

Supporting Information

Efficient organic solar cells with benzo[*b*]phenazine-core acceptors:

Insights into the effects of halogenation

Han Tian,^{‡a} Kangbo Sun,^{‡b} Yufei Wang,^b Zhanxiang Chen,^a Guangye Zhang,^{*b}
Zhenghui Luo^{*a}

^aH. Tian, Z. Luo, Z. Chen, C. Yang,
Guangdong Provincial Key Laboratory of New Energy Materials Service Safety,
Shenzhen Key Laboratory of New Information Display and Storage Materials, College of
Materials Science and Engineering, Shenzhen University, Shenzhen 518060, China.
Email: zhhuiluo@szu.edu.cn; clyang@szu.edu.cn

^bK. Sun, Y. Wang, G. Zhang
College of New Materials and New Energies Shenzhen Technology University, Shenzhen
518118, China
E-mail: zhangguangye@sztu.edu.cn

[‡] These authors contributed equally to this work.

Materials and Measurements

All solvents and reagents were used as received from commercial sources and used without further purification unless otherwise specified. All reactions were heated by metal sand bath (WATTCAS, LAB-500, <https://www.wattcas.com>). ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were measured on a MERCURYVX300 spectrometers. Mass spectra were recorded on a Shimadzu spectrometer. High-resolution mass spectrometry was carried out on Thermo Scientific TM Q-Exactive. Cyclic voltammetry (CV) measurements were carried out on a CHI voltammetric analyzer at room temperature. Tetrabutylammonium hexafluorophosphate ($n\text{-Bu}_4\text{NPF}_6$, 0.1 M) was used as the supporting electrolyte. The conventional three-electrode configuration consists of a platinum working electrode with a 2 mm diameter, a platinum wire counter electrode, and an Ag/AgCl wire reference electrode. Cyclic voltammograms were obtained at a scan rate of 100 mV/s. The film morphology was measured using an atomic force microscope (AFM, Bruker Dimension ICON) using the tapping mode. The RMS values of the surface AFM images are averaged based on five times testing on different areas for each sample. DFT calculations were performed by using Gaussian 16 at the B3LYP-D3(BJ)/def2-SVP level, and the long alkyl chain was simplified as methyl.

Device fabrication and characterization

Solar cells were fabricated in a conventional device configuration of ITO/PEDOT:PSS/PM6/acceptors/PNDIT-F3N/Ag. The ITO substrates were first

scrubbed by detergent and then sonicated with deionized water, acetone and isopropanol subsequently, and dried overnight in an oven. The glass substrates were treated by UV-Ozone for 30 min before use. PEDOT:PSS (Heraeus Clevios P VP AI 4083) was spin-cast onto the ITO substrates at 4000 rpm for 30 s, and then dried at 170 °C for 15 min in air. PM6 is dissolved in chloroform (7 mg mL⁻¹) and stirred in a nitrogen-filled glove box at 100 °C for one hour. Acceptors are dissolved in chloroform (9 mg mL⁻¹) and stirred in a nitrogen-filled glove box at 50 °C for one hour with 7mg/ml 1,4-diiodobenzene as additive. The precursors are spin-cast at 2000-2500 rpm onto substrates for 30·s with layer-by-layer method. The average thickness values of PM6/acceptors layers are 119.3 (117.0 ± 3.4) nm measured by Surface Profiler (ProfilierD-300). The active layers were then treated by 100°C thermal annealing for 5 min. A thin PFN-Br layer was coated on the active layer, followed by the deposition of Ag (100 nm) (evaporated under 1×10⁻⁴ Pa through a shadow mask). The current density-voltage (*J-V*) curves of devices were measured using a Keysight B2901A Source Meter in glove box under AM 1.5G (100 mW cm⁻²) using a Enlitech solar simulator. The device contact area was 0.042 cm², device illuminated area during testing was 0.041 cm², which was determined by a mask. The EQE spectra were measured using a Solar Cell Spectral Response Measurement System QE-R3011 (Enlitech Co., Ltd.). The light intensity at each wavelength was calibrated using a standard monocrystalline Si photovoltaic cell.

Mobility Measurements

The electron- and hole-mobilities were evaluated using the space-charge limited current

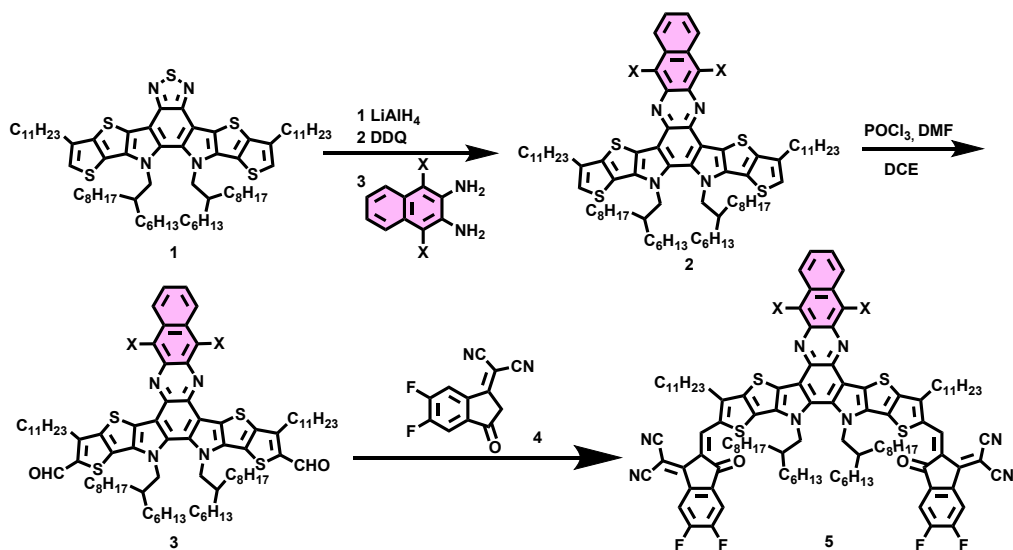
(SCLC) method. The device architecture of the electron-only devices was ITO/ZnO/active layer/PNDIT-F3N/Ag and that of the hole-only devices was ITO/PEDOT:PSS/active layer/MoOx/Ag. The charge carrier mobilities were determined by fitting the dark current into the model of a single carrier SCLC according to the equation: $J = 9\epsilon_0\epsilon_r\mu V^2/8d^3$, where J is the current density, d is the film thickness of the active layer, μ is the charge carrier mobility, ϵ_r is the relative dielectric constant of the transport medium, and ϵ_0 is the permittivity of free space. The V used in the equation is defined by: $V = V_{\text{app}} - V_{\text{bi}}$, where V_{app} is the applied voltage, V_{bi} is the built-in voltage. The carrier mobilities were calculated from the slope of the $J \sim V^2$ curves.

TPC and TPV measurements

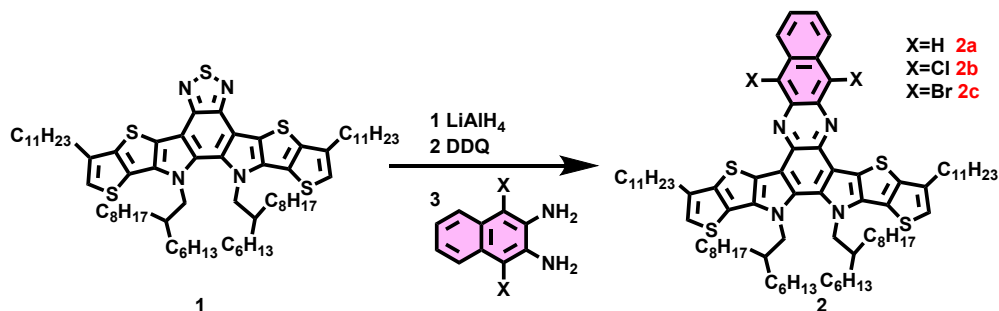
In TPV measurements, the devices were placed under background light bias enabled by a focused Quartz Tungsten-Halogen Lamp with an intensity of similar to working devices, i.e., the device voltage matches the open-circuit voltage under solar illumination conditions. Photo-excitations were generated with an 8 ns pulses from a laser system (Oriental Spectra, NLD520). The wavelength for the excitation was tuned to 518 nm with a spectral width of 3 nm. A digital oscilloscope was used to acquire the TPV signal at the open-circuit condition. TPC signals were measured under short-circuit conditions under the same excitation wavelength without background light bias.

