Electronic Supplementary Information for

Development of benzo[*cd*]indolenyl cyanine dyes for NIR-absorbing films and elucidation of molecular structure–spectroscopic relationship

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Supporting Information includes:

S1. Supporting Figures and Tables

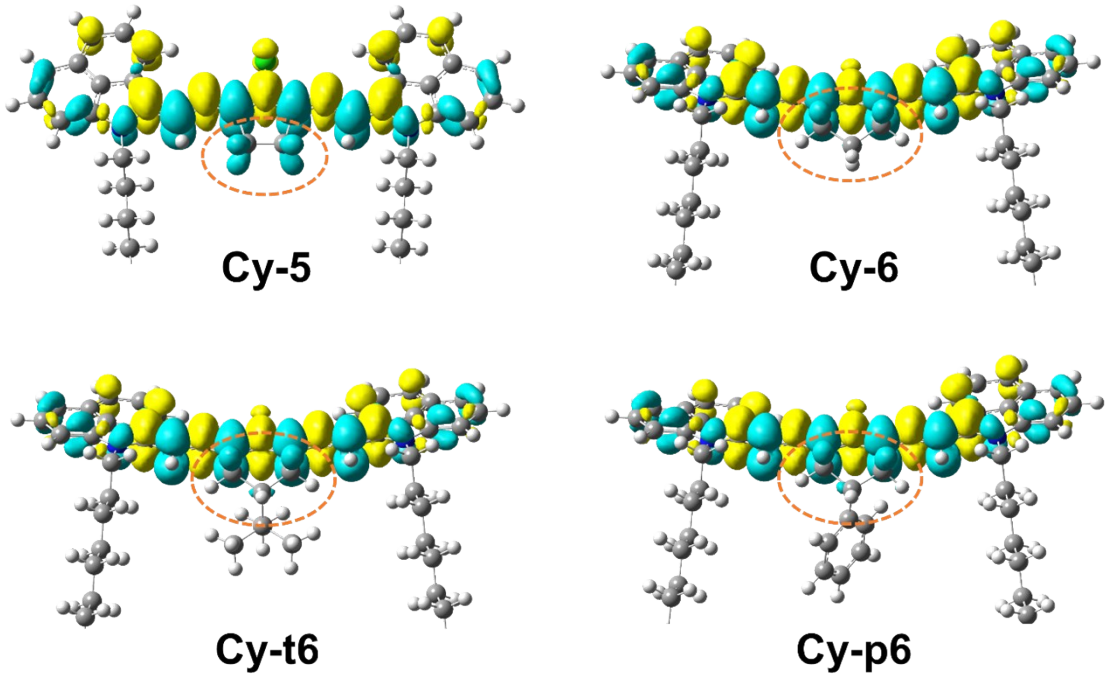
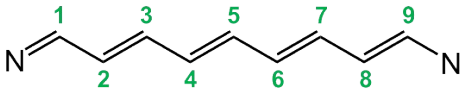


Fig. S1. Side view of charge density differences of cyanine dyes at the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO).

Table S1. Bond lengths and bond length alternation (BLA) along the polymethine chain of cyanine as calculated by DFT in the ground state.



	Bond length (Å)			
	Cy-5	Cy-6	Cy-t6	Cy-p6
L1	1.3962	1.3979	1.3979	1.3985
L2	1.3938	1.3928	1.3930	1.3924
L3	1.3911	1.4009	1.4011	1.4015
L4	1.4014	1.4097	1.4068	1.4079
L5	1.4014	1.4097	1.4068	1.4078
L6	1.3911	1.4009	1.4010	1.4006
L7	1.3938	1.3928	1.3930	1.3927
L8	1.3962	1.3979	1.3979	1.3981
L_{avg}	1.3956	1.4003	1.3997	1.3999
$L_{max-min}$	0.0103	0.0169	0.0138	0.0155
BLA	0.0044	0.0063	0.0053	0.0060

BLA was defined following the equation below,

$$BLA = \frac{|L1 - L2| + |L2 - L3| + |L3 - L4| + |L4 - L5| + |L5 - L6| + |L6 - L7| + |L7 - L8|}{7}$$

(1)

where L1 is the bond length between carbons 1 and 2.

