Electronic Supplementary Information (ESI) for:

Tuning Supramolecular Chirality and Optoelectronic Performance of Chiral Perylene Diimides Nanowires via *N*-Substituted Side Chain Engineering

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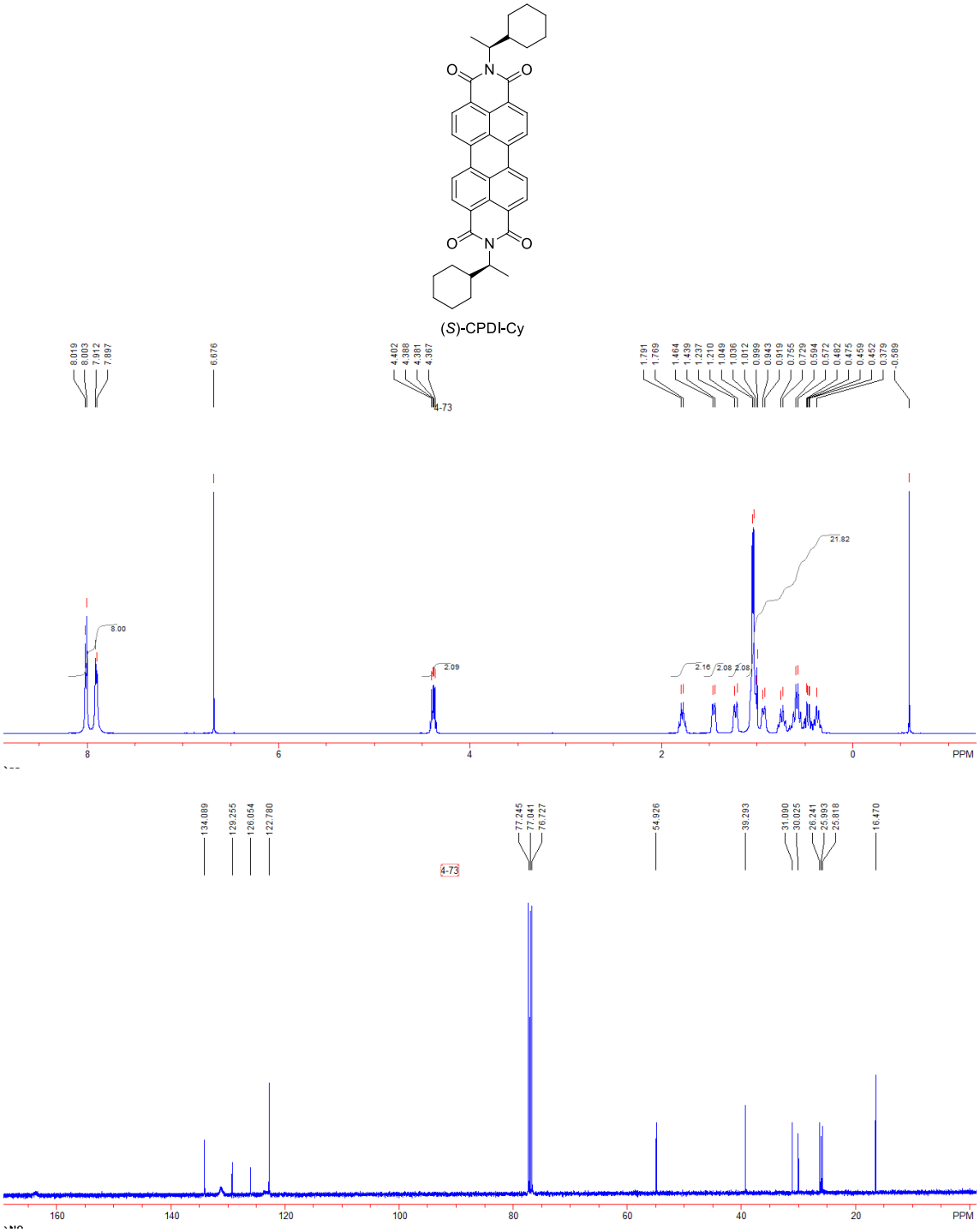
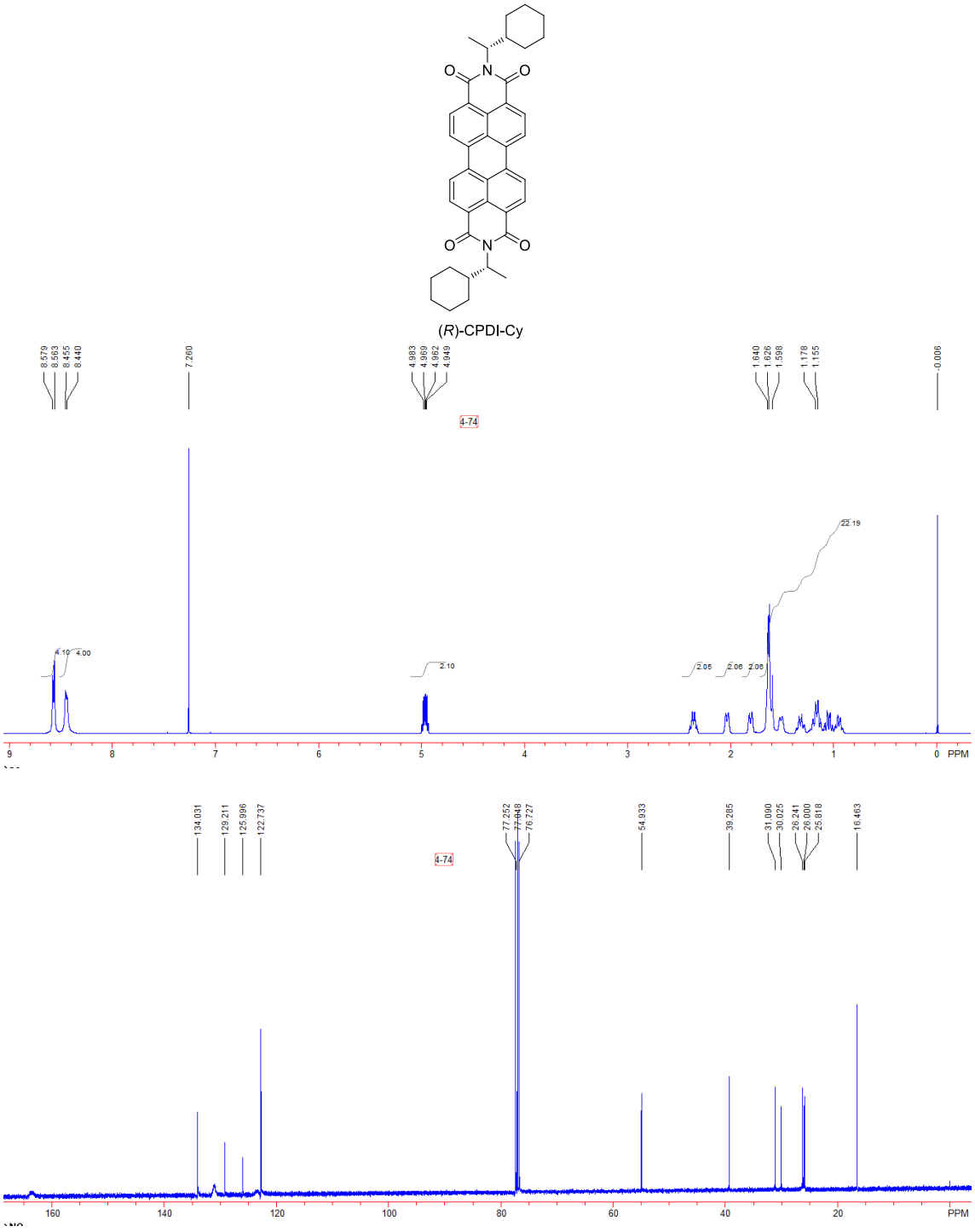
Supplementary Contents