GIWAXS measurements

2D GIWAXS measurement was performed on an XEUSS 3.0 UHR SAXS/WAXS system (XENOCSS, France). A Eiger2 R 1M 2-dimensional detector with 0.075 mm×0.075 mm active pixels were utilized in integration mode. The sample-to-detector distance is settled at 100 mm for GIWAXS measurement. The samples for GIWAXS test were prepared by casting solution onto silicon wafer substrates (ca. 10 mm × 10 mm), and the active layers were prepared using exactly the same concentration and same procedures as those for $J-V$ measurements.



Scheme S1. The overall synthetic route to NA9, NA10 and NA11.



Scheme S2. The synthetic route of three central cores.

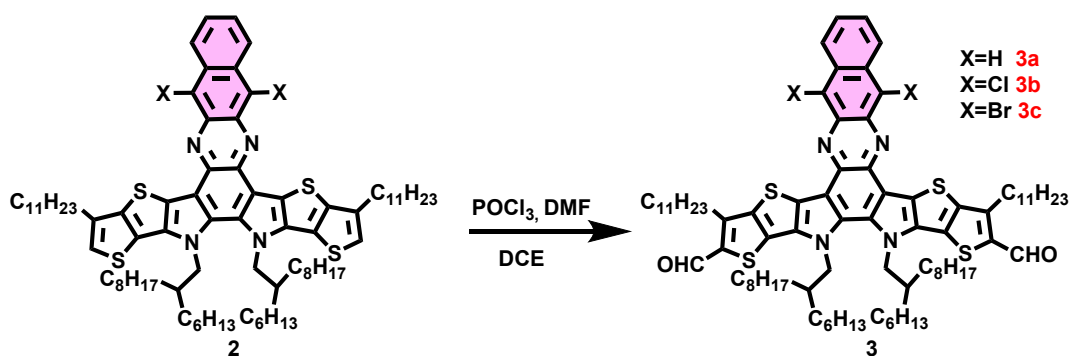
Synthesis of compound 2. Under the protection of nitrogen, compound **1** (1.0 eq.) was dissolved in anhydrous THF, then, a solution of LiAlH₄ (1M/L, 8.0 eq.) was slowly added to the mixed solution. The resulting mixture was stirred and heated to 70 °C overnight, afterthat, the mixture was added to the ice cube and extracted with dichloromethane. The organic phase was dried over anhydrous Na₂SO₄. The crude product was dissolved in chloroform (30 mL), then 3-dichloro-5,6-dicyano-1, 4-benzoquinone (DDQ, 0.95 eq.) and 3,4-Diaminopyridine (2.0 eq.) were added to the solution in turn. The mixture was stirred at room temperature for 3 hours, and then the mixture was extracted with dichloromethane. Finally, the crude product was purified by column chromatography over silica gel to afford viscous dark green solid.

2a: ¹H NMR (500 MHz, CDCl₃) δ 9.06 (s, 2H), 8.22 (dd, *J* = 6.4, 3.2 Hz, 2H), 7.56 (dd, *J* = 6.6, 3.1 Hz, 2H), 7.02 (s, 2H), 4.64 (d, *J* = 7.7 Hz, 4H), 2.89 (t, *J* = 7.7 Hz, 4H), 2.22 – 2.15 (m, 2H), 1.94 – 1.90 (m, 4H), 1.32 – 0.92 (m, 86H), 0.76 (t, *d* = 7.3 Hz, 6H), 0.66 (d, *J* = 7.2 Hz, 6H). ¹³C NMR (125 MHz, CDCl₃) δ 143.02 (s), 140.26 (s), 138.80 (s), 136.96 (s), 136.71 (s), 133.13 (s), 131.91 (s), 128.41 (s), 127.01 (s), 125.68 (s), 124.07 (s), 123.51 (s), 118.82 (s), 117.00 (s), 55.10 (s), 38.79 (s), 37.15 (s), 32.80 (s), 31.99 (s), 31.91 – 31.44 (m), 30.51 (d, *J* = 6.6 Hz), 30.14 (d, *J* = 10.6 Hz), 29.97 – 29.30 (m), 29.19 (s), 29.01 (s), 27.14 (s), 25.59 (s), 22.85 – 22.40 (m), 19.76 (s), 14.26 – 13.89 (m).

2b: ¹H NMR (500 MHz, CDCl₃) δ 8.82 (dd, *J* = 6.8, 3.2 Hz, 2H), 7.74 (dd, *J* = 6.8, 3.1 Hz, 2H), 7.04 (s, 2H), 4.67 (d, *J* = 7.7 Hz, 4H), 2.92 (t, *J* = 7.6 Hz, 4H), 2.22 – 2.17 (m, 2H), 1.95 – 1.91 (m, 4H), 1.40 – 0.80 (m, 70H), 0.89 (m, 86H), 0.78 (d, *J* = 7.3 Hz, 6H), 0.70 (t, *J* = 6.9 Hz, 6H). ¹³C NMR (125 MHz, CDCl₃) δ 143.62 (s), 139.90 (s), 137.03 (d, *J* = 17.5 Hz), 135.17 (s), 132.40 (s), 130.09 (s), 128.41 (s), 127.15 (s), 125.47 (s), 124.42 (s), 123.44 (d, *J* = 18.1 Hz), 119.00 (s), 116.75 (s), 55.27 (s), 38.83 (s), 35.02 (s), 32.07 – 31.65 (m), 31.54 (s), 30.39 (dd, *J* = 28.3, 18.8 Hz), 30.06 – 29.22 (m), 29.19 (s), 28.92 (s), 25.65 (s), 22.85 – 22.42 (m), 14.27 – 13.92 (m).

2c: ¹H NMR (500 MHz, CDCl₃) δ 8.86 (dd, *J* = 6.8, 3.1 Hz, 2H), 7.73 (dd, *J* = 6.8, 3.0

Hz, 2H), 7.04 (s, 2H), 4.65 (t, $J = 15.2$ Hz, 4H), 2.92 (t, $J = 7.6$ Hz, 4H), 2.23 – 2.17 (m, 2H), 1.96 – 1.90 (m, 4H), 1.38 – 1.10 (m, 86H), 0.77 (t, $J = 7.3$ Hz, 6H), 0.69 (t, $J = 7.0$ Hz, 6H). ^{13}C NMR (125 MHz, CDCl_3) δ 143.68 (s), 140.21 (s), 137.03 (d, $J = 15.6$ Hz), 136.37 (s), 132.39 (s), 132.05 (s), 128.43 (s), 127.45 (s), 124.42 (s), 123.81 (s), 123.36 (s), 118.98 (s), 116.55 (s), 55.28 (s), 38.81 (s), 37.14 (s), 32.79 (s), 31.99 (s), 31.91 – 31.35 (m), 30.49 (d, $J = 10.8$ Hz), 30.12 (d, $J = 11.4$ Hz), 29.95 – 29.13 (m), 28.90 (s), 27.13 (s), 25.64 (s), 22.93 – 22.32 (m), 19.76 (s), 14.27 – 13.90 (m).



Scheme S3. The synthetic route of three dialdehyde compounds.

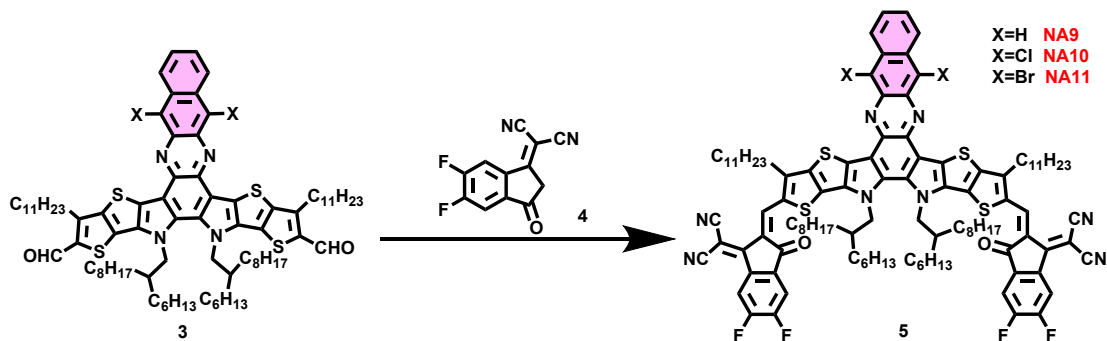
Synthesis of compound 3. POCl_3 (3 mL) was added dropwise to a solution of anhydrous *N,N*-dimethylformamide (DMF) (8 mL) at 0°C under N_2 atmosphere and stirred at room temperature for 30 min. Compound **2** dissolved in 20 mL anhydrous 1,2-dichloroethane (DCE) was added to the above solution and stirred at 70°C for 12 h under N_2 atmosphere. Then, the reaction mixture is quenched by stirring with water and extracted with dichloromethane. Finally, the crude product was purified by column chromatography over silica gel to afford red solid.