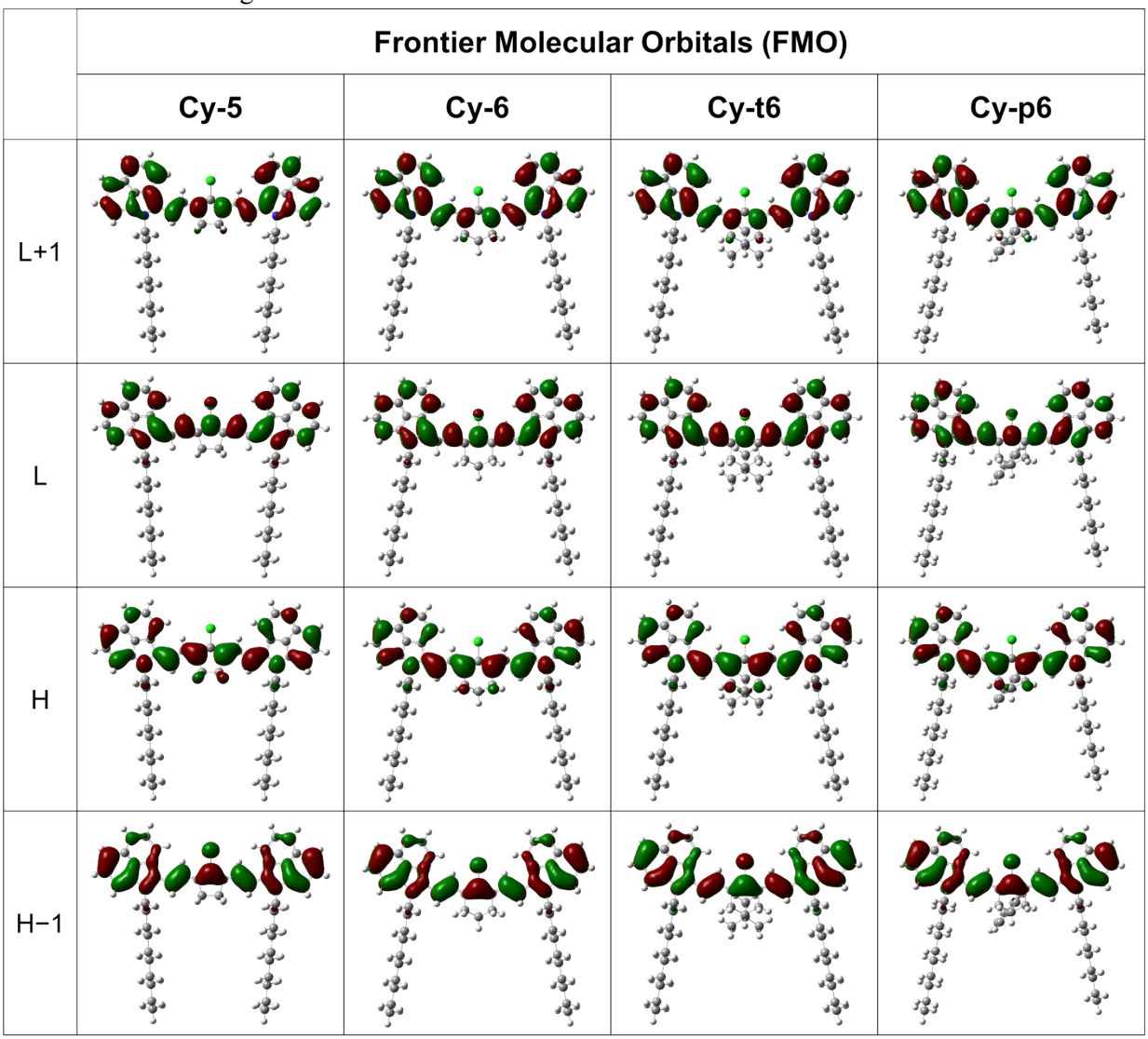


Fig. S2. Frontier molecular orbital plots of the synthesized cyanine dyes. H and L denote the HOMO and LUMO, respectively.

Table S2. Calculated values of orbital energies of the prepared cyanine dyes.