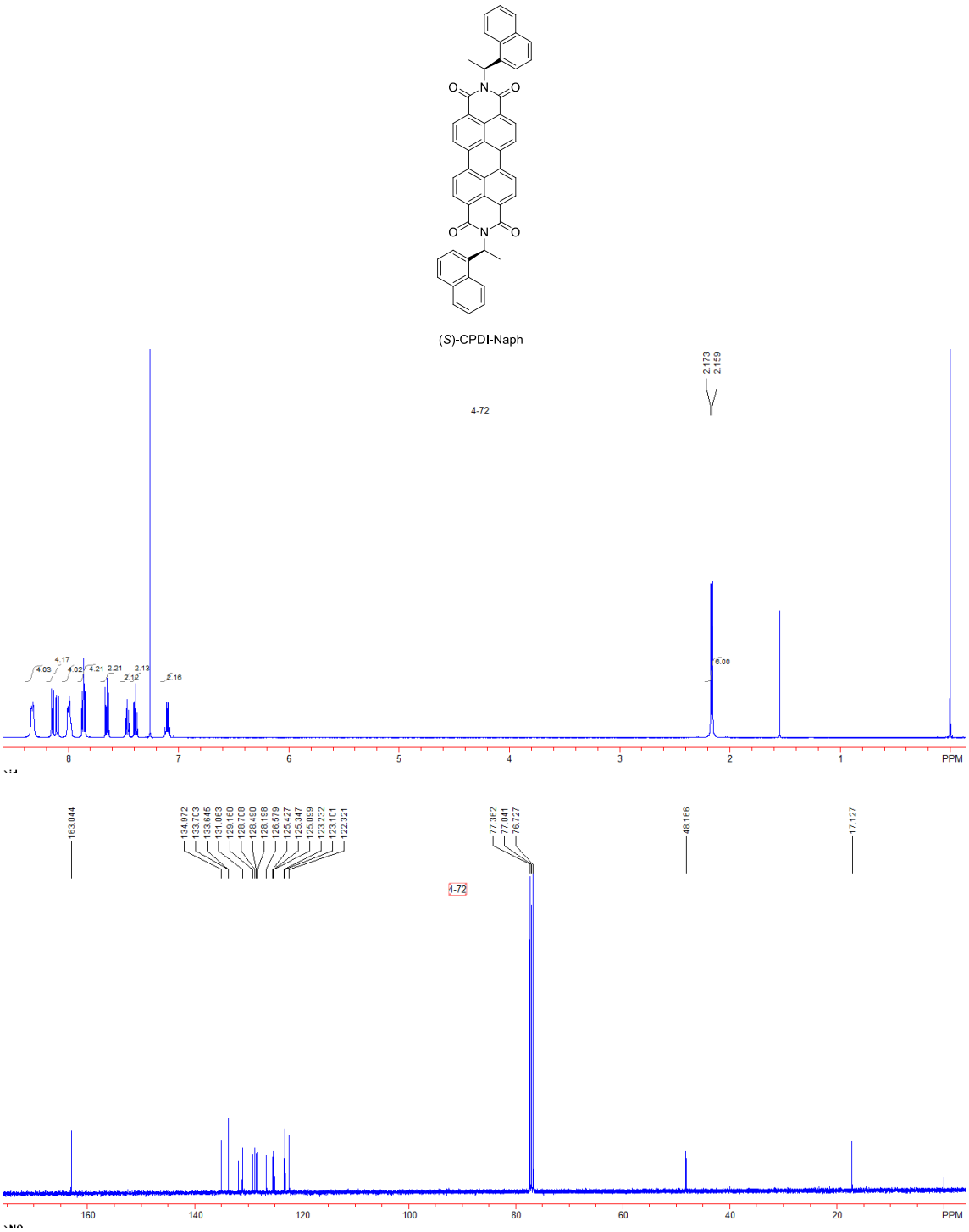
Characterization of Synthesized Molecules