3a: ^1H NMR (500 MHz, CDCl_3) δ 10.16 (s, 2H), 9.07 (s, 2H), 8.23 (dd, $J = 6.4, 3.2$ Hz, 2H), 7.60 (dd, $J = 6.6, 3.1$ Hz, 2H), 4.66 (d, $J = 7.9$ Hz, 4H), 3.26 (t, $J = 7.7$ Hz, 4H), 2.18 – 2.10 (m, 2H), 1.99 (dt, $J = 15.3, 7.7$ Hz, 4H), 1.33 – 0.91 (m, 86H), 0.77 (t, $J = 7.3$ Hz, 6H), 0.66 (t, $J = 7.1$ Hz, 6H). ^{13}C NMR (125 MHz, CDCl_3) δ 181.70 (s), 147.03 (d, J

= 13.9 Hz), 144.17 (s), 139.81 (s), 138.75 (s), 136.67 (s), 136.45 (s), 133.46 (s), 133.06 (s), 129.58 (s), 128.69 (s), 128.34 (s), 127.12 (s), 126.14 (s), 124.48 (s), 124.00 (s), 119.13 (s), 117.91 (s), 55.36 (s), 39.07 (s), 34.89 (s), 31.94 (s), 31.77 (s), 31.53 (d, $J = 18.3$ Hz), 30.79 – 30.25 (m), 30.22 (s), 29.55 (ddd, $J = 15.3, 13.5, 4.3$ Hz), 29.17 (s), 28.23 (s), 25.61 (d, $J = 4.4$ Hz), 22.81 – 22.39 (m), 14.23 – 13.88 (m).

3b: ^1H NMR (500 MHz, CDCl_3) δ 10.17 (s, 2H), 8.81 (dd, $J = 6.8, 3.2$ Hz, 2H), 7.79 (dd, $J = 6.8, 3.1$ Hz, 2H), 4.68 (d, $J = 7.8$ Hz, 4H), 3.28 (t, $J = 7.7$ Hz, 4H), 2.19 – 2.10 (m, 2H), 2.01 – 1.96 (m, 4H), 1.50-1.00 (m, 86H), 0.76 (t, $J = 7.3$ Hz, 6H), 0.68 (t, $J = 6.9$ Hz, 6H). ^{13}C NMR (125 MHz, CDCl_3) δ 181.84 (s), 147.14 (s), 144.58 (s), 139.67 (s), 136.92 (s), 136.70 (s), 135.25 (s), 133.56 (s), 130.51 (s), 129.50 (s), 128.98 (s), 128.70 (s), 127.72 (s), 125.52 (s), 124.48 (s), 123.99 (s), 119.12 (s), 117.55 (s), 55.50 (s), 53.43 (s), 39.04 (s), 34.88 (s), 34.54 (s), 31.94 (s), 31.76 (s), 31.69 – 31.35 (m), 30.80 – 29.96 (m), 29.51 (ddd, $J = 12.7, 12.2, 7.0$ Hz), 29.15 (s), 28.13 (s), 25.58 (s), 22.79 – 22.38 (m), 14.22 – 13.86 (m).

3c: ^1H NMR (500 MHz, CDCl_3) δ 10.17 (s, 2H), 8.83 (dd, $J = 6.8, 3.2$ Hz, 2H), 7.75 (dd, $J = 6.8, 3.1$ Hz, 2H), 4.70 (d, $J = 7.8$ Hz, 4H), 3.28 (t, $J = 7.6$ Hz, 4H), 2.20 – 2.14 (m, 2H), 2.02 – 1.96 (m, 4H), 1.32 – 0.80 (m, 86H), 0.76 (t, $J = 7.3$ Hz, 6H), 0.69 (t, $J = 7.0$ Hz, 6H). ^{13}C NMR (125 MHz, CDCl_3) δ 181.79 (s), 147.05 (s), 144.62 (s), 139.92 (s), 136.91 (s), 136.69 (s), 136.39 (s), 133.50 (s), 132.40 (s), 129.46 (s), 128.95 (s), 128.40 (s), 127.95 (s), 124.00 (s), 117.38 (s), 55.52 (s), 39.09 (s), 34.89 (s), 31.94 (s), 31.89 – 31.44 (m), 31.44 – 31.35 (m), 30.46 (dd, $J = 29.9, 19.7$ Hz), 30.20 – 30.04 (m), 30.04 – 29.21 (m), 29.18 (s), 28.10 (s), 25.66 (s), 22.90 – 22.32 (m), 14.32 – 13.80 (m).



Scheme S4. The synthesis route of three SMAs.

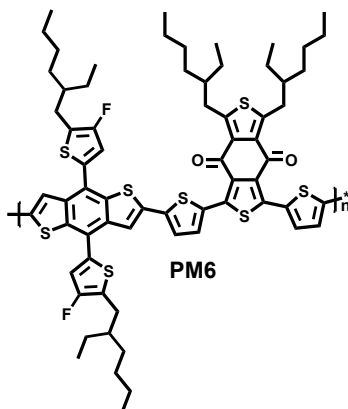
Synthesis of three SMAs. Compound **3** (1.0 eq.) and Compound **4** (8.0 eq.) were added dissolved in chloroform (30 mL), then 1mL pyridine was added, the reaction mixture was stirred for 3 h under 70 °C. The reaction mixture was allowed to cool down to room temperature. The residue was purified by column chromatography on silica gel to afford dark blue solid.

NA9: ^1H NMR (500 MHz, CDCl_3) δ 9.10 (s, 2H), 8.96 (s, 2H), 8.51 (dd, $J = 9.7, 6.5$ Hz, 2H), 8.16 (dd, $J = 6.3, 3.1$ Hz, 2H), 7.68 (t, $J = 7.4$ Hz, 2H), 7.59 (dd, $J = 6.6, 3.0$ Hz, 2H), 4.81 (d, $J = 7.8$ Hz, 4H), 3.22 (t, $J = 7.8$ Hz, 4H), 2.26 (s, 2H), 1.92 – 1.86 (m, 4H), 1.40 – 1.35 (m, 4H), 1.30 – 1.01 (m, 76H), 0.85 (t, $J = 6.9$ Hz, 6H), 0.73 (t, $J = 7.2$ Hz, 6H), 0.68 (t, $J = 6.8$ Hz, 6H). ^{13}C NMR (125 MHz, CDCl_3) δ 186.11 (s), 153.84 (s), 146.61 (s), 139.58 (s), 138.44 (s), 137.65 (s), 136.07 (s), 134.02 (s), 133.48 (s), 133.19 (s), 132.15 (s), 119.36 (s), 119.16 (s), 114.75 (s), 67.72 (s), 31.92 (s), 31.74 (s), 31.45 (s), 30.58 (s), 30.13 (d, $J = 19.7$ Hz), 30.01 – 29.41 (m), 29.34 (d, $J = 7.5$ Hz), 25.88 (s), 22.75 – 22.41 (m), 14.07 (d, $J = 3.0$ Hz). HRMS (m/z) $[\text{M}+\text{H}]^+$ calcd. for ($\text{C}_{108}\text{H}_{124}\text{F}_4\text{N}_8\text{O}_2\text{S}_4$): 1768.8666. Found: 1769.8688.