	Calculated (B3LYP/6-311G+(d,p))			
Dyes	HOMO−1 (eV)	HOMO (eV)	LUMO (eV)	LUMO+1 (eV)
Cy-5	−6.60	−5.43	−3.93	−2.78
Cy-6	−6.60	−5.48	−3.91	−2.83
Cy-t6	−6.59	−5.46	−3.90	−2.82
Cy-p6	−6.61	−5.49	−3.91	−2.85

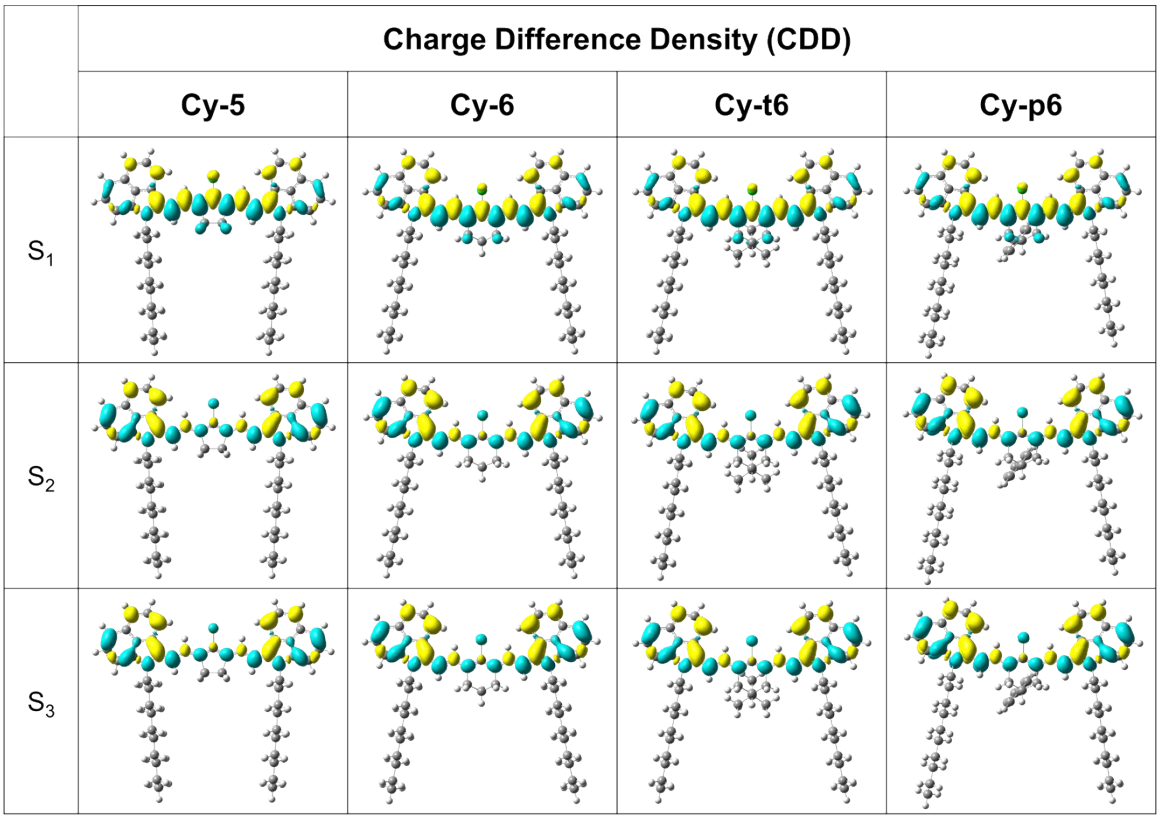


Fig. S3. Charge difference density of the synthesized cyanine dyes associated to the first three singlet excited states from the ground state.