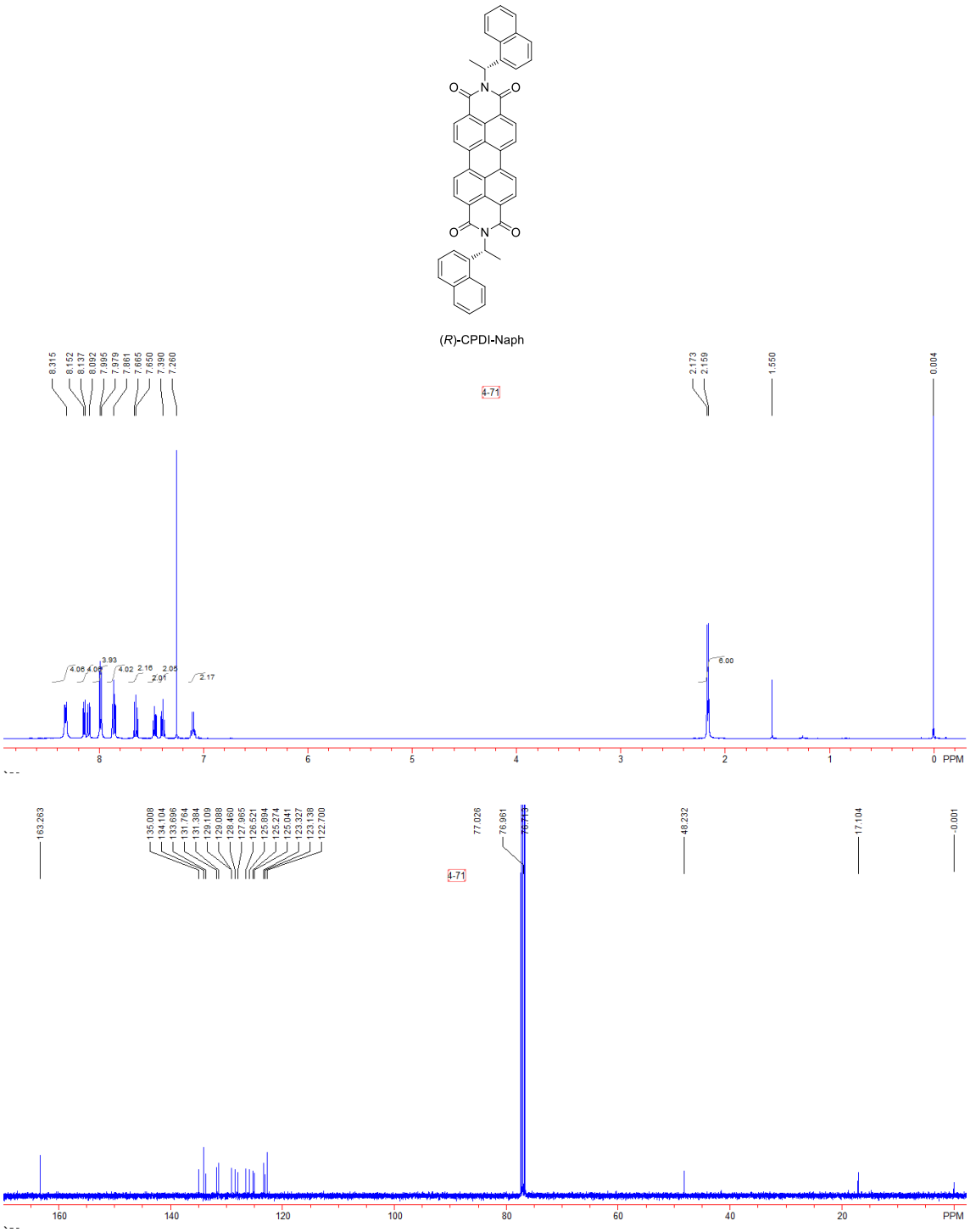
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (d, *J* = 6.4 Hz, 4 H), 7.90 (d, *J* = 6.0 Hz, 4 H), 4.34-4.43 (m, 2 H), 1.72-1.84 (m, 2 H), 1.17-1.50 (m, 4 H), 0.30-1.15 (m, 22 H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.4, 134.1, 131.3, 129.3, 126.1, 122.8, 54.9, 39.3, 31.1, 30.0, 26.2, 26.0, 25.8, 16.5 ppm. Anal. Calcd. For $C_{40}H_{38}N_2O_4$ (%): C, 78.66, H, 6.27, N, 4.59. Found (%): C, 78.55, H, 6.20, N, 4.46. HRMS (*m*/*z*): [M^+] calcd for 610.2832, found: 611.2909.