NA10: ^1H NMR (500 MHz, CDCl_3) δ 9.12 (s, 2H), 8.74 (dd, $J = 6.7, 2.9$ Hz, 2H), 8.51 (dd, $J = 9.6, 6.6$ Hz, 2H), 7.79 (dd, $J = 6.8, 3.0$ Hz, 2H), 7.68 (t, $J = 7.4$ Hz, 2H), 4.84 (d, $J = 7.9$ Hz, 4H), 3.26 (t, $J = 7.6$ Hz, 4H), 2.27 (s, 2H), 1.95-1.86 (m, 4H), 1.31 – 1.01 (m, 76H), 0.88-0.82 (t, $J = 6.8$ Hz, 6H), 0.73 – 0.69 (m, 12H). ^{13}C NMR (125 MHz, CDCl_3) δ

185.91 (s), 167.78 (s), 153.87 (s), 146.78 (s), 139.39 (s), 137.81 (s), 135.96 (s), 134.74 (s), 134.32 (s), 133.20 (s), 132.47 (s), 130.89 (s), 130.34 (s), 128.82 (s), 124.78 (s), 124.38 (s), 123.49 (s), 119.03 (s), 114.08 (s), 68.17 (s), 39.72 (s), 38.75 (s), 34.99 (s), 34.38 (d, $J = 17.8$ Hz), 31.95 (s), 31.78 (s), 31.48 (d, $J = 8.8$ Hz), 30.74 (s), 30.26 (dd, $J = 21.9, 7.4$ Hz), 29.97 – 29.22 (m), 28.95 (s), 25.94 (s), 23.77 (s), 23.00 (s), 22.67 (dd, $J = 6.4, 3.7$ Hz), 14.10 (dd, $J = 5.1, 3.1$ Hz), 10.97 (s), 1.04 (s). HRMS (m/z) $[M+H]^+$ calcd. for (C₁₀₈H₁₂₂Cl₂F₄N₈O₂S₄): 1836.7887. Found: 1837.7825.

NA11: ¹H NMR (500 MHz, CDCl₃) δ 9.11 (s, 2H), 8.78 (dd, $J = 6.7, 3.2$ Hz, 2H), 8.49 (dd, $J = 9.7, 6.5$ Hz, 2H), 7.77 (dd, $J = 6.8, 3.0$ Hz, 2H), 7.67 (t, $J = 7.3$ Hz, 2H), 4.84 (d, $J = 7.9$ Hz, 4H), 3.25 (t, $J = 7.7$ Hz, 4H), 2.28 (s, 2H), 1.95 – 1.86 (m, 4H), 1.40 (d, $J = 6.9$ Hz, 4H), 1.32 – 0.98 (m, 76H), 0.88-0.80 (m, 6H), 0.76-0.68 (m, 12H). ¹³C NMR (125 MHz, CDCl₃) δ 185.84 (s), 157.64 (s), 153.82 (s), 147.63 (s), 146.86 (s), 139.67 (s), 139.29 (s), 137.85 (s), 135.94 (s), 134.29 (s), 133.21 (s), 132.26 (s), 128.18 (s), 124.43 (d, $J = 11.9$ Hz), 123.99 (s), 119.22 – 118.57 (m), 114.72 (s), 114.07 (s), 67.87 (s), 53.43 (s), 39.82 (s), 34.89 (s), 34.54 (s), 33.84 (s), 31.91 (t, $J = 11.0$ Hz), 31.43 (t, $J = 11.4$ Hz), 30.35 (t, $J = 33.1$ Hz), 30.13 – 29.99 (m), 29.99 – 29.35 (m), 29.18 (s), 28.97 (s), 26.00 (s), 22.67 (d, $J = 5.3$ Hz), 14.11 (d, $J = 5.6$ Hz). HRMS (m/z) $[M+H]^+$ calcd. for (C₁₀₈H₁₂₂Br₂F₄N₈O₂S₄): 1924.6876. Found: 1925.6984.



Scheme S5. The chemical structure of PM6.

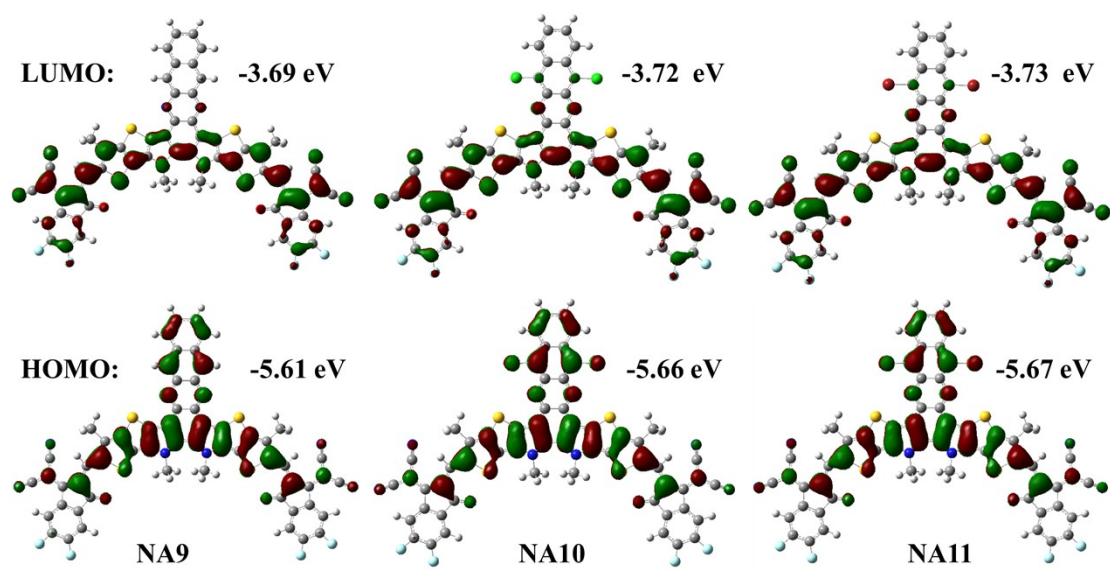


Figure S1. The calculated HOMO and LUMO for NA9, NA10 and NA11.

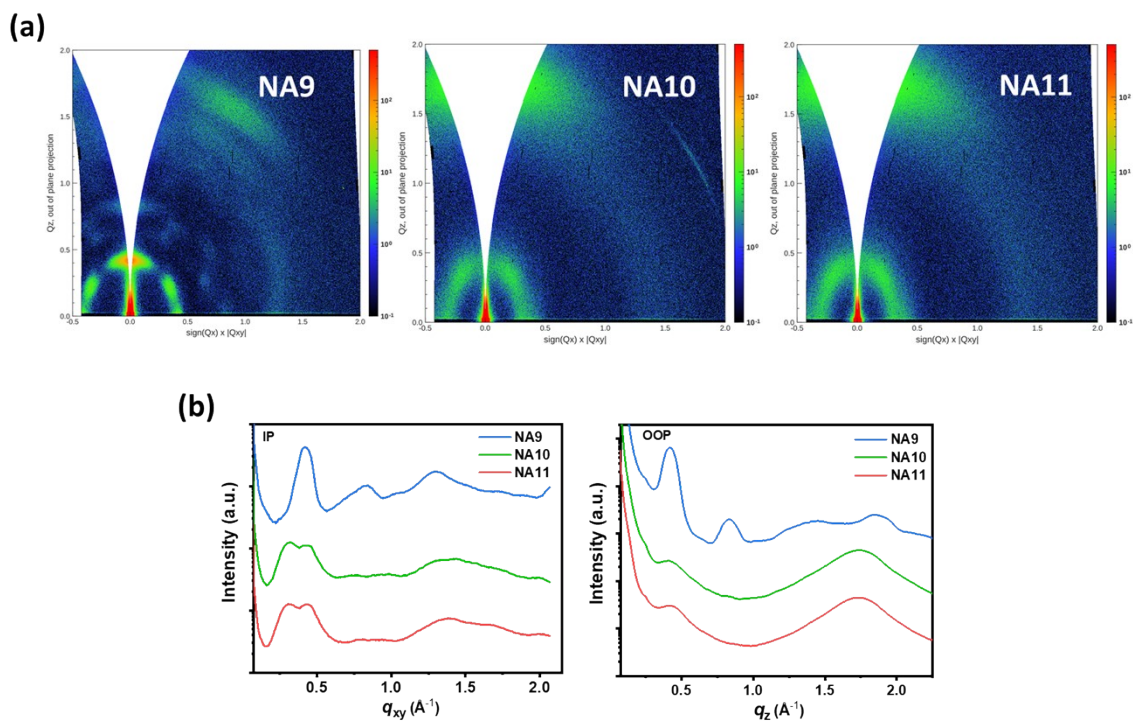


Figure S2. (a) 2D GIWAXS patterns and (b) the in-plane and out-of-plane line-cut profiles of NA9, NA10 and NA11 neat films.