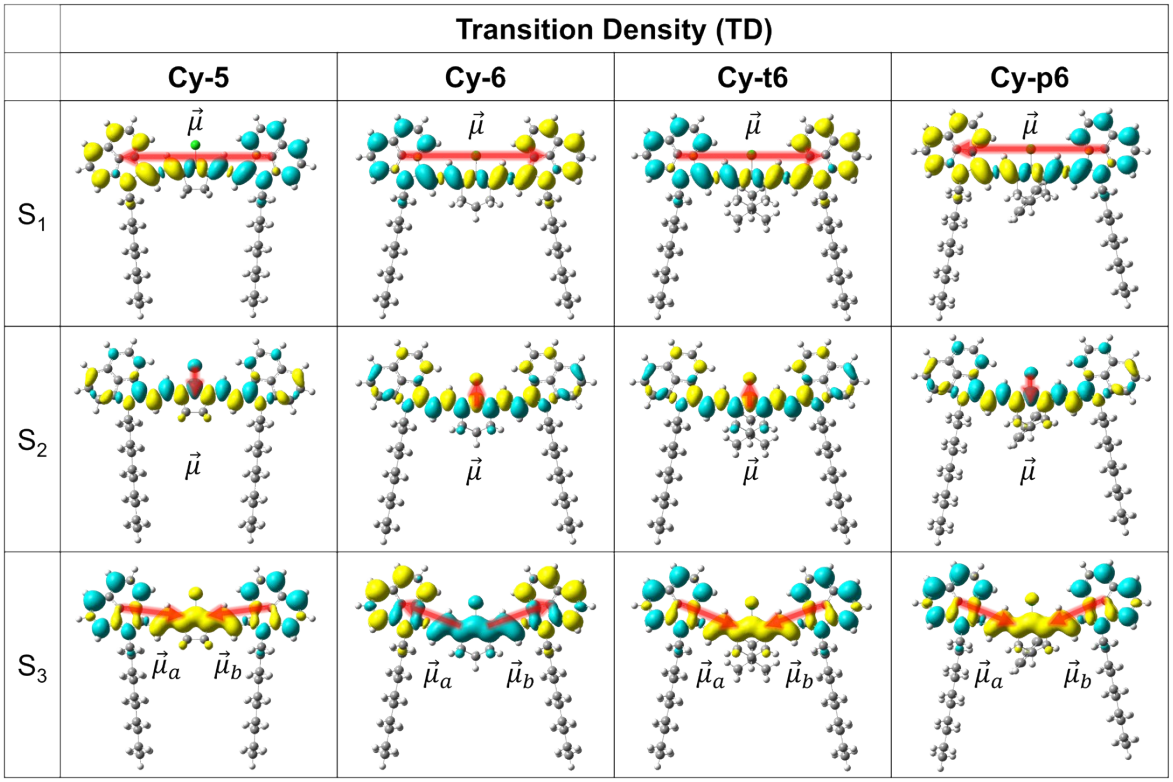


Fig. S4. Transition density for cyanine dyes from the ground state to the first three excited states (S_1, S_2, and S_3) during excitation. The yellow and cyan regions represent holes and electrons, respectively. The isosurface value of the plot is 0.0005 a.u. The red arrows indicate the transition dipole moment of the corresponding excitation.

