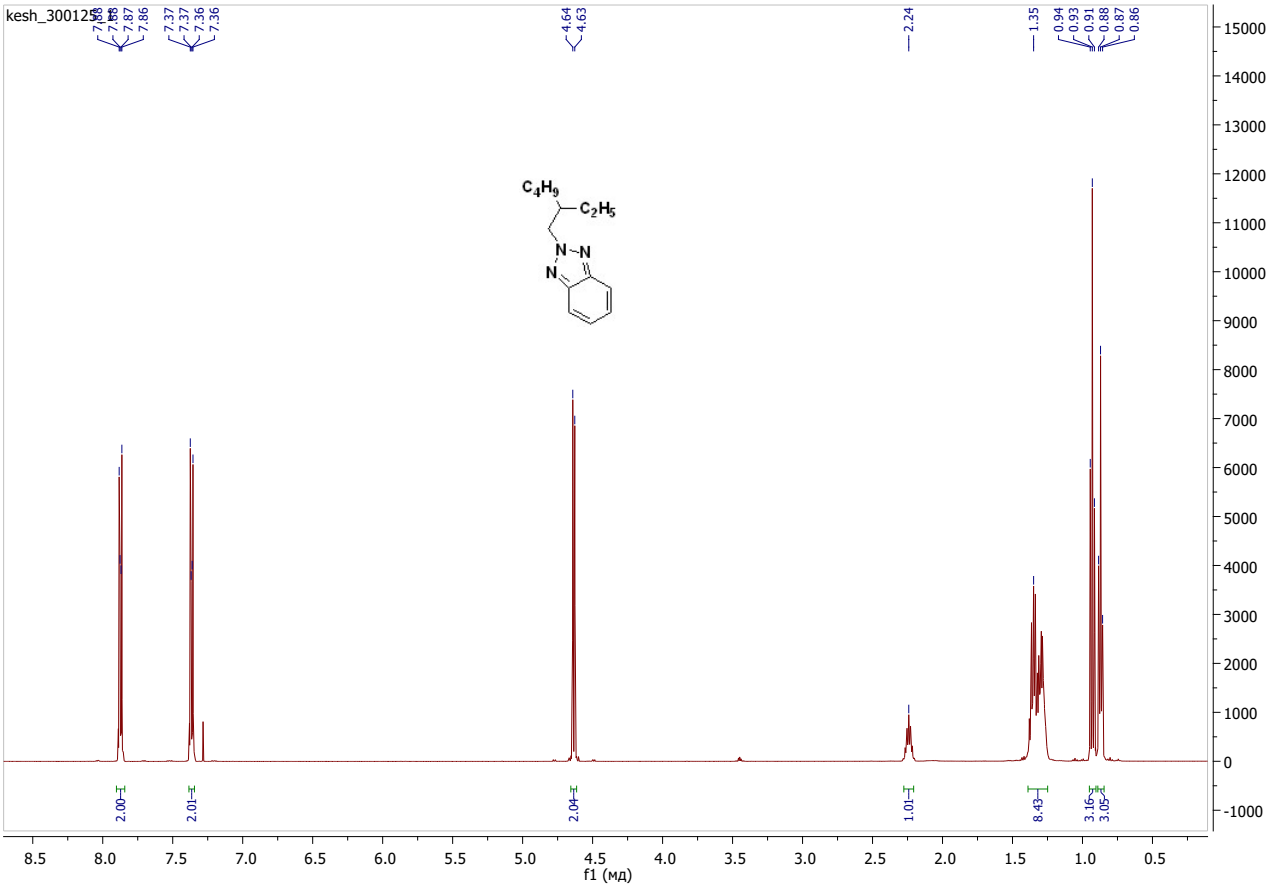

Figure S1.[1]H NMR spectrum of compound 1

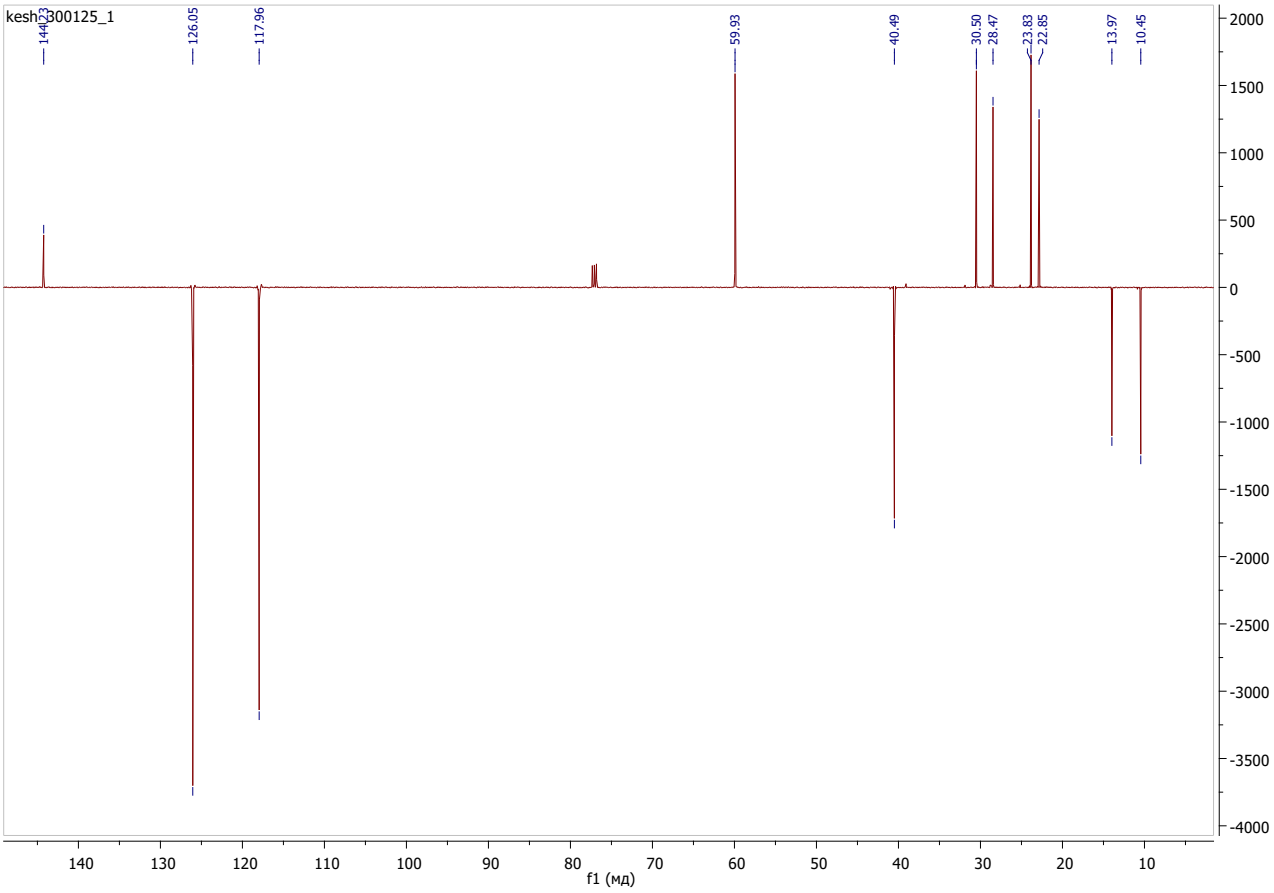

Figure S2.[13]C NMR spectrum of compound **1**

4,7-Dibromo-2-(2-ethylhexyl)-2H-benzo[d][1,2,3]triazole (2). 2-(2-Ethylhexyl)-2H-benzo[d][1,2,3]triazole (66.8 g, 289 mmol) was added to 400 mL of aqueous HBr solution and stirred for 1 h at 100°C. Then Br_2 (42 mL, 838 mmol) was added dropwise to the mixture and the reaction mixture was refluxed for 12 h. After cooling to room temperature, an aqueous $NaHCO_3$ solution was added to the mixture and it was extracted with chloroform three times. The organic layer was dried over $MgSO_4$, and the solvent was evaporated on a rotary evaporator. The crude product was purified by column chromatography on silica gel with petroleum ether:1,2-dichloromethane (4:1 v/v) as eluent. Compound **2** was obtained as an orange viscous oil in yield 103.50 g (92%). ^{1}H NMR (500 MHz, $CDCl_3$), δ: 7.42 (s, 2H), 4.68 (d, J = 7.3 Hz, 2H), 2.31 (s, 1H), 1.35 (s, 8H), 0.92 (t, J = 7.5 Hz, 3H), 0.86 (t, J = 7.1 Hz, 3H). 13C NMR (126 MHz, CDCl3), δ: 13C NMR (126 MHz, $CDCl_3$), δ: 143.64, 129.68, 109.99, 60.79, 40.24, 30.23, 28.22, 23.70, 22.85, 13.97, 10.36