Table S1. Device data of PM6/acceptors based devices. Values in parentheses are averages based on 10 independent devices.

Active layer	V_{oc} [V]	FF [%]	J_{sc} [mA cm^{-2}]	PCE [%]
PM6/NA10	0.912 (0.912±0.001)	61.84 (67.58±0.71)	20.68 (20.55) ^{a)} (20.66±0.11)	11.66 (11.56±0.08)
PM6/NA10	0.886 (0.884±0.002)	68.42 (67.58±0.71)	25.82 (25.09) ^{a)} (25.69±0.12)	15.65 (15.35±0.15)
PM6/NA11	0.897 (0.893±0.002)	70.57 (69.94±0.37)	26.29 (25.74) ^{a)} (26.27±0.07)	16.64 (16.41±0.11)

a) Integrated from EQE spectra.

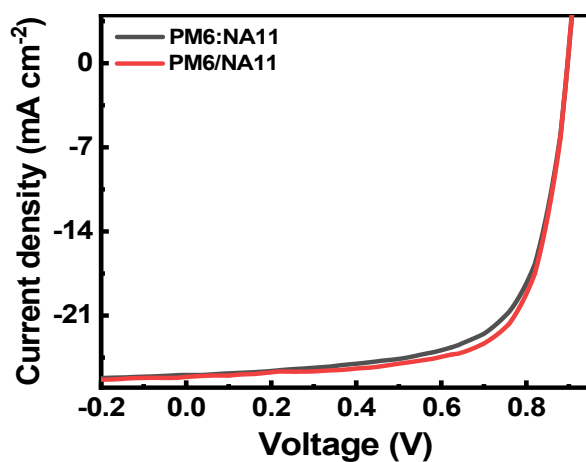


Figure S3. J - V curves of PM6:NA11 and PM6/NA11 devices.

Table S2. Photovoltaic performance of PM6:NA11 and PM6/NA11 devices.

Active layer	V_{oc} [V]	FF [%]	J_{sc} [mA/cm^{-2}]	PCE [%]
PM6:NA11	0.896 (0.894±0.002)	68.79 (68.44±0.35)	26.05 (26.01±0.06)	16.05 (15.91±0.13)
PM6/NA11	0.897 (0.893±0.002)	70.57 (69.94±0.37)	26.29 (26.27±0.07)	16.64 (16.41±0.11)

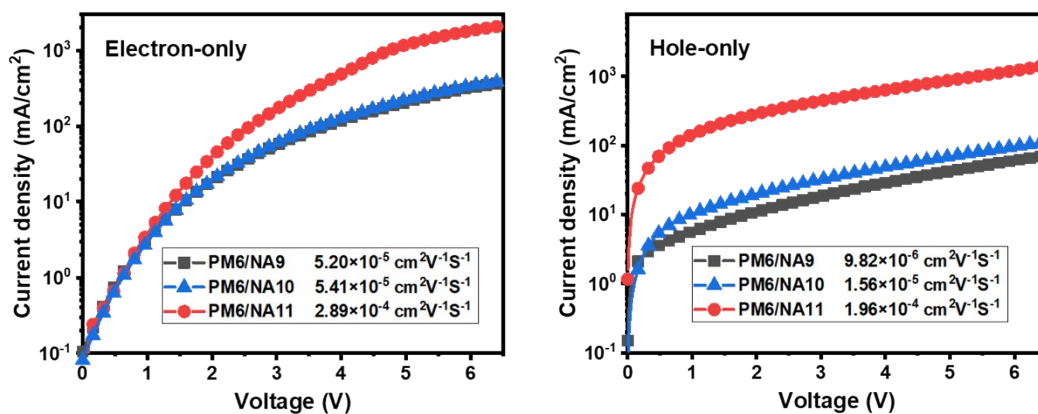


Figure S4. J - V characteristics in dark for electron-only and hole-only devices based on PM6/NA9, PM6/NA10, and PM6/NA10 blends.

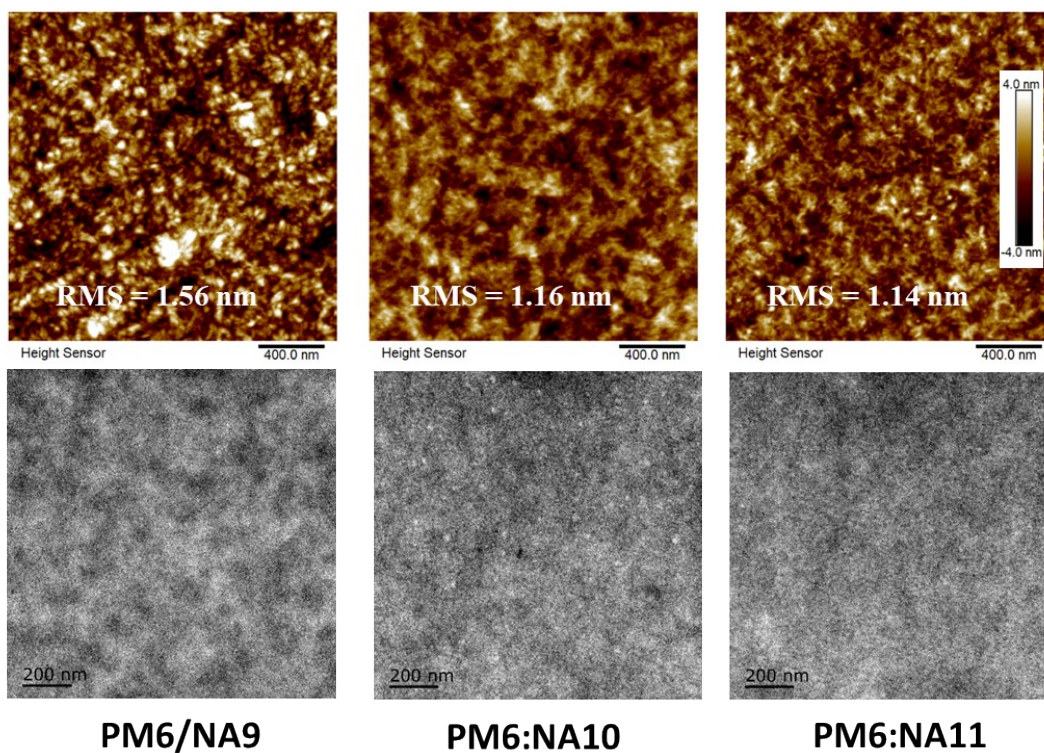


Figure S5. AFM images (upper) and TEM images (down) for PM6/NA9, PM6/NA10, and PM6/NA10 blends.

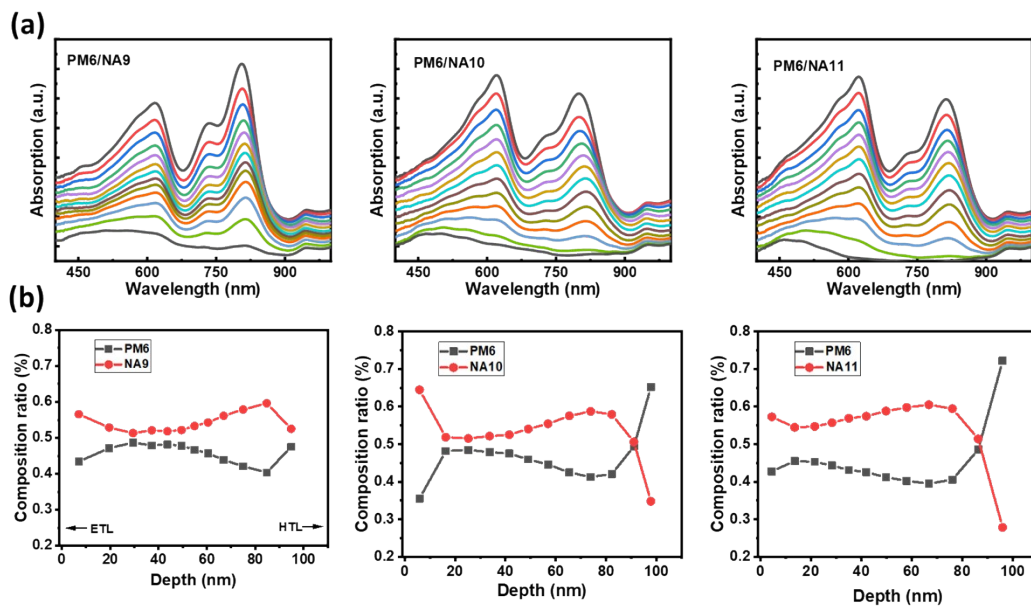


Figure S6. (a) Film-depth-dependent absorption spectra and (b) Calculated component distribution profiles of PM6/NA9, PM6/NA10, and PM6/NA10 blends.