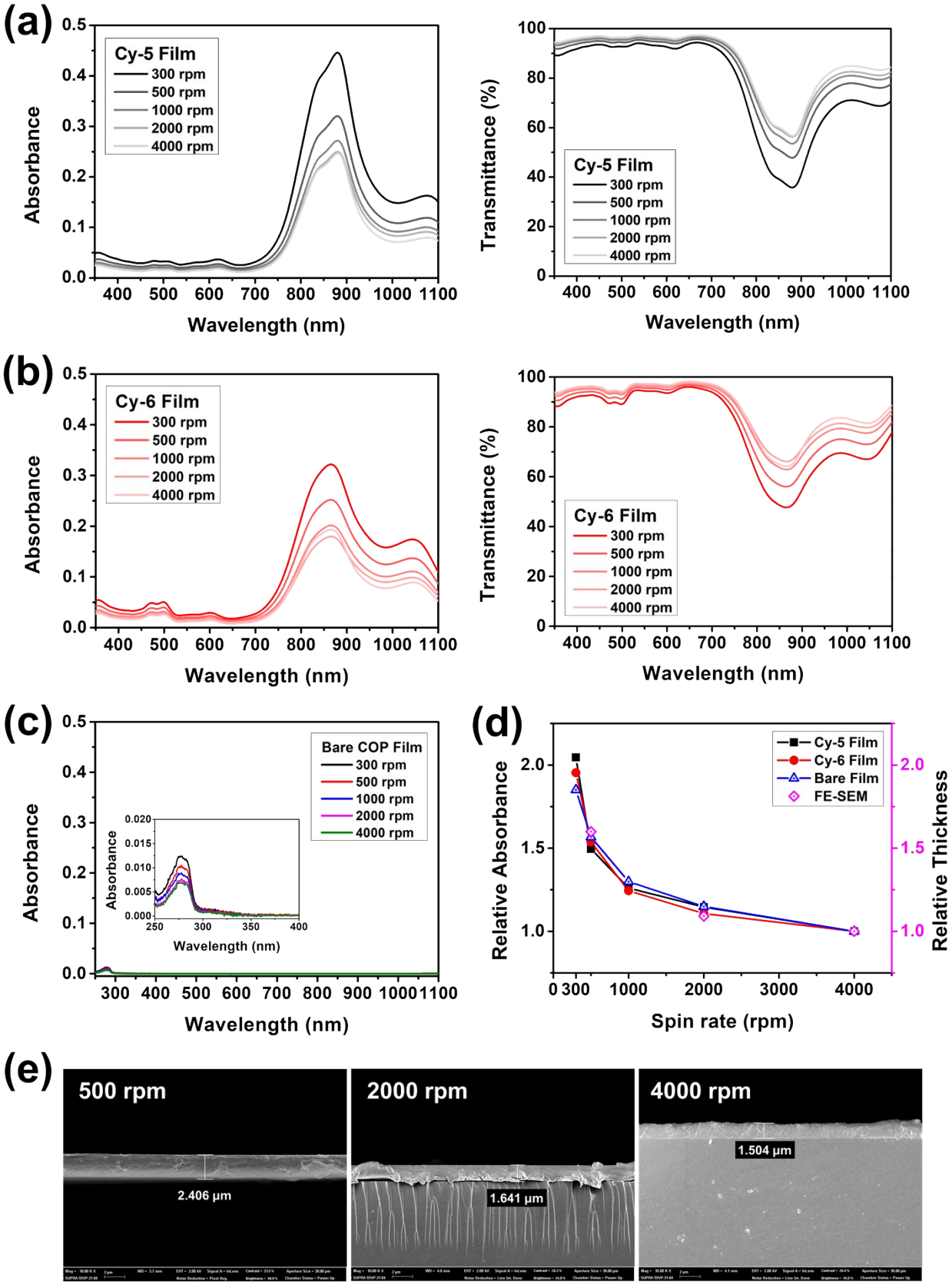


Fig. S5. Changes in absorbance and transmittance for films of (a) Cy-5 and (b) Cy-6 corresponding to variations in film thickness. (c) Absorbance spectra of bare COP films without dye addition. (d) Relative absorbance changes according to spinning rate, using the film fabricated at 4000 rpm as a reference. The film thickness determined by cross-sectional FE-SEM analysis was compared, showing good agreement. (e) Cross-sectional FE-SEM images of the COP films at different spin rates, acquired at 10,000× magnification.