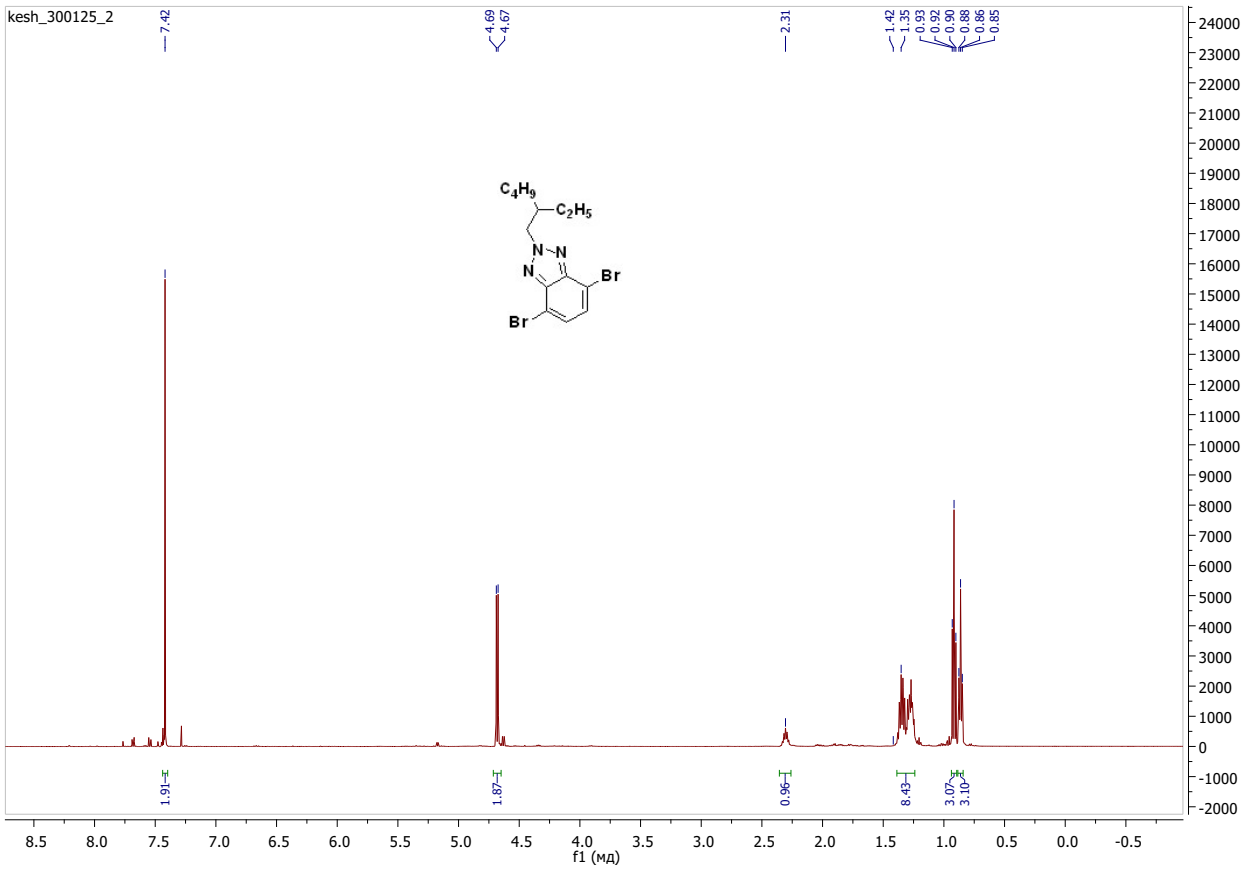

Figure S3.^{1}H NMR spectrum of compound 2

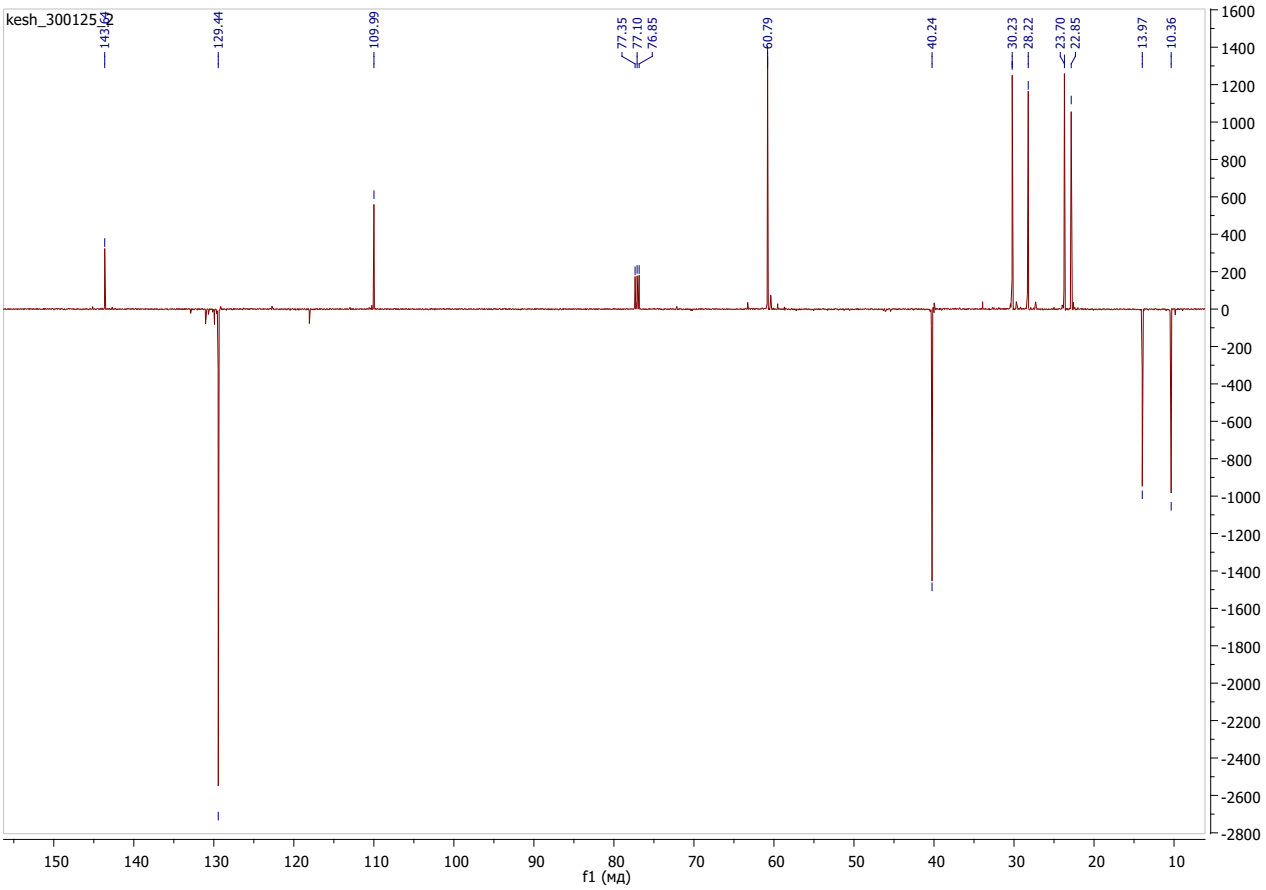

Figure S4.^{13}C NMR spectrum of compound **2**

4,7-Dibromo-2-(2-ethylhexyl)-5-nitro-2H-benzo[d][1,2,3]triazole (3). 4,7-Dibromo-2-(2-ethylhexyl)-2H-benzo[d][1,2,3]triazole (102.2 g, 263 mmol) was added to trifluoromethanesulfonic acid (84 mL, 1069 mmol). After cooling to 5°C, HNO_3 (97.3 mL, 1069 mmol, 60%) was slowly added dropwise and the mixture was stirred at the same temperature for 1 h. The reaction mixture was then warmed to room temperature and stirred overnight. The reaction was then neutralized with aqueous $NaHCO_3$ and extracted with 1,2-dichloromethane. The organic layer was washed three times with distilled water and dried over $MgSO_4$, the solvent was evaporated under vacuum. After drying, the product was purified by column chromatography on silica gel with petroleum ether:1,2-dichloromethane (4:1 v/v) as eluent. Compound **3** was obtained as a light-brown viscous oil in a yield of 86 g (75%). ^{1}H NMR (500 MHz, CDCl3), δ: 8.11 (s, 1H), 4.75 (d, J = 7.2 Hz, 2H), 2.32 (s, 1H), 1.37 (s, 8H), 0.96 (t, J = 7.5 Hz, 3H), 0.90 (t, J = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, CDCl3), δ: 147.27, 143.86, 143.46, 125.28, 110.95, 106.53, 61.43, 40.41, 30.25, 28.21, 23.75, 22.81, 13.96, 10.36.