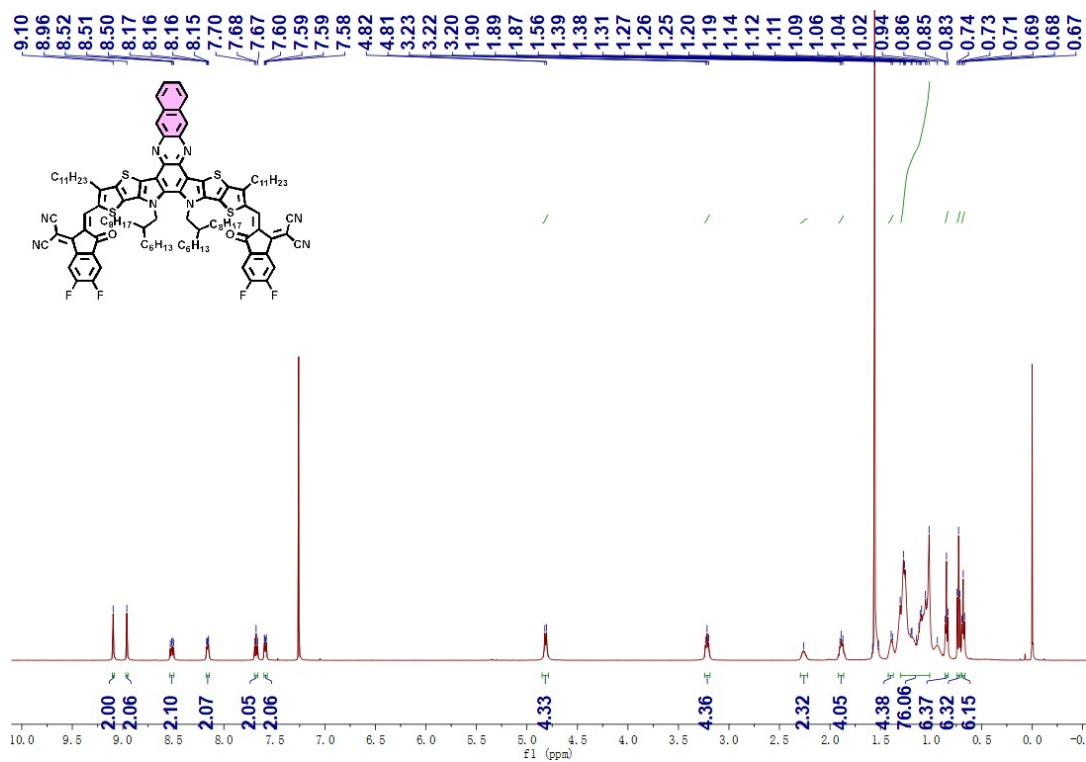


Figure S7. ¹H NMR spectrum of compound NA9 in CDCl₃.

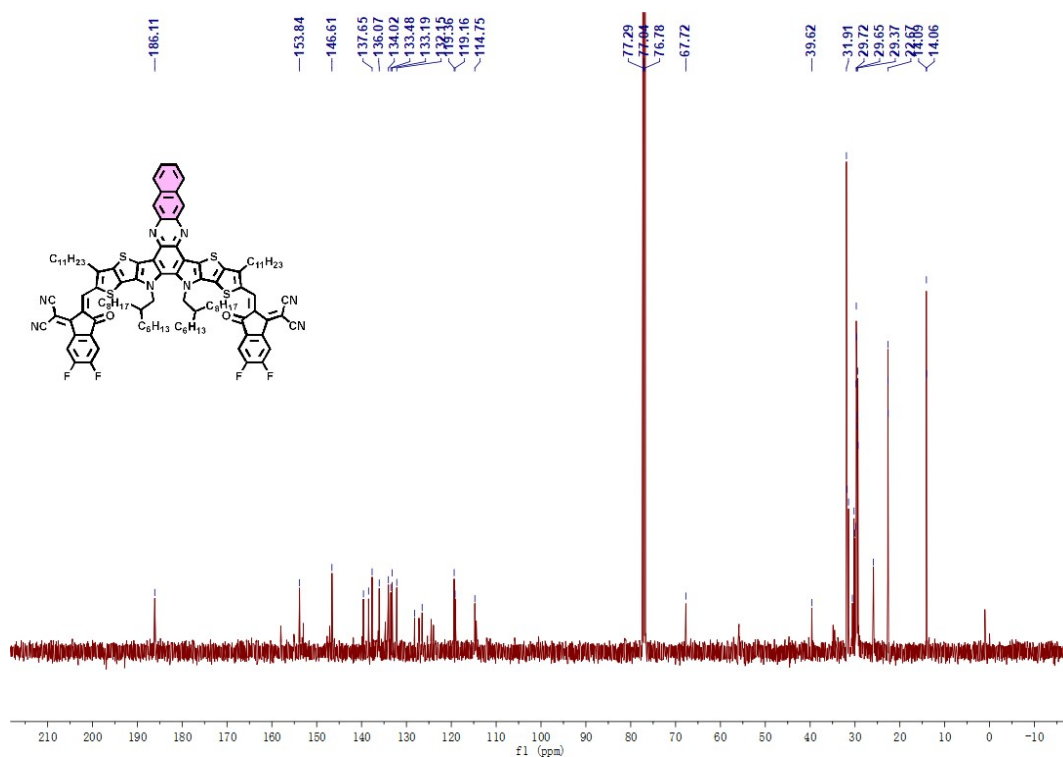


Figure S8. ¹³C NMR spectrum of compound NA9 in CDCl₃.

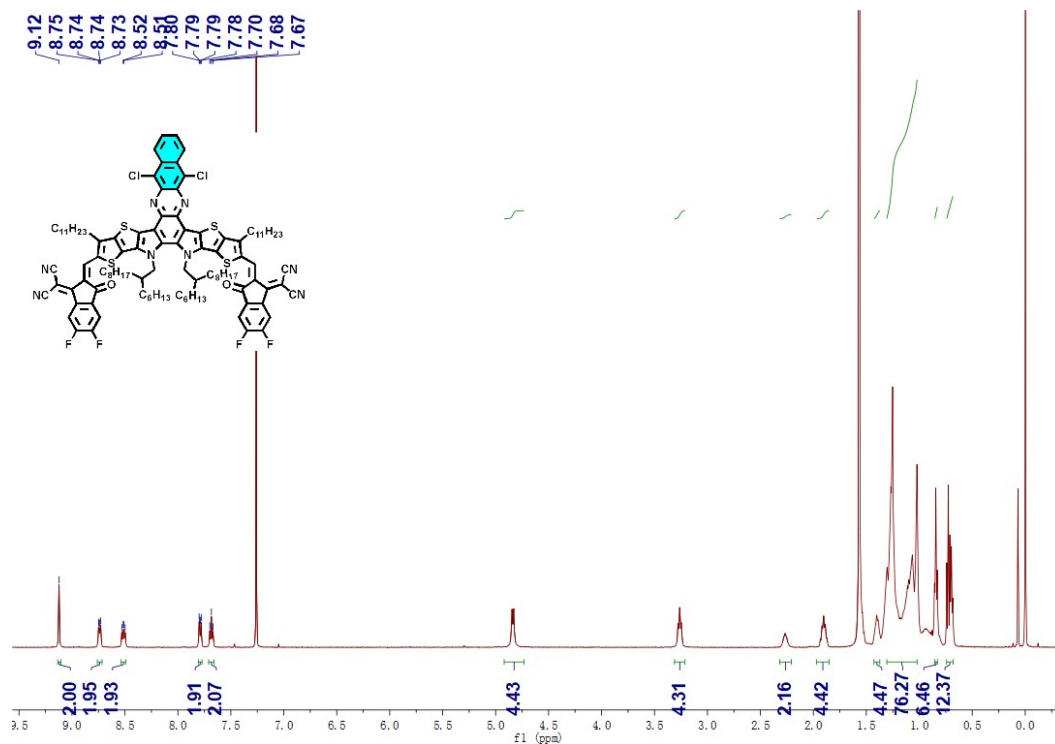


Figure S9. ¹H NMR spectrum of compound NA10 in CDCl₃.