^{1}H NMR (400 MHz, $CDCl_3$): δ 8.57 (d, *J* = 6.4 Hz, 4 H), 8.45 (d, *J* = 6.0 Hz, 4 H), 4.93-5.01 (m, 2 H), 2.30-2.42 (m, 2 H), 1.75-2.08 (m, 4 H), 0.90-1.72 (m, 22 H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.0, 134.0, 131.0, 129.2, 126.0, 122.7, 54.9, 39.3, 31.1, 30.0, 26.2, 26.0, 25.8, 16.5 ppm. Anal. Calcd. For $C_{40}H_{38}N_2O_4$ (%): C, 78.66, H, 6.27, N, 4.59. Found (%): C, 78.53, H, 6.18, N, 4.48. HRMS (*m*/*z*): [M^+] calcd for 610.2832, found: 611.2910.



^{1}H NMR (400 MHz, $CDCl_3$): δ 8.33 (d, J = 6.0 Hz, 4 H), 8.12 (dd, J_1 = 16.8 Hz, J_2 = 6.4 Hz, 4 H), 8.00 (d, J = 6.4 Hz, 4 H), 7.83-7.89 (m, 4 H), 7.62-7.67 (m, 2 H), 7.36-7.50 (m, 4 H), 7.10 (q, J = 5.6 Hz, 2 H), 2.17 (d, J = 5.6 Hz, 6 H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.0, 135.0, 133.7, 133.6, 131.1, 129.2, 128.7, 128.5, 128.2, 126.6, 125.4, 125.3, 125.1, 123.2, 123.1, 122.3, 48.2, 17.1 ppm. Anal. Calcd. For $C_{48}H_{30}N_2O_4$ (%): C, 82.50, H, 4.33, N, 4.01. Found (%): C, 82.45, H, 4.43, N, 4.16. HRMS (m/z): [M^+] calcd for 698.2206, found: 699.2282.



^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (d, J = 6.4 Hz, 4 H), 8.16 (dd, J_1 = 17.2 Hz, J_2 = 6.4 Hz, 4 H), 8.02 (d, J = 6.8 Hz, 4 H), 7.87-7.93 (m, 4 H), 7.66-7.72 (m, 2 H), 7.39-7.53 (m, 4 H), 7.14 (q, J = 5.6 Hz, 2 H), 2.20 (d, J = 5.6 Hz, 6 H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.3, 135.0, 134.1, 133.7, 131.8, 131.4, 129.1, 129.1, 128.5, 128.0, 126.5, 125.9, 125.3, 125.0, 123.3, 123.1, 122.7 ppm. Anal. Calcd. For $C_{48}H_{30}N_2O_4$ (%): C, 82.50, H, 4.33, N, 4.01. Found (%): C, 82.39, H, 4.44, N, 4.20. HRMS (*m*/*z*): [M^+] calcd for 698.2206, found: 699.2281.