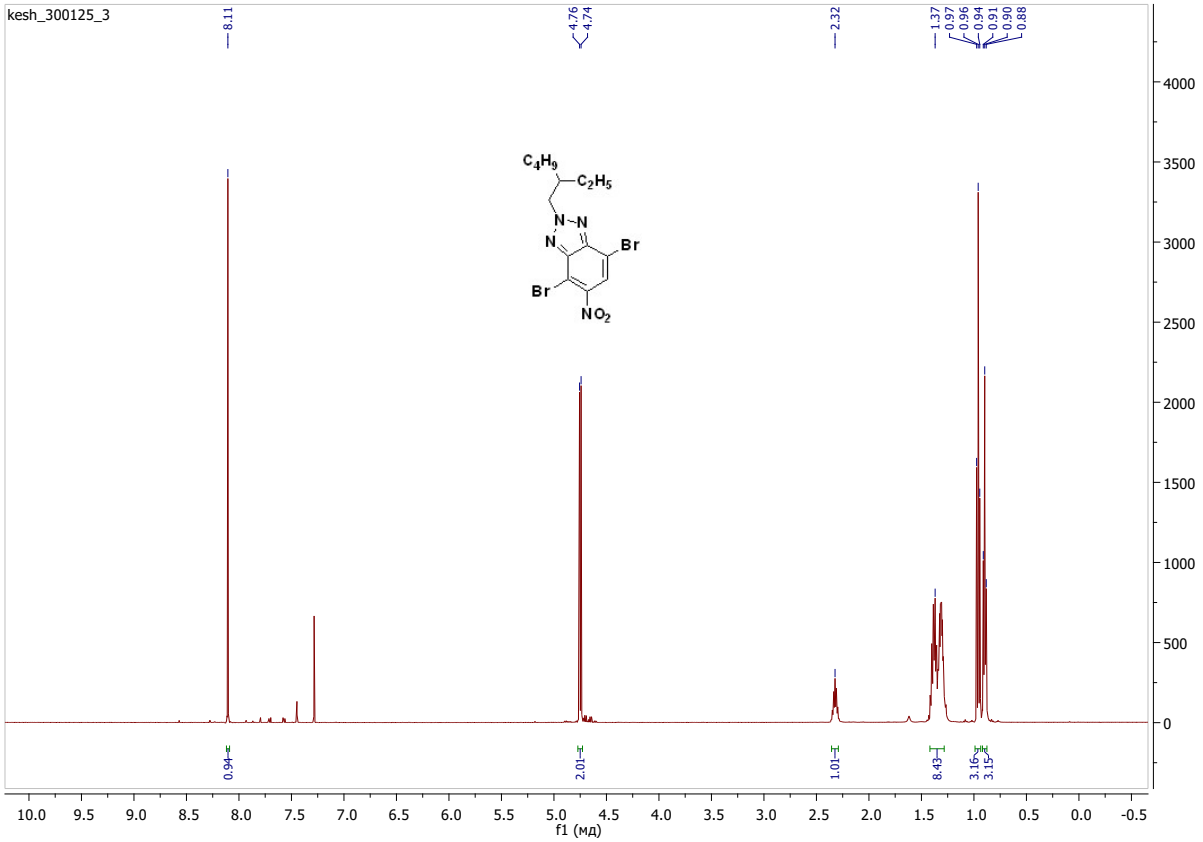

Figure S5.[1]H NMR spectrum of compound **3**

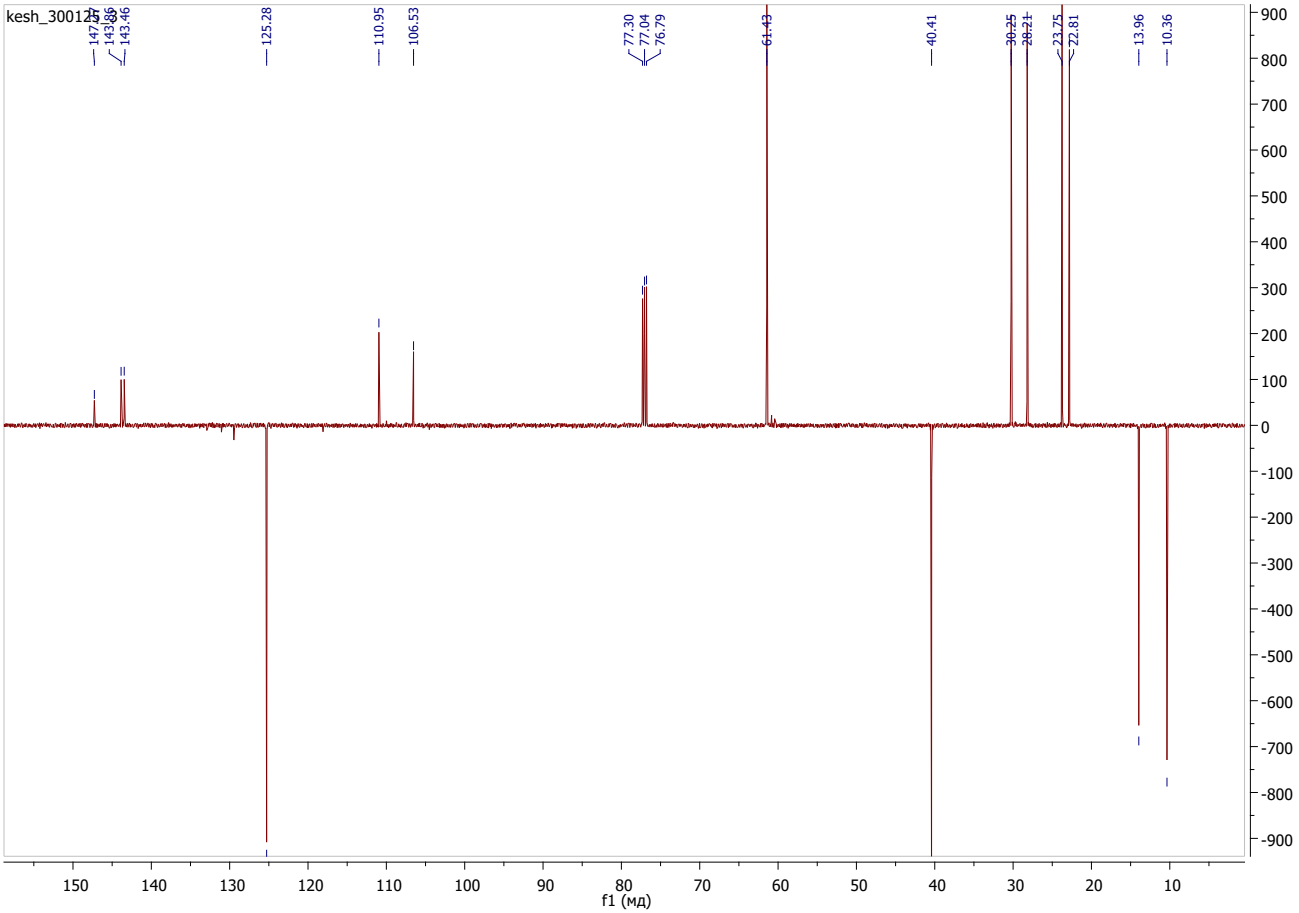

Figure S6.[13]C NMR spectrum of compound **3**

2-(2-,Ethylhexyl)-5-nitro-4,7-di(thiophen-2-yl)-2H-benzo[d][1,2,3]triazole (4). 4,7-Dibromo-2-(2-ethylhexyl)-5-nitro-2H-benzo[d][1,2,3]triazole (48.30 g, 111 mmol), 2-(tributylstannyl)thiophene (83.10 g, 223 mmol), and $PdCl_2(PPh_3)_2$ (3.1 g, 4.4 mmol) were dissolved in 700 mL of anhydrous THF under argon atmosphere. The resulting mixture was then refluxed overnight. After cooling to room temperature, the solvent was evaporated under vacuum. The product was purified by column chromatography on aluminum oxide with petroleum ether-acetone (50:1v/v). Compound **4** was obtained as a dark yellow viscous oil with a yield of 34.20 g (70%). ^{1}H NMR (600 MHz, $CDCl_3$), δ: 8.16 (d, J = 2.6 Hz, 1H), 7.92 (s, 1H), 7.61 (d, J = 5.1 Hz, 1H), 7.50 (dd, J = 10.3, 4.9 Hz, 2H), 7.27 – 7.18 (m, 2H), 4.76 (d, J = 6.8 Hz, 2H), 2.28 (s, 1H), 1.39 (s, 8H), 1.00 (t, J = 7.4 Hz, 3H), 0.91 (t, J = 7.2 Hz, 3H). ^{13}C NMR (151 MHz, CDCl3), δ: 146.30, 143.38, 141.70, 137.68, 131.82, 129.50, 128.82, 128.67, 128.34, 127.56, 127.48, 125.34, 117.76, 117.18, 60.45, 40.46, 30.54, 28.39, 23.98, 22.89, 13.98, 10.52.