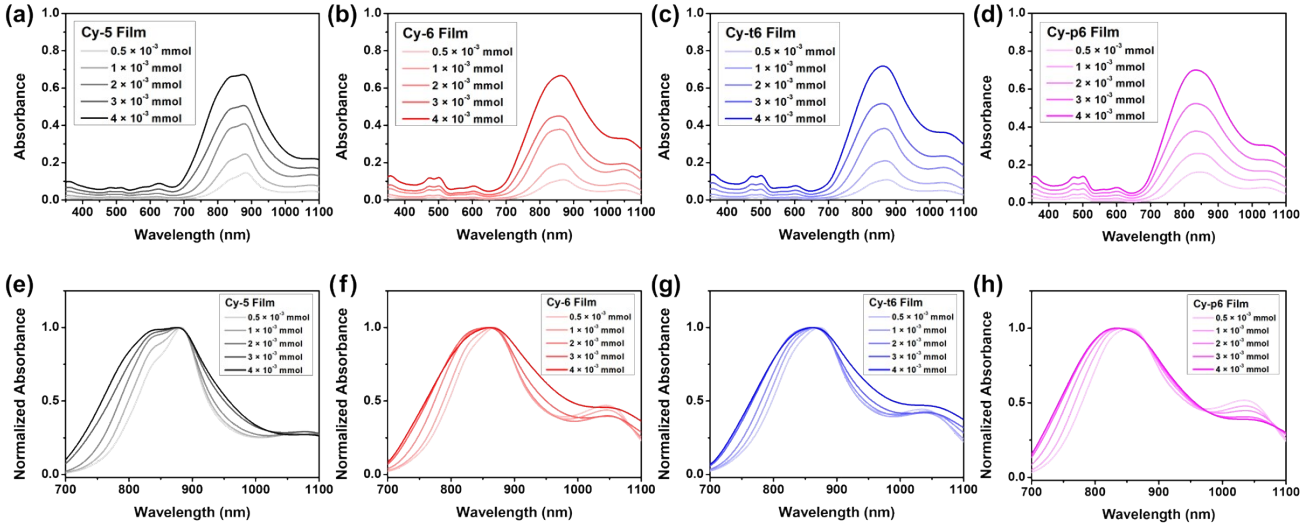


Fig. S6. Alterations in the absorption spectra of COP films fabricated at various dye concentrations. (a) Cy-5, (b) Cy-6, (c) Cy-t6, (d) Cy-p6. Normalized absorbance graphs in the NIR region of the films are shown at the lower part of the figure (10e–10h). Coating solutions were prepared by mixing the corresponding amount of cyanine dyes with 1.6 g of a 5 wt% chloroform COP solution.

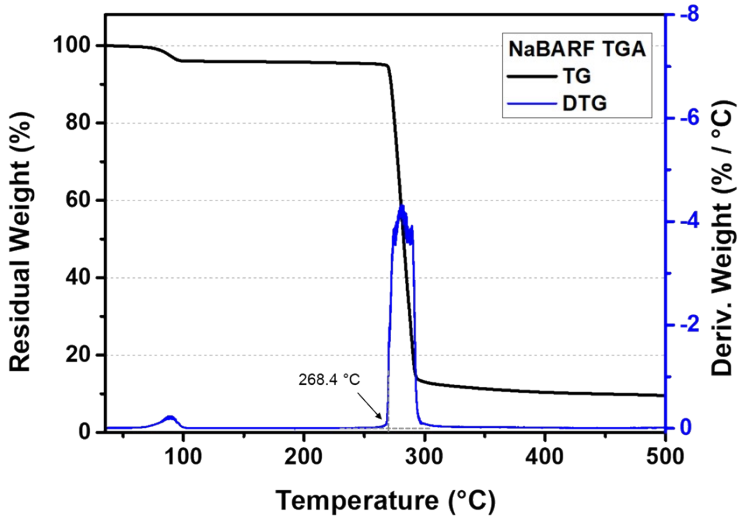


Fig. S7. TGA curve (black) and first derivative TG curve (blue) of NaBARF.

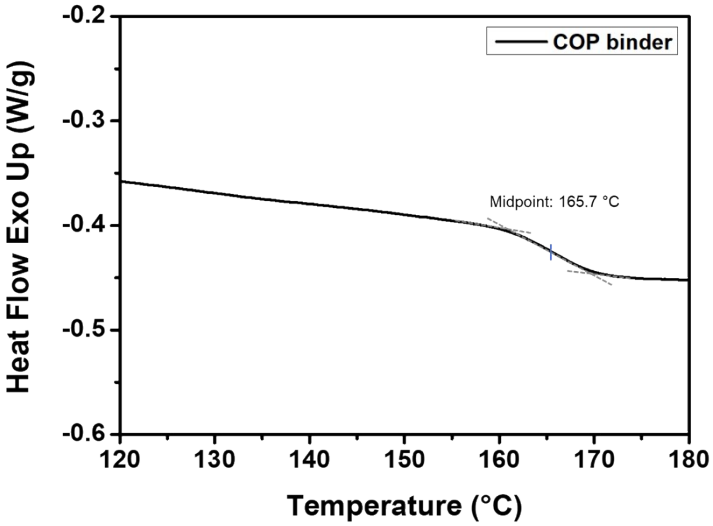
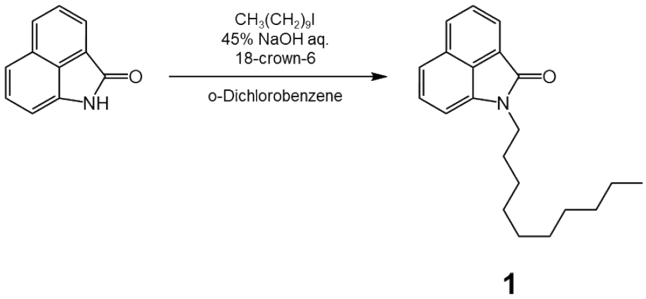