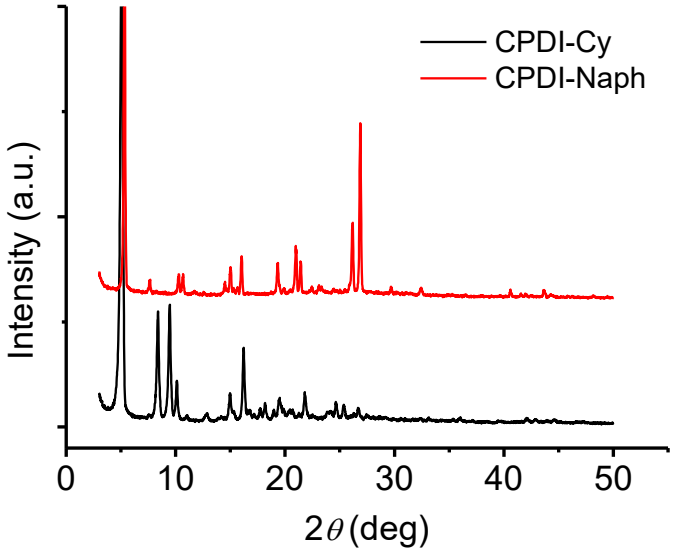


Fig. S1 PXRD results of (*S*)-CPDI-Cy and (*S*)-CPDI-Naph NWs.

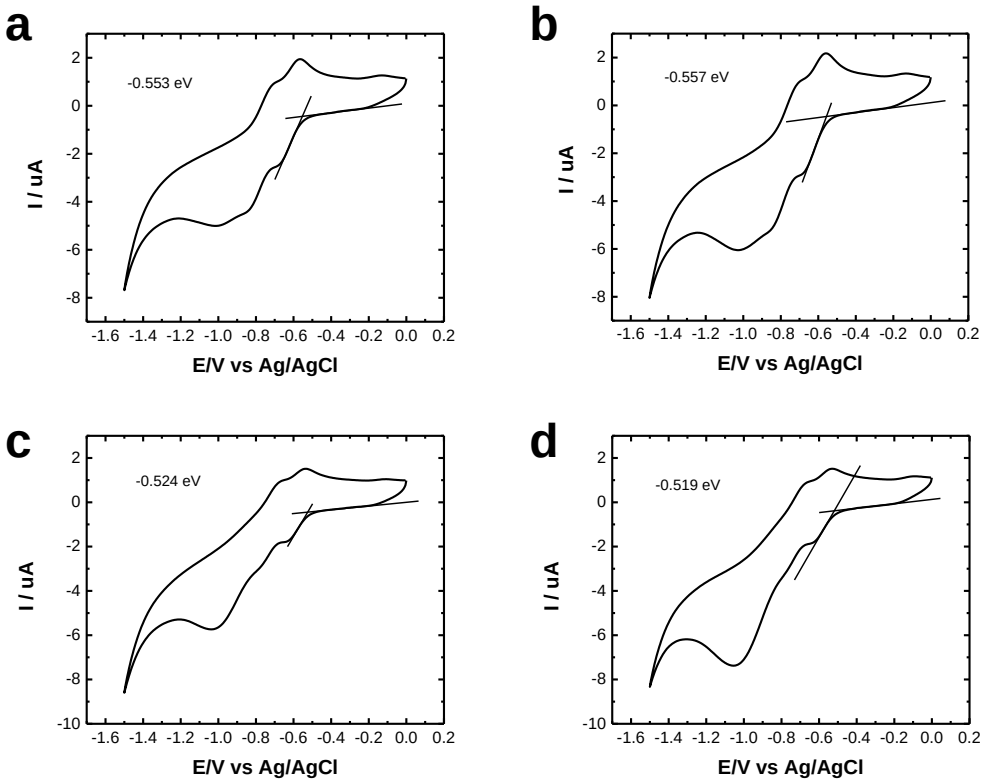


Fig. S2 Cyclic voltammetric results of (a) (*S*)-CPDI-Cy, (b) (*R*)-CPDI-Cy, (c) (*S*)-CPDI-Naph and (d) (*R*)-CPDI-Naph.