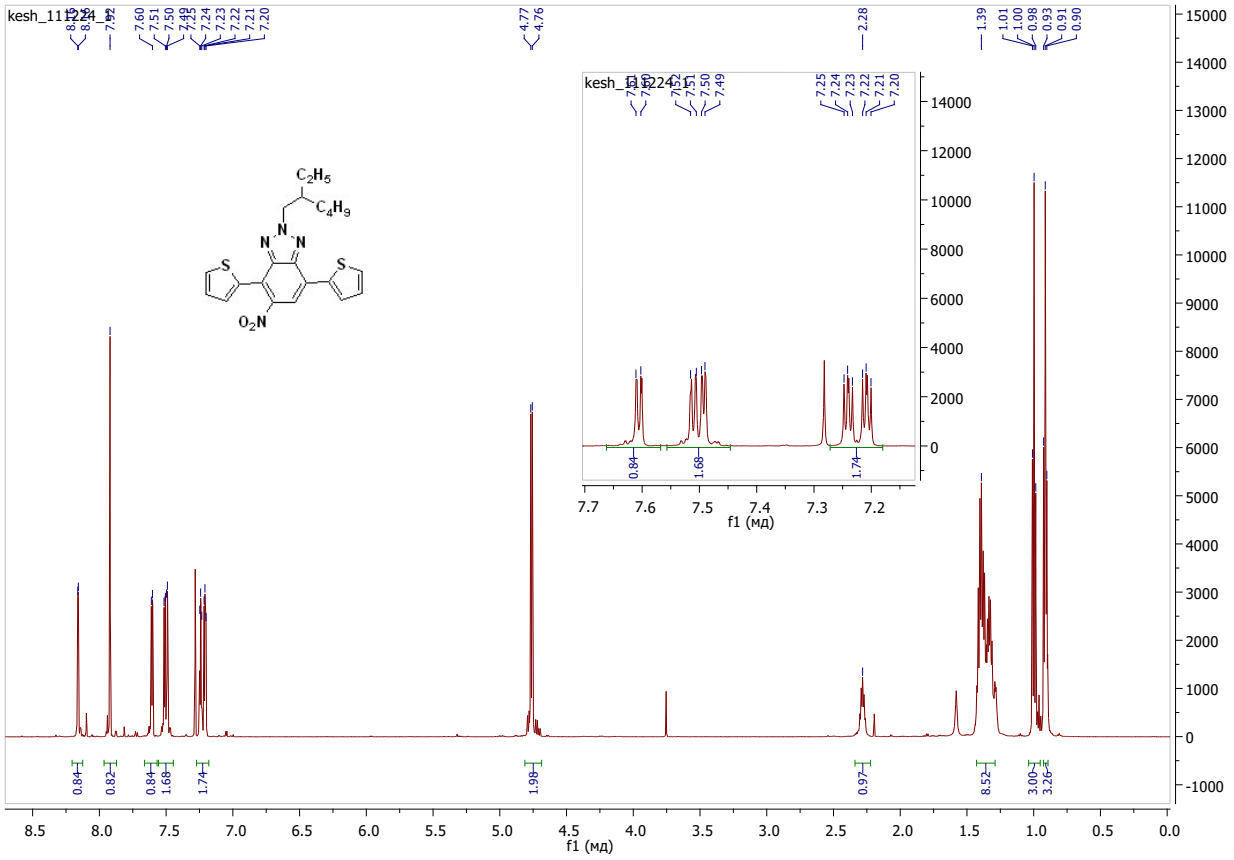

Figure S7.^{1}H NMR spectrum of compound **4**

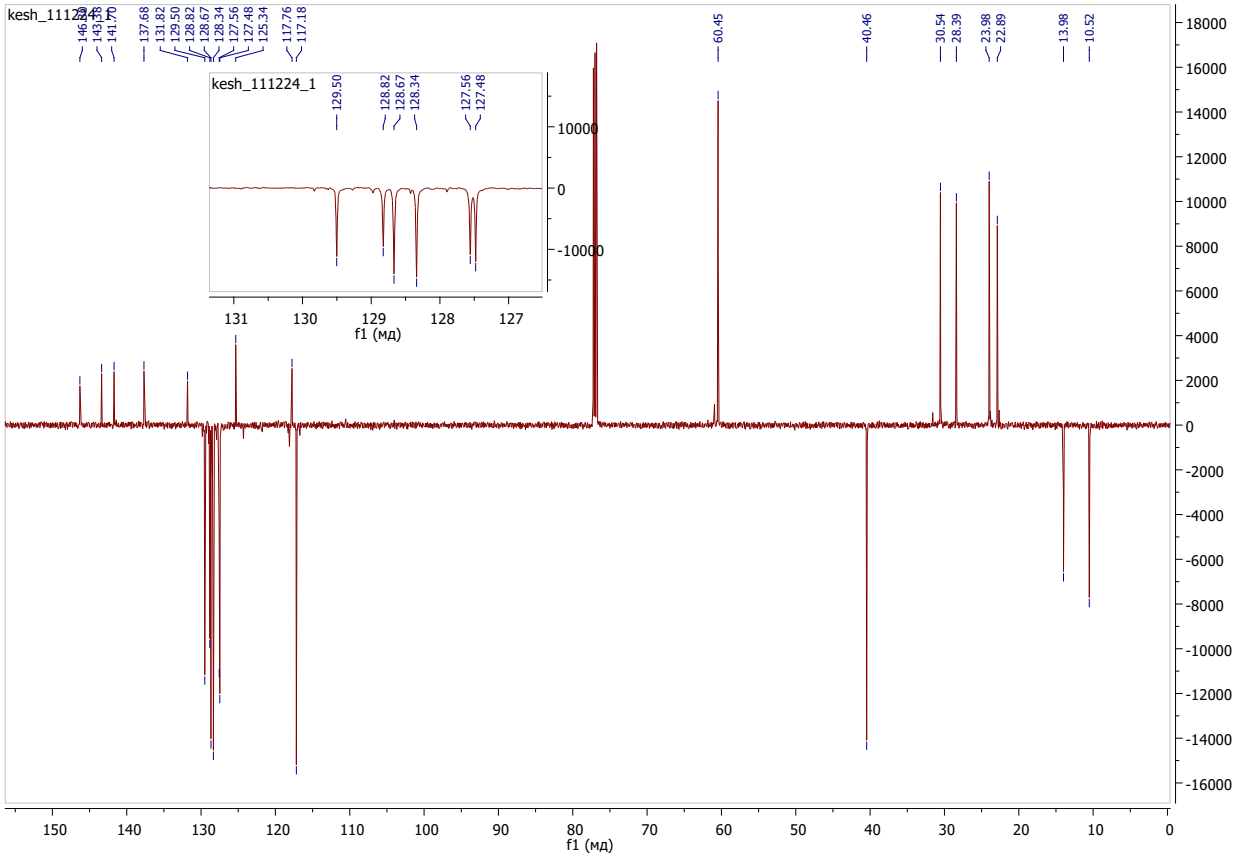

Figure S8.^{13}C NMR spectrum of compound **4**

2-(2-Ethylhexyl)-4-(thiophen-2-yl)-2,6-dihydrothieno[3,2-b][1,2,3]triazole[4,5-e]indole (5). 2-(2-Ethylhexyl)-5-nitro-4,7-di(thiophen-2-yl)-2H-benzo[d][1,2,3]triazole (13.2 g, 30 mmol) and triphenylphosphine (27.3 g, 104 mmol) were dissolved in 130 mL of anhydrous chlorobenzene under argon atmosphere. The reaction mixture was heated to 135 °C and stirred for 17 h. After cooling to room temperature, it was poured into distilled water and extracted with chloroform. The organic layer was dried over $MgSO_4$, and the solvent was evaporated under vacuum. The product was purified by column chromatography on silica gel with hexane:methylene (1:1 v/v) as eluent. Compound **5** was obtained as a dark-yellow viscous oil with a yield of 8.30 g (68%). 1H NMR (500 MHz, CDCl3), δ:8.73 (s, 1H), 8.13 (d, J = 4.7 Hz, 1H), 7.75 (s, 1H), 7.42 (d, J = 5.2 Hz, 1H), 7.35 (d, J = 5.1 Hz, 1H), 7.25 – 7.17 13C NMR (126 MHz, CDCl3), δ: 142.14, 140.92, 138.63, 138.21, 137.98, 128.07, 127.48, 126.42, 124.53, 119.73, 118.04, 111.28, 110.74, 108.23, 59.57, 40.29, 30.49, 28.44, 23.91, 22.97, 14.07, 10.54.