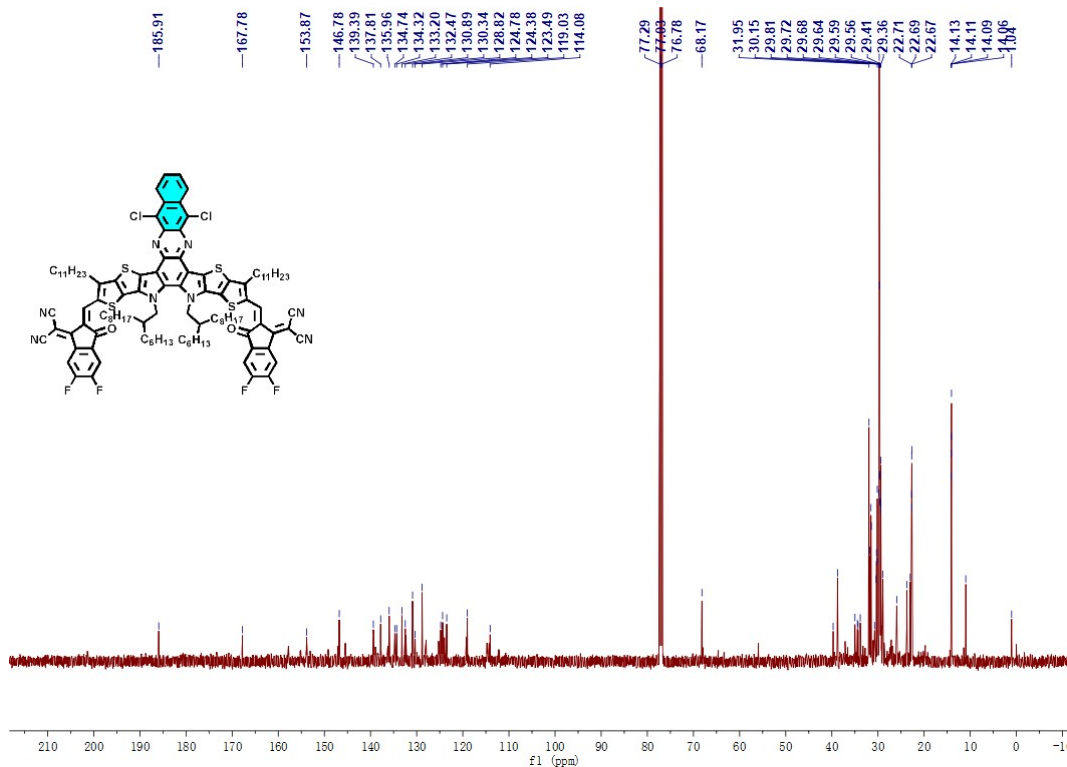


Figure S10. ^{13}C NMR spectrum of compound NA10 in CDCl_3 .

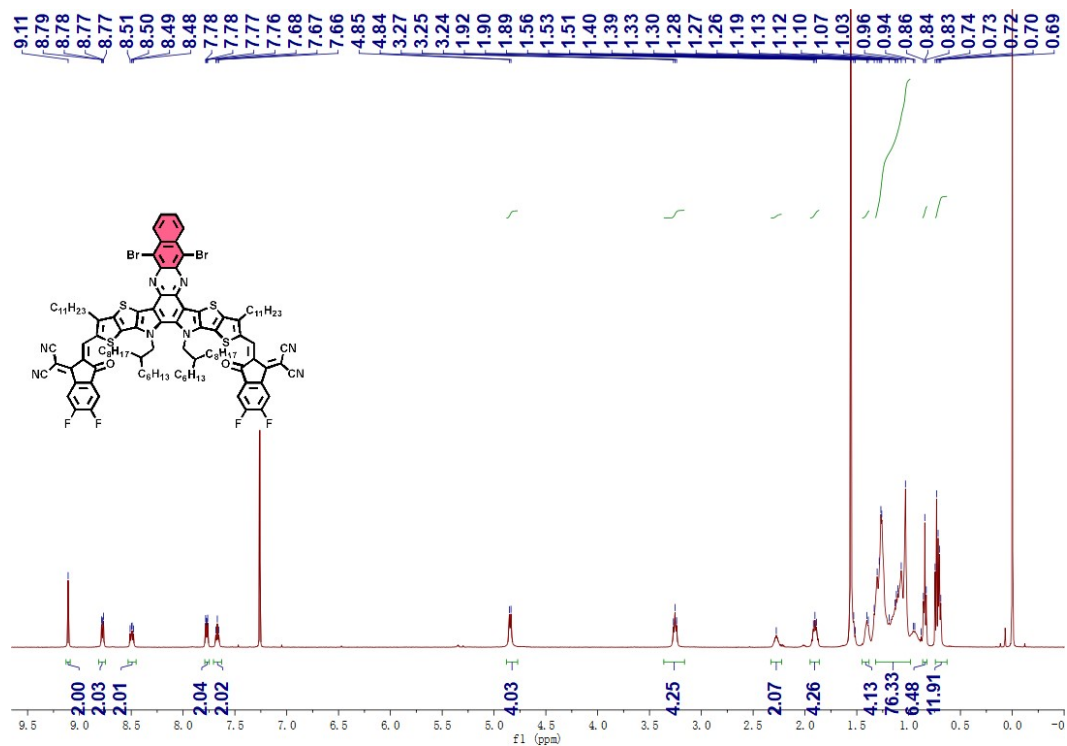


Figure S11. ^1H NMR spectrum of compound NA11 in CDCl_3 .

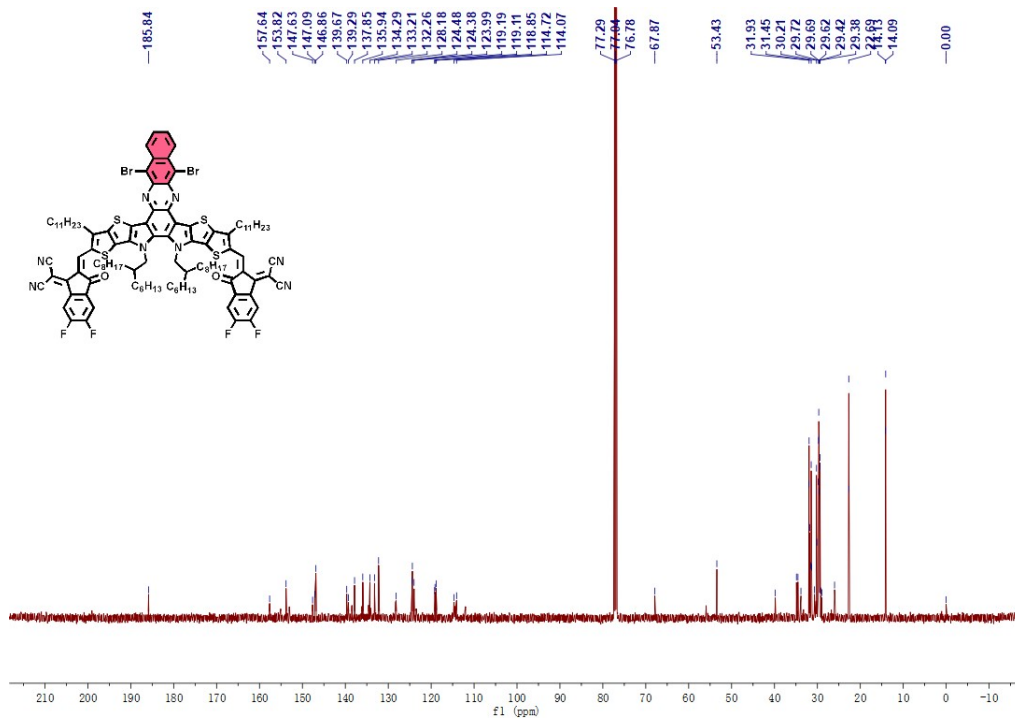


Figure S12. ^{13}C NMR spectrum of compound NA11 in CDCl_3 .