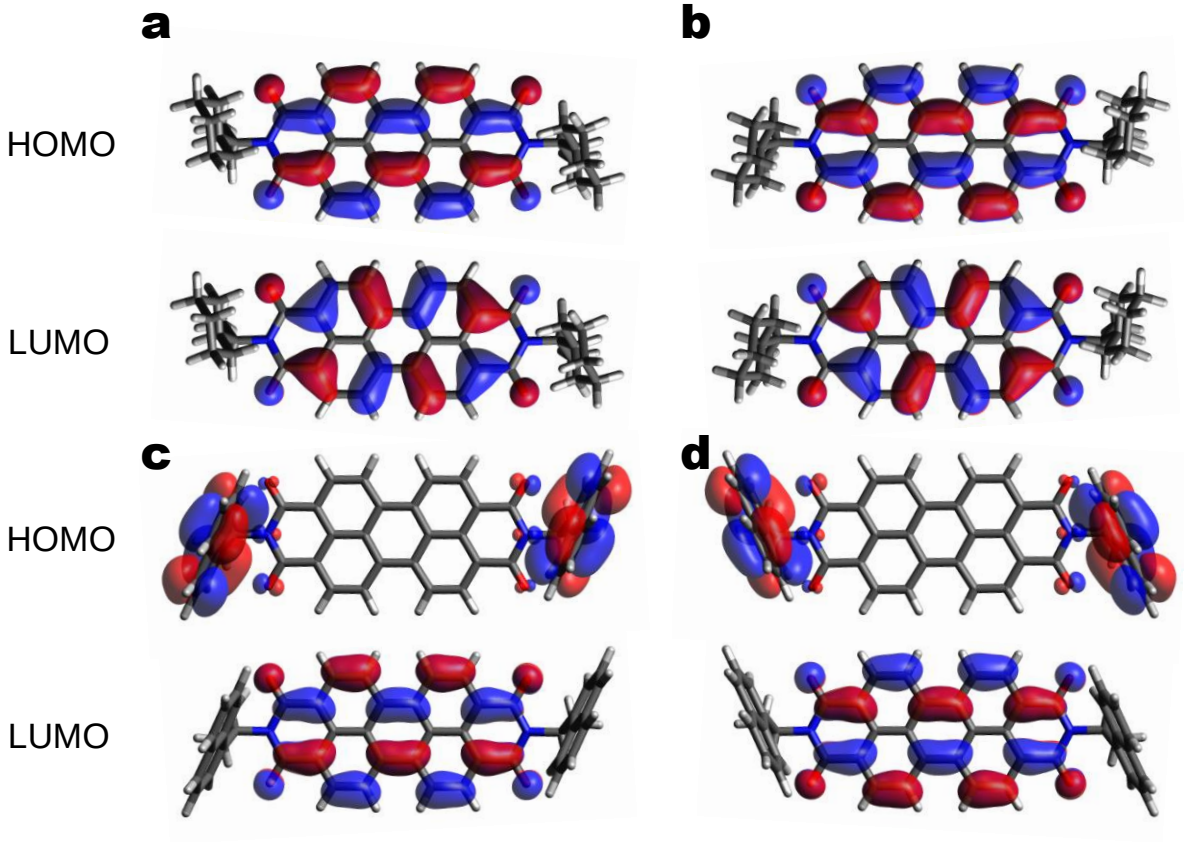


Fig. S3 HOMO and LUMO electron distributions of (a) (*S*)-CPDI-Cy, (b) (*R*)-CPDI-Cy, (c) (*S*)-CPDI-Naph, and (d) (*R*)-CPDI-Naph monomers obtained by DFT calculations. The carbon, hydrogen, oxygen, and nitrogen atoms are shown by gray, white, red, and blue sticks, respectively.