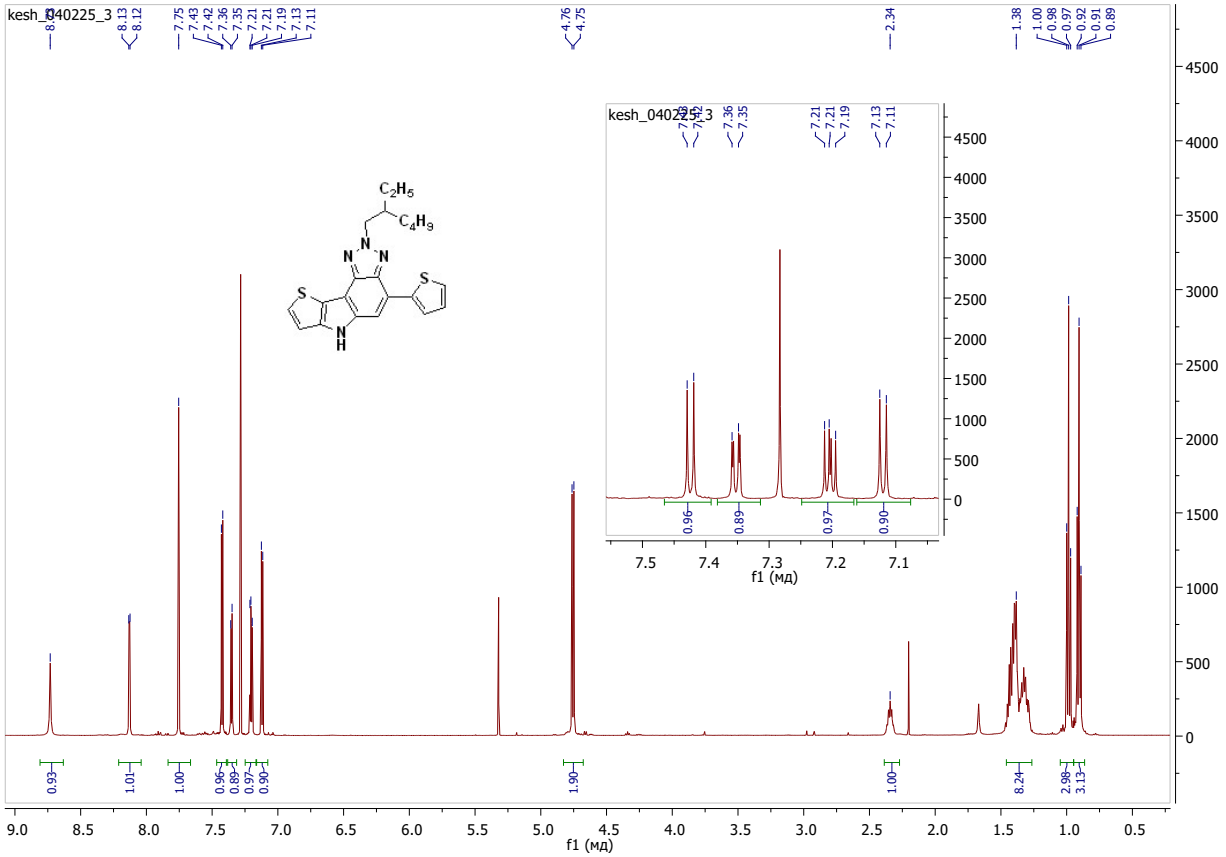

Figure S9.[1]H NMR spectrum of compound **5**

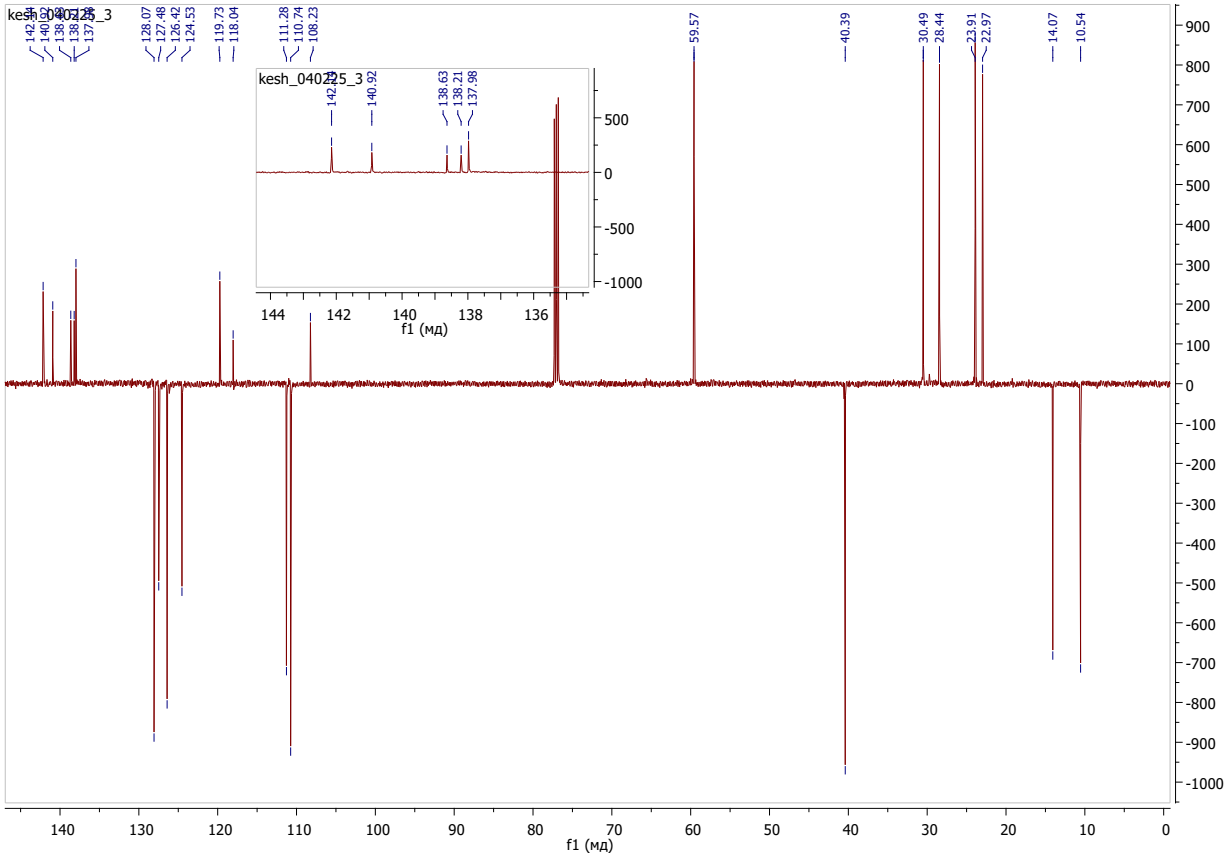

Figure S10.[13]C NMR spectrum of compound **5**

2-(2-Ethylhexyl)-6-(2-hexyldecyl)-4-(thiophen-2-yl)-2,6-dihydrothieno[3,2-b][1,2,3]triazole[4,5-e]indole (6). 2-(2-Ethylhexyl)-4-(thiophen-2-yl)-2,6-dihydro thieno[3,2-b][1,2,3]triazole[4,5-e]indole (12.70 g, 31 mmol), K_2CO_3 (8.20 g, 59 mmol), KI (1.70 g, 10 mmol), and (7-bromomethyl)pentadecane (15 g, 49 mmol) were added to 155 mL of anhydrous DMF under argon atmosphere. The reaction was then heated to 80°C and stirred for 17 h. The reaction mixture was then extracted with 1,2-dichloromethane and washed with an aqueous NaCl solution and distilled water. The mixture was dried over $MgSO_4$. The solvent was evaporated under vacuum. The product was purified by gradient column chromatography on silica gel eluting with hexane:1,2-dichloromethane (4:1v/v) to hexane:1,2-dichloromethane (1:1v/v). Compound **6** was obtained as a yellow oil in 12.00 g (61.0%) yield. ^{1}H NMR (500 MHz, CDCl3): δ 8.15 (d, J = 3.6 Hz, 1H), 7.75 (s, 1H), 7.44 (d, J = 5.2 Hz, 1H), 7.37 (d, J = 6.2 Hz, 1H), 7.26 – 7.19 (m, 1H), 7.12 (d, J = 5.2 Hz, 1H), 4.76 (d, J = 7.0 Hz, 2H), 4.27 (d, J = 7.3 Hz, 2H), 2.36 (s, 1H), 2.12 (s, 1H), 1.24 (s, 32H), 1.00 (t, J = 7.4 Hz, 3H), 0.93 (s, 9H).^{13}CNMR (126 MHz, CDCl3), δ; 144.88, 141.35, 138.45, 138.42, 138.36, 128.10, 127.10, 126.28, 124.29, 119.10, 115.94, 110.46, 109.30, 107.67, 66.68, 59.52, 50.16, 40.38, 39.15, 37.25, 31.87, 31.82, 31.81, 29.91 29.59, 29.54, 29.27, 23.89, 23.89, 23.00, 22.66, 22.62, 14.13, 14.08, 10.54.