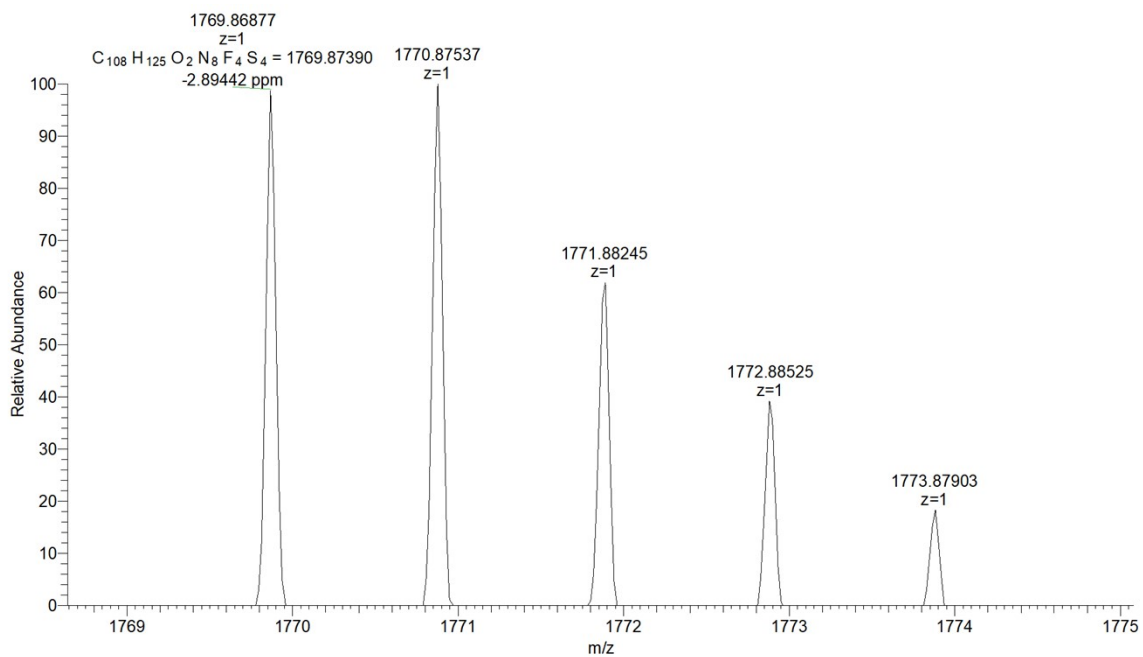


Figure S13. HRMS spectrum of NA9.

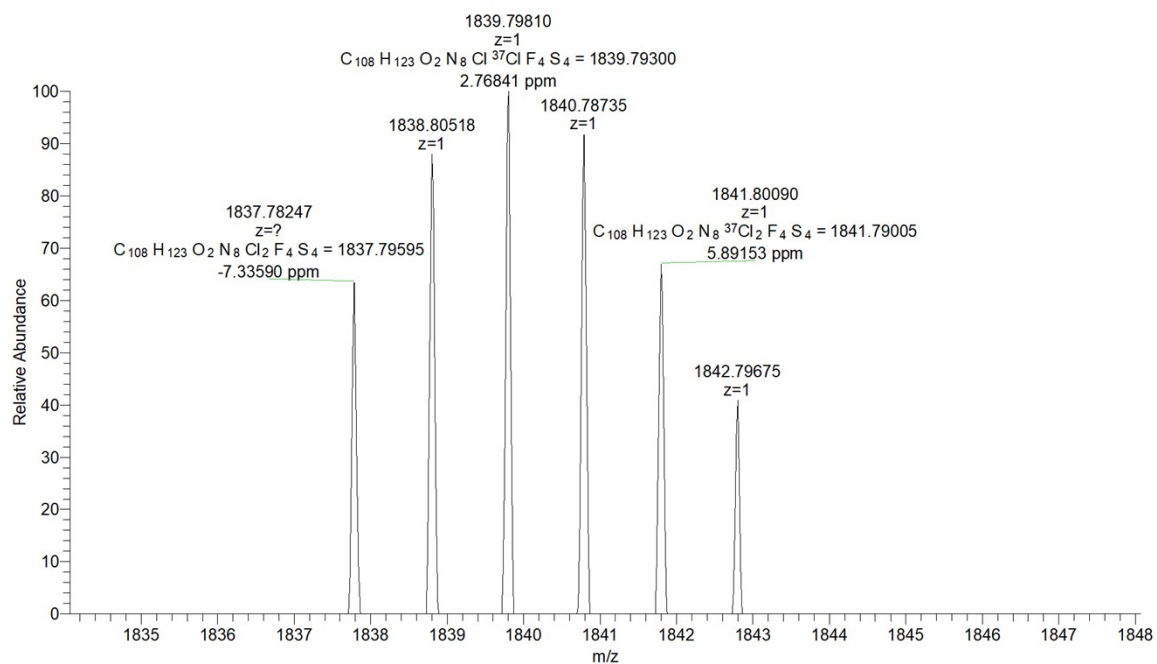


Figure S14. HRMS spectrum of NA10.

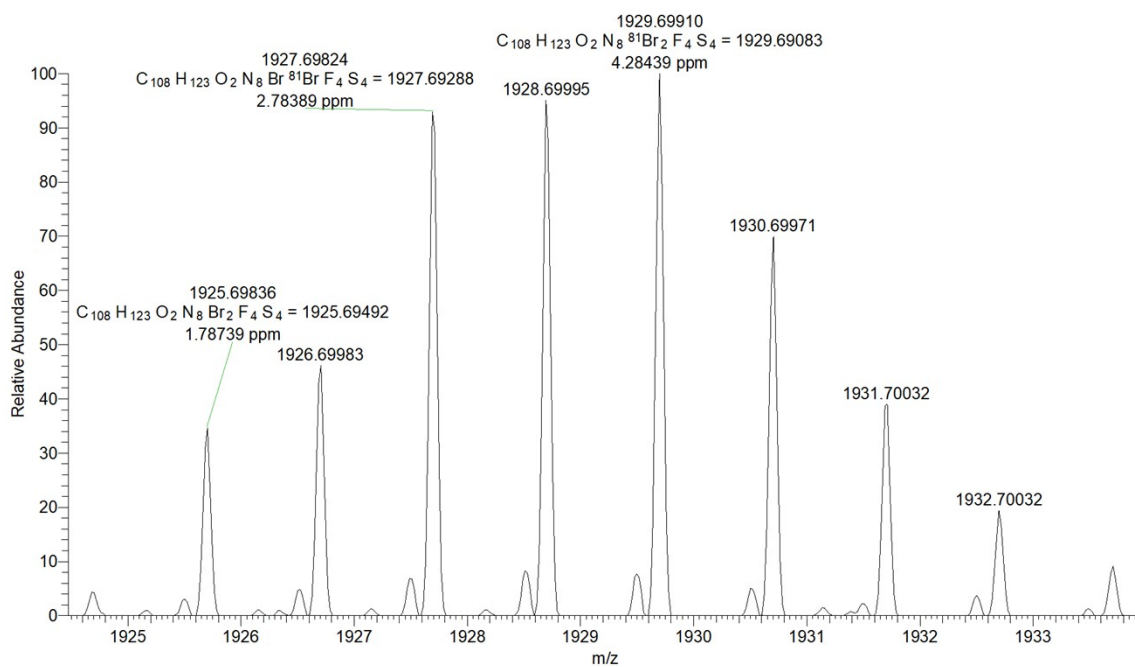


Figure S15. HRMS spectrum of NA11.