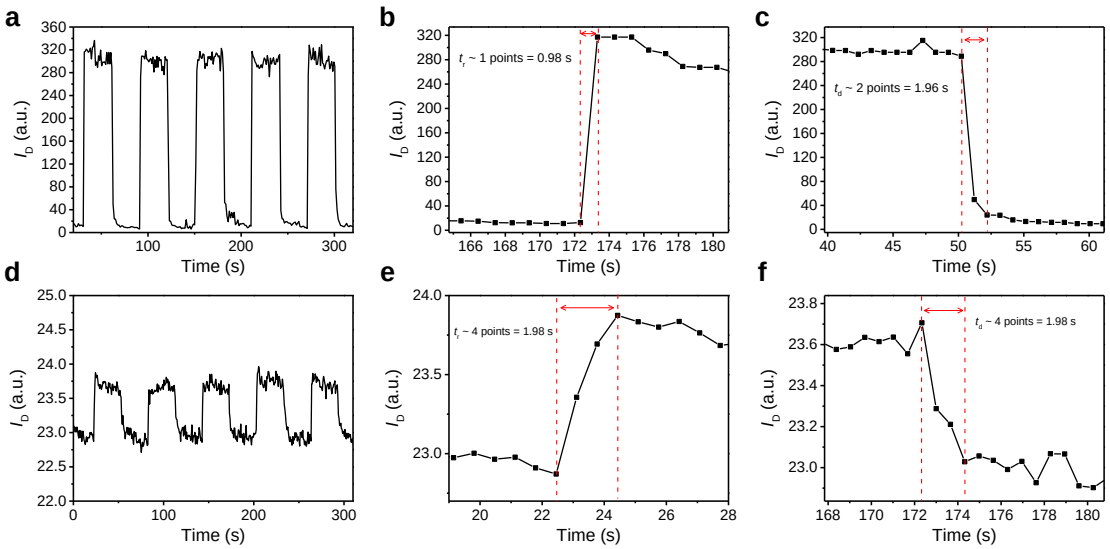


Fig. S4 (a) On/off photoswitching of (*S*)-CPDI-Cy NW-based OPTs (b-c) Rise time and decay time of (*S*)-CPDI-Cy NW-based OPTs. (d) On/off photoswitching of (*S*)-CPDI-Naph NW-based OPTs (e-f) Rise time and decay time of (*S*)-CPDI-Naph NW-based OPTs.

Table S1. Energy levels of enantiomeric CPDI-Cy, CPDI-Naph from CV measurement and DFT calculation.

Material	Chirality	Orbital	Energy level (eV)	
			CV	DFT
CPDI-Cy	(*S*)	LUMO	−3.82	−3.42
		HOMO	−6.11	−5.95
	(*R*)	LUMO	−3.81	−3.42
		HOMO	−6.10	−5.95
CPDI-Naph	(*S*)	LUMO	−3.85	−3.46
		HOMO	−6.13	−5.67
	(*R*)	LUMO	−3.85	−3.46
		HOMO	−6.13	−5.67

Table S2. Summary of field-effect mobilities (μ), on/off ratio (I_{on}/I_{off}), and threshold voltages (V_t) under dark condition.

Material	I_{on}/I_{off}	V_t (V)	μ ($cm^2V^{-1}s^{-1}$)
CPDI-Cy	$>10^3$	3.47 [a] (± 4.2)[b]	0.17 [a] (± 0.06)[b]
CPDI-Naph	$>10^1$	-22.1 [a] (± 6.1)[b]	0.00052 [a] (± 0.00016)[b]

[a]The average values obtained for at least nine devices from more than three different batches.
[b]The standard deviation values obtained for at least nine devices from more than three different batches.

Table S3. Summary of DFT results for the calculation of electron reorganization energy.

Material	E_0 (Ha)	E_- (Ha)	E_0^* (Ha)	E_-^* (Ha)	λ_0 (eV)	λ_- (eV)	λ (eV)
CPDI-Cy	−1957.718	−1957.805	−1957.713	−1957.799	0.145	0.148	0.293
CPDI-Naph	−2257.719	−2257.838	−2257.743	−2257.832	0.155	0.158	0.313

Table S4. Optoelectronic characteristics of CPDI-Cy and CPDI-Naph NWs-based OPTs.

Material	R^a (A W^{-1})	P^a	EQE^a (%)	D^{*a} (Jones)
CPDI-Cy	7.0	6.5×10^4	1.8×10^3	1.8×10^{13}
CPDI-Naph	0.0036	24.4	0.88	6.7×10^9

[a] Maximum values were obtained under monochromic light illumination (λ = 460 nm, 400 μW cm^{-2}).