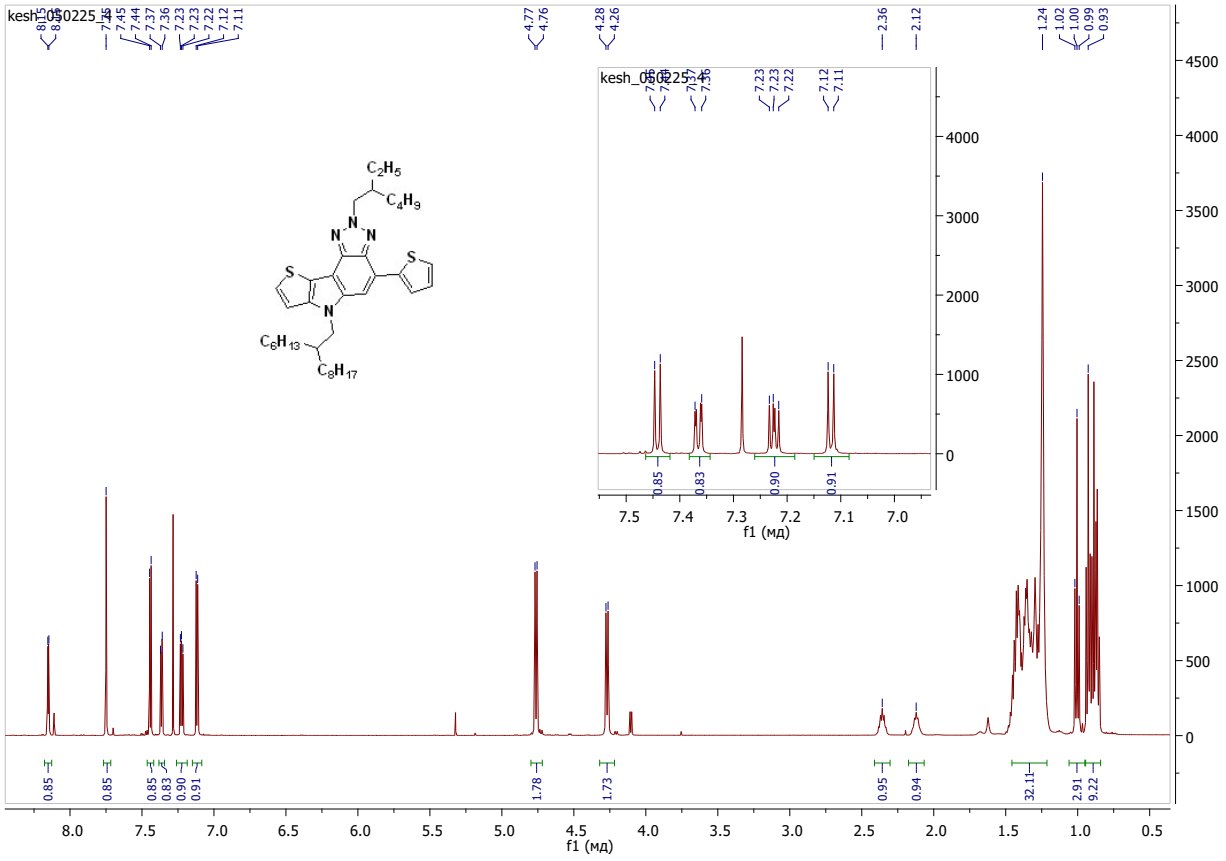

Figure S11.^{1}H NMR spectrum of compound **6**

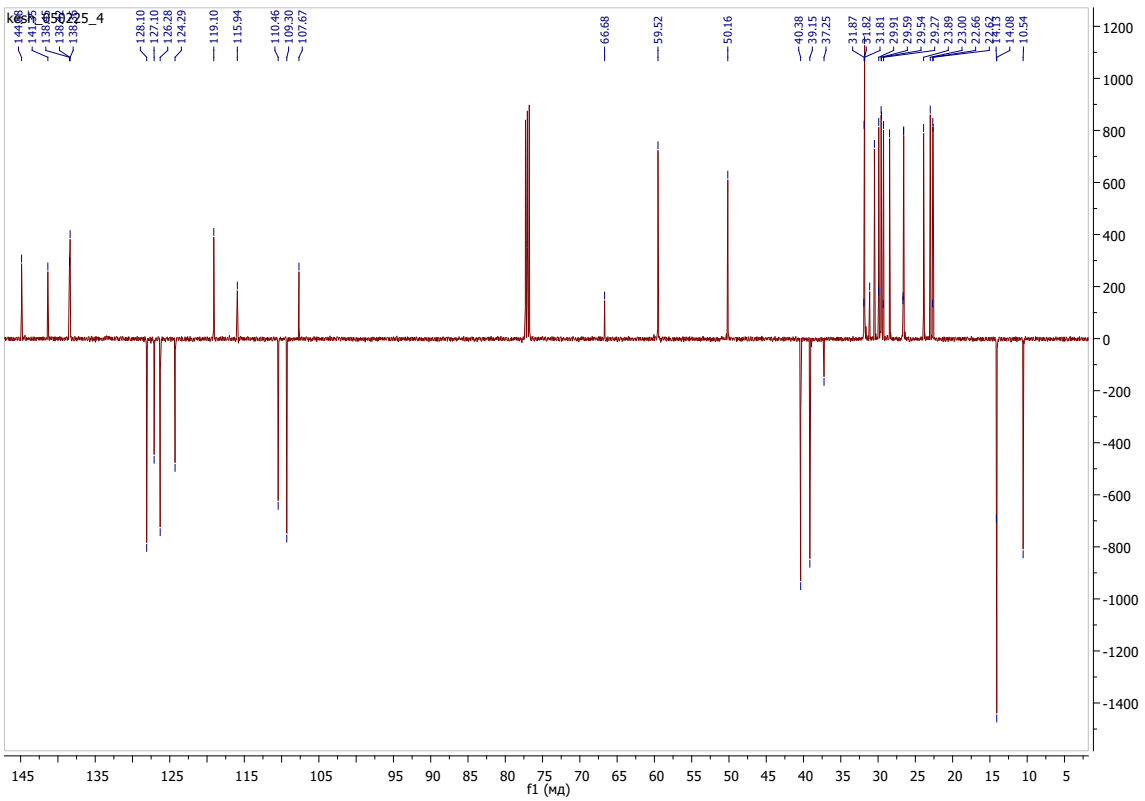

Figure S12.^{13}C NMR spectrum of compound **6**

8-**Bromo-4-(5-bromothiophen-2-yl)-2-(2-ethylhexyl)-6-(2-hexyldecyl)-2,6-dihydrothieno [3,2-b][1,2,3]triazolo[4,5-e]indole (M1).** 2-(2-Ethylhexyl)-6-(2-hexyldecyl)-4-(thiophen-2-yl)-2,6-dihydrothieno[3,2-b][1,2,3]triazolo[4,5-e]indole (6.3 g, 10 mmol) was dissolved in 200 ml of CHCl3-AcOH (1:1 v/v) and sprinkled portionwise with NBS (3.60 g, 20 mmol) under argon atmosphere and in the dark. The reaction was stirred for 2 h, then poured into distilled water and extracted with 1,2-dichloromethane. The organic layer was washed with an aqueous solution of NaHCO3 and dried over MgSO4. The product was purified by column chromatography on alumina with hexane as eluent. The target product **M1** was obtained as a light-yellow viscous oil with a yield of 7.00 g (88%). ^{1}HNMR (500 MHz, CDCl3), δ: 7.96 (s, 1H), 7.46 (d, J = 5.4 Hz, 1H), 7.18 (t, J = 5.2Hz, 2H), 4.71 (d, J = 7.1 Hz, 2H), 4.22 (d, J = 7.5 Hz, 2H), 2.32 (s, 1H), 2.12 (s, 1H), 1.22 (s, 32H), 0.98 (t, J = 7.4 Hz, 3H), 0.88 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$), δ: 142.72, 139.37, 137.83, 136.68, 134.62, 131.18, 126.16, 116.78, 115.89, 114.27, 113.90, 113.64, 108.59, 108.18, 59.64, 50.52, 40.38, 39.15, 31.86, 31.76, 29.92, 29.60, 29.50,29.26, 28.43, 26.52, 22.99, 22.65, 22.61, 14.12, 14.08, 10.53. Anal. Calcd. for $C_{38}H_{54}Br2N_4S_2$,%: C, 57.71; H, 6.88; Br, 20.21; N, 7.08; S, 8.11. Found,%: C, 57.92; H, 6.82; Br, 20.02; N, 6.96; S, 8.10. MALDI-TOF: m/z: 790.17 [M + H]+ (Calcd: 790.80)

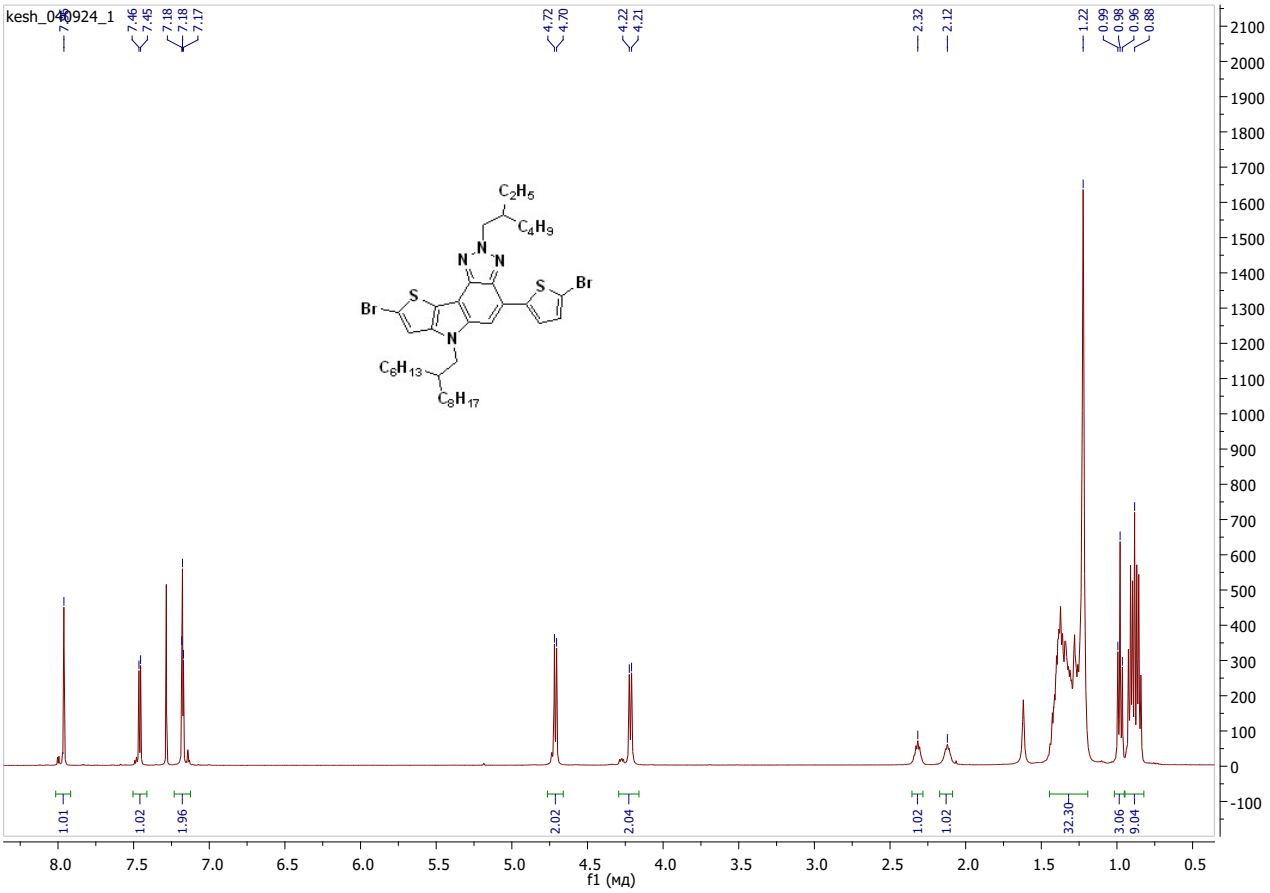

Figure S13.[1]H NMR spectrum of M2

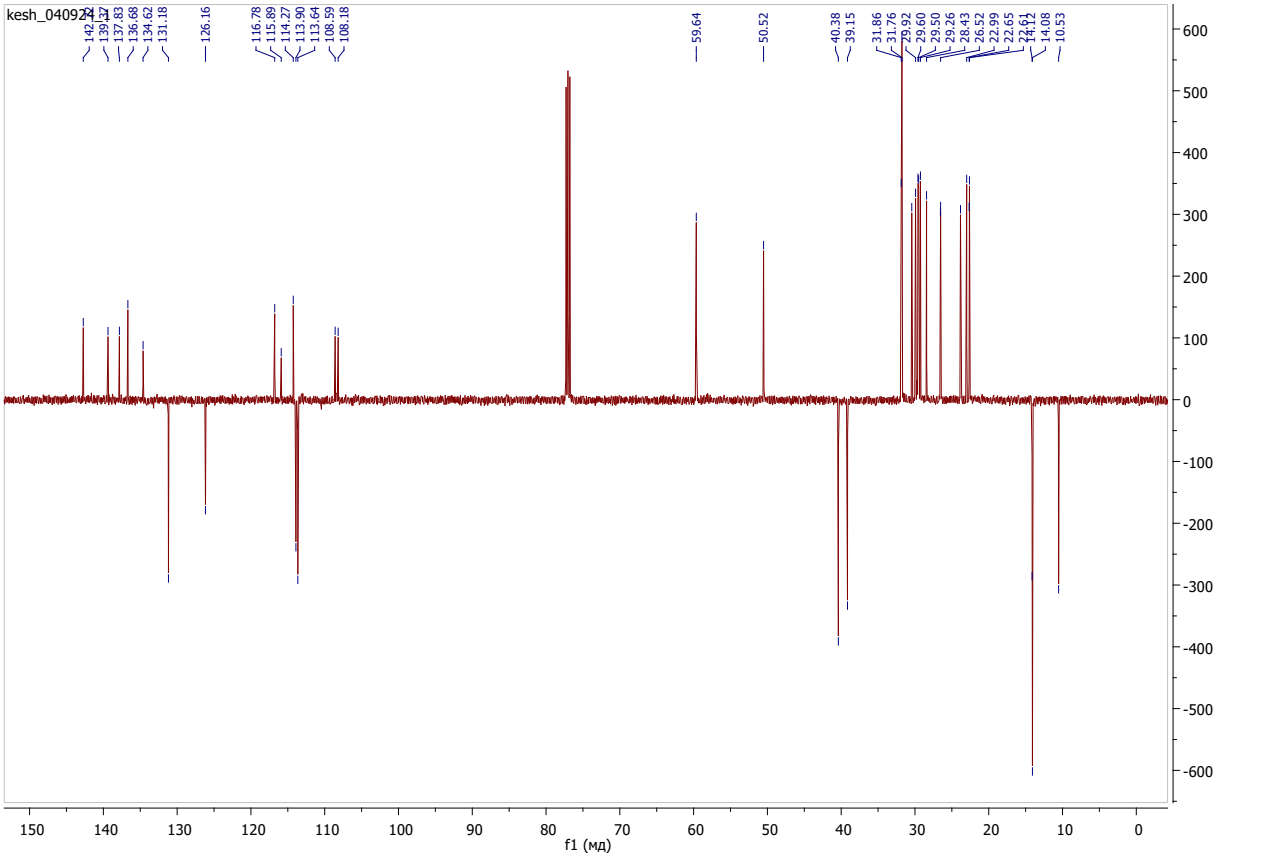

Figure S14.[13]C NMR spectrum of M1

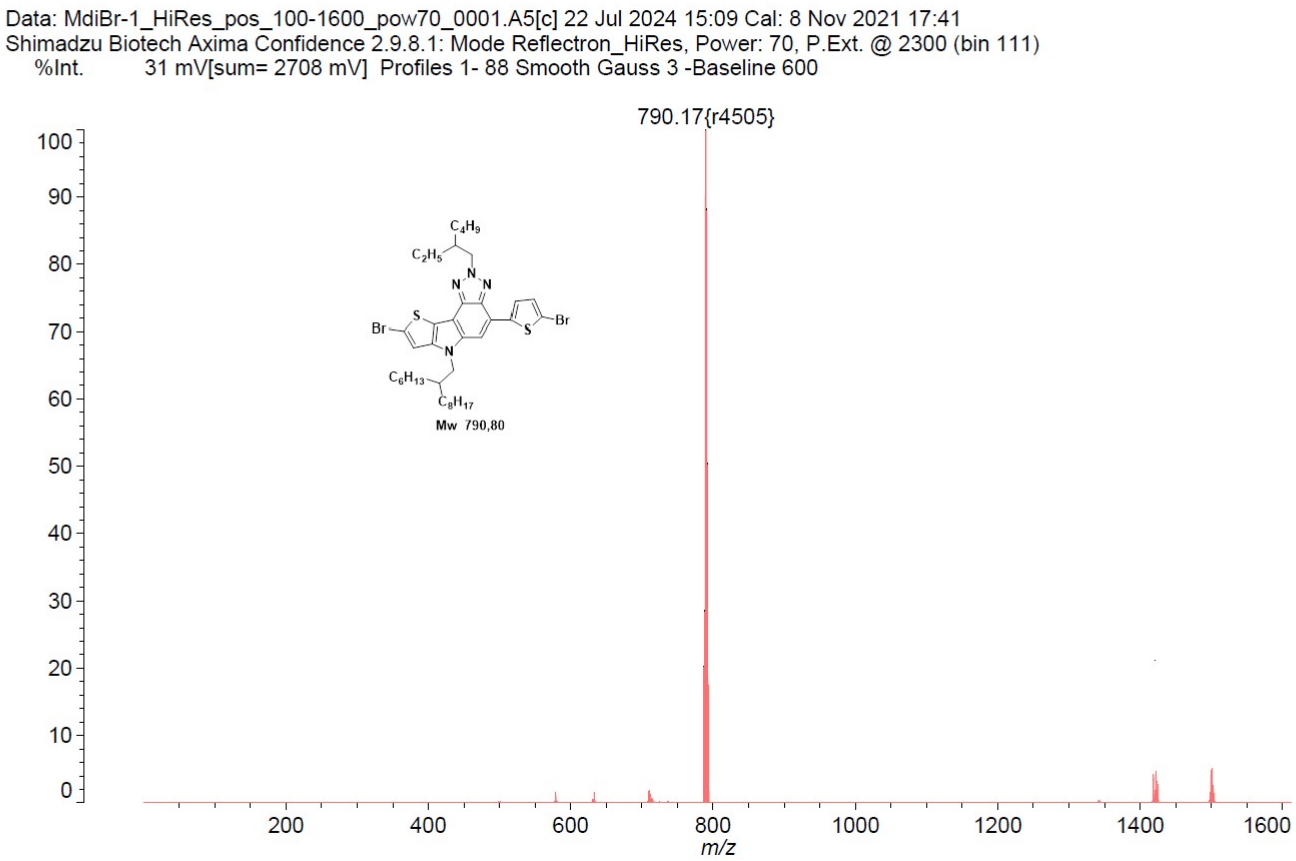

Figure S15. MALDI-TOF spectrum of M1

Poly[2,2'-(2,6-(benzo[1,2-b:4,5-b']dithiophene-4,8-diyl)bis(4,5-diundecylthiazole)-*alt*-8-4-(5-thiophen-2-yl)-2-(2-ethylhexyl)-6-(2-hexyldecyl)-2,6-dihydrothieno[3,2-b] [1,2,3] triazolo [4,5-e]indole] P154. A mixture of **M1** (1.1501 g, 0.885 mmol), **M2** (0.7000 g, 0.885 mmol) and 20 mL of toluene was charged into a 25 mL round-bottomed flask with a reflux condenser under nitrogen atmosphere. After degassing for 30 min, palladium catalyst $Pd[Pn_3P]_4$ (30 mg) was added to the flask. The mixture was additionally purged with argon for 20 min and heated to 110°C for 48 h. The reaction was quenched by adding 0.20 mmol of 2-bromothiophene and 0.2 mmol of 2-tributylstannylthiophene in that order. After completion of the reaction, the crude polymer was precipitated in methanol, and the precipitate was collected. Then it was extracted sequentially by Soxhlet extraction with acetone, hexane, and chloroform. The final polymer was obtained by precipitation from a solution of chloroform in methanol as a blue solid powder in a yield of 1.18 g (83%). ^{1}H NMR (400 MHz, $CDCl^3$, δ: 8.65-8.31 (br, 1H), 8.01-7.68 (br, 2H), 7.65-7.36 (m, 3H), 4.75-4.50 (m, 2H), 4.25-3.81 (m, 2H), 3.63-0.01 (m, 138H) Anal. Calcd. for $C_{98}H_{148}N_6S_6$. C, 73.44; H, 9.31; N, 5.24; S, 12.00. Found: C, 73.16; H, 9.27; N, 5.13,. S, 11.56

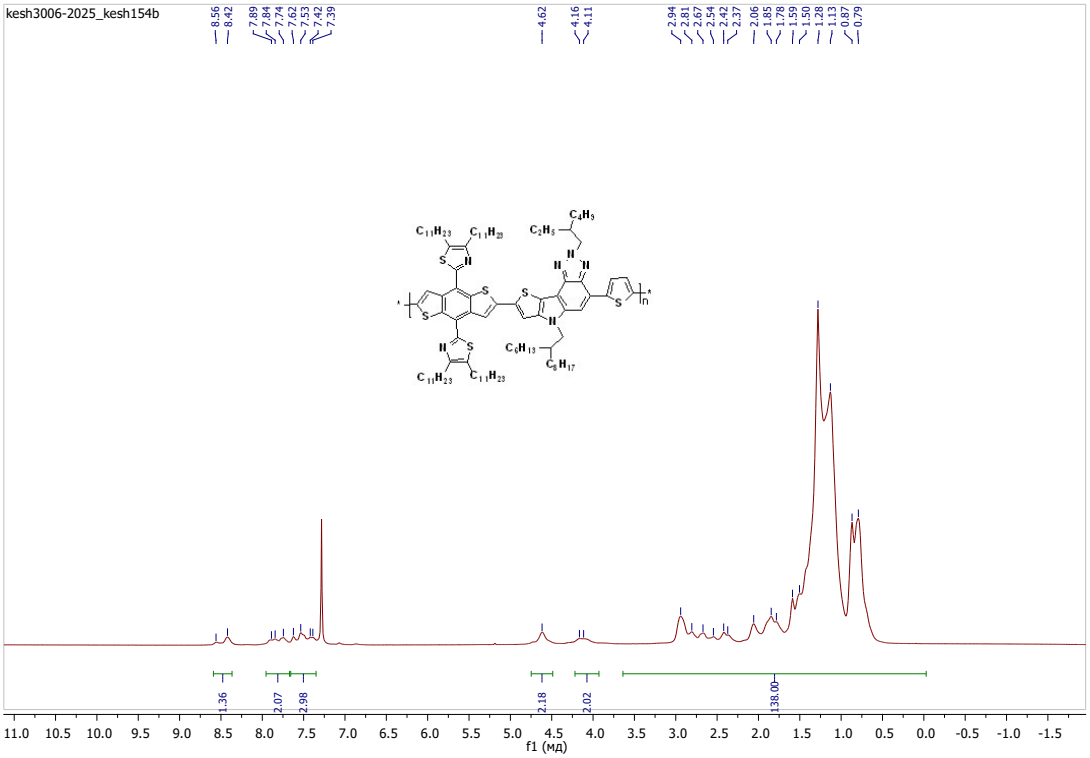

Figure S16.[1]HNMR spectrum of **P154**

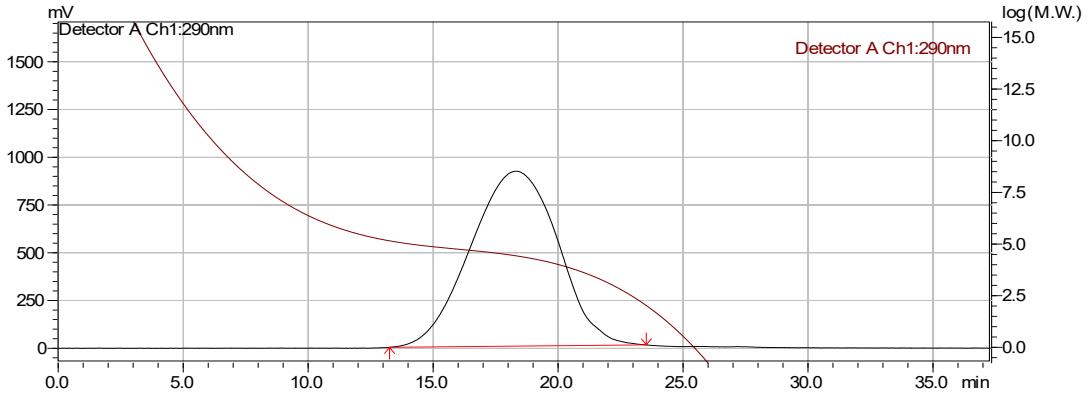

Figure S17. GPC curves for **P154**.

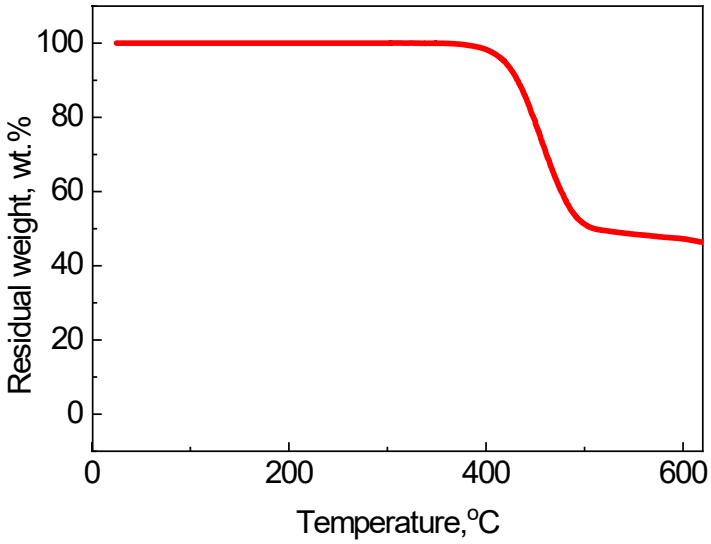

Figure S18. TGA plots of **P154.**

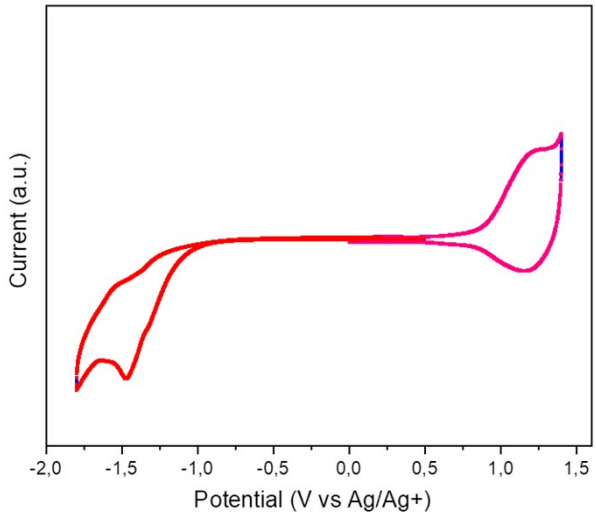

Figure S19. Cyclic voltammetry curves for **P154**. Assuming the absolute energy level of Fc/Fc+ to be - 4.44 eV versus vacuum level

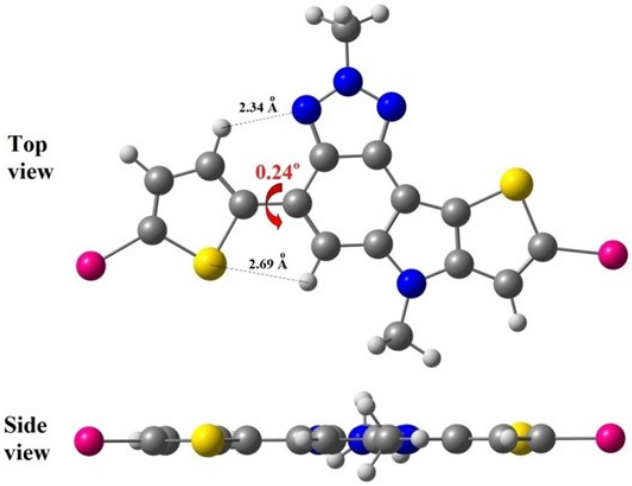

Figure S20. Optimized molecular geometry of M1. The alkyl side chains were replaced with a methyl group to simplify the calculations.

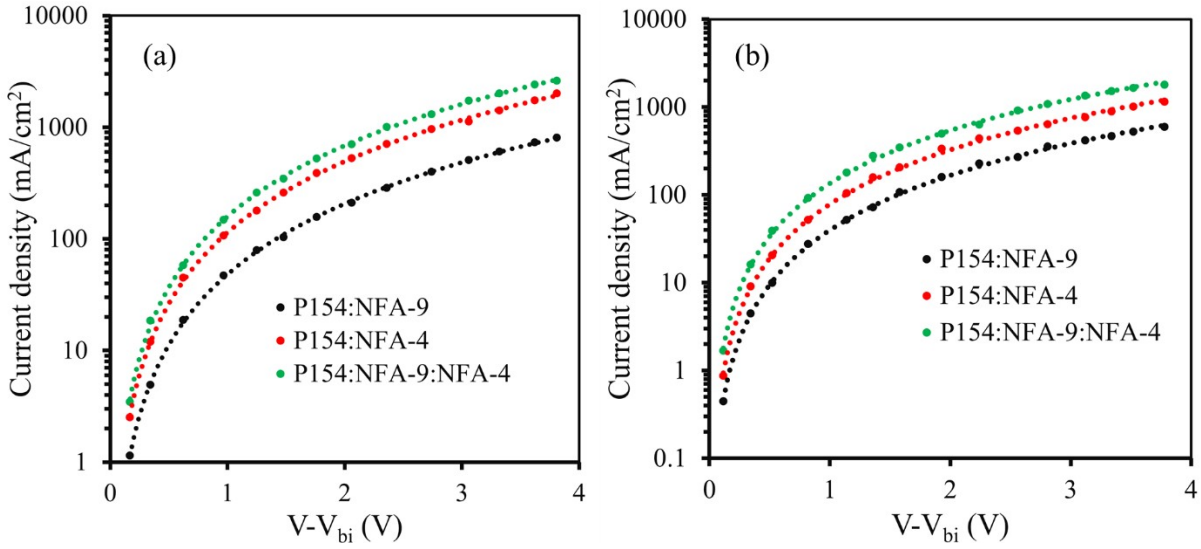

Figure S21. Dark J-V characteristics of (a) hole-only and (b)electron-only devices based on binary and ternary active layers.

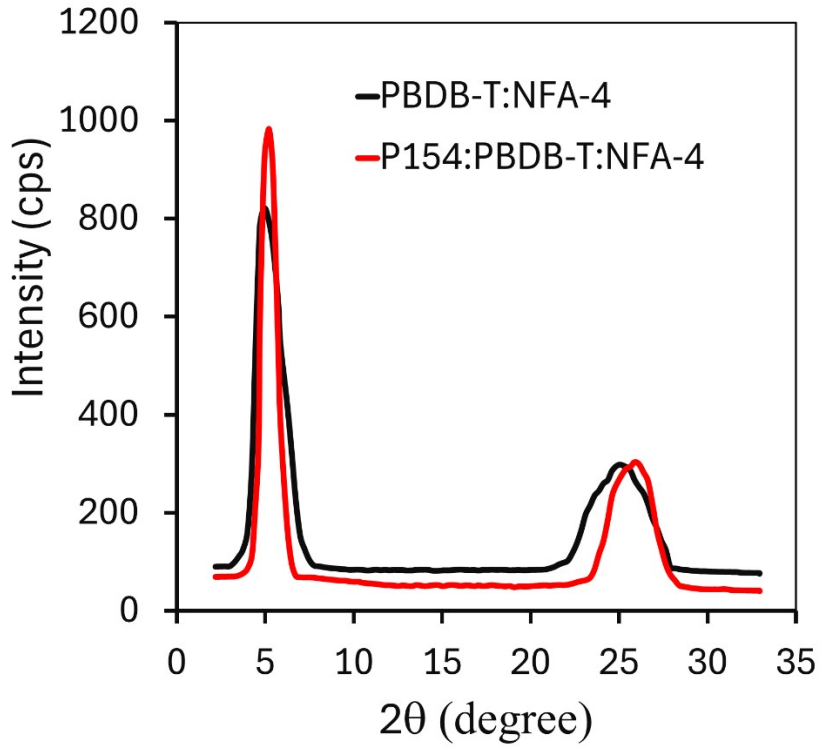

Figure 22. X-ray diffraction patterns for binary PBDB-T:NFA-4 and ternary **P154**:PBDB-T:NFA-4 thin films.

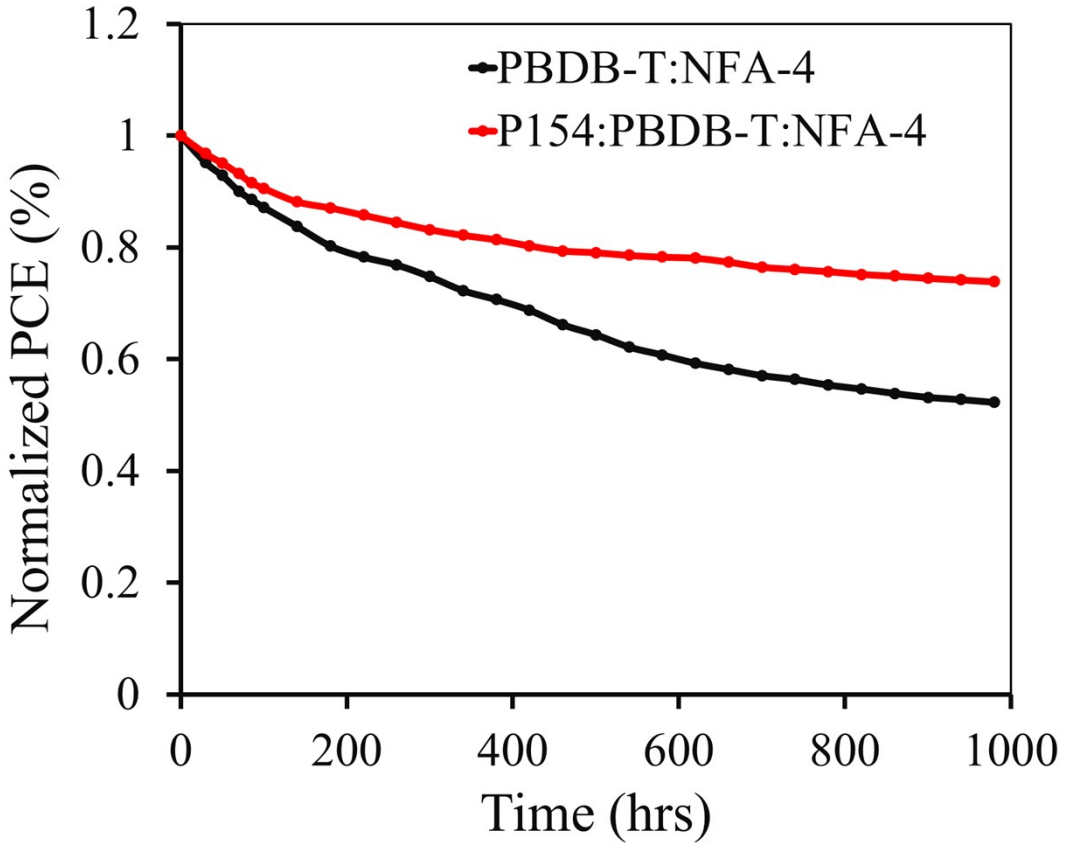

Figure S23. Stability test of the binary and ternary devices under ambient conditions.

Table S1. Photovoltaic parameters of **P154**:NFA-4 based OSCs, with different weight ratios between **P154** and NFA-4

P154:NFA-4 Weight ratio	J_{SC} (mA/cm^2)	V_{OC} (V)	FF	PCE (%)
1:0.4	16.08	0.958	0.596	9.18
1:0.8	17.78	0.962	0.622	10.64
1.1.2	**18.65**	**0.962**	**0.645**	**11.57**
1:1.4	17.94	0.959	0.617	10.62

Table S2. Photovoltaic parameters of **P154**:PBDB-T:NFA-4 based OSCs, with different weight ratios between **P154** and PBDB-T.

Weight ratio between **P154**:PBDB-T	J_{SC} (mA/cm^2)	V_{OC} (V)	FF	PCE (%)
0.2:1.0	18.74	0.923	0.674	11.66
0.4:0.8	**20.87**	**0.927**	**0.698**	**13.50**
0.8:0.4	20.02	0.923	0.664	12.27
1.0:0.2	19.43	0.916	0.653	11.62

References

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