Fig. S8. Differential scanning calorimetry (DSC) curve of the selected cyclic olefin polymer (COP) binder.

S2. Supporting experimental section

S2.1. Synthesis of precursors of NIR cyanine dyes

S2.1.1 Synthesis of 1-decylbenzo[*cd*]indol-2(1*H*)-one (**1**)



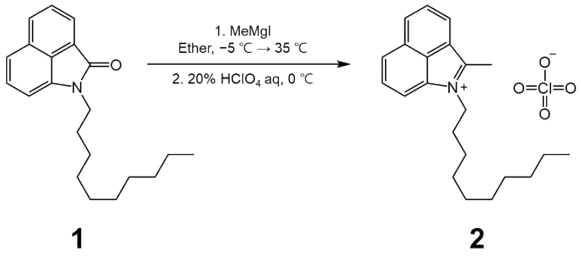
1

Scheme S1. Synthesis of 1-decylbenzo[*cd*]indol-2(1*H*)-one.

A solution of benzo[*cd*]indol-2(1*H*)-one (5 g, 29.55 mmol) and 1-iododecane 12.61 mL (15.85 g, 59.11 mmol) in 150 mL of *o*-dichlorobenzene was added to a 500 mL three-neck flask. Subsequently, 18-crown-6 (0.146 g, 0.552 mmol) and 45% sodium hydroxide solution (120 mL) were introduced into the reaction flask and heated at 120 ℃ for 2 hours under vigorous stirring. Over time, the color of the solution gradually changed from yellow to orange-brown. After the reaction, the mixture was cooled to room temperature and extracted with hexane (100 mL × 3). The organic extracts were dried over anhydrous magnesium sulfate, and the solvent was removed using a rotary evaporator. The resulting crude product was purified through column chromatography on silica

gel with ethyl acetate/hexane (1:7) as the eluent to afford 8.60 g of compound **1** as a bright yellow oil (Yield: 94%). LC/TOF-MS (ESI+) found: *m/z* 310.2968. Calcd for $C_{21}H_{28}NO$: [M+H], 310.2171.

S2.1.2. Synthesis of 1-decyl-2-methylbenzo[*cd*]indol-1-ium perchlorate (**2**)



Scheme S2. Synthesis of 1-decyl-2-methylbenzo[*cd*]indol-1-ium perchlorate.

1-Decylbenzo[*cd*]indol-2(1*H*)-one (**1**) (8 g, 25.85 mmol) was dissolved in anhydrous diethyl ether (70 mL) and cooled to −5 ℃ in an ice bath. Methyl magnesium iodide 16.67 mL (50 mmol, 3.0 M in diethyl ether) was placed in a 250 mL 1-neck flask, and the prepared solution of **1** was added dropwise using a syringe. After stirring for 15 min, the ice bath was removed, and the reaction flask was warmed to room temperature. Then, the reaction temperature was raised to 35 ℃ and stirred for 1 hour. The color gradually changed from dark yellow to dark green during this time. The flask was then returned to the ice bath and cooled to below 0 ℃, followed by a slow addition of 20% perchloric acid solution (70 mL). After further stirring for 30 minutes, the resulting precipitate was filtered and washed with diethyl ether to obtain 5.695 g of compound **2** as a pale yellow solid (Yield: 54%). LC/TOF-MS (ESI+) found: *m/z* 308.3174. Calcd for $C_{22}H_{30}N$: [M–ClO_4], 308.2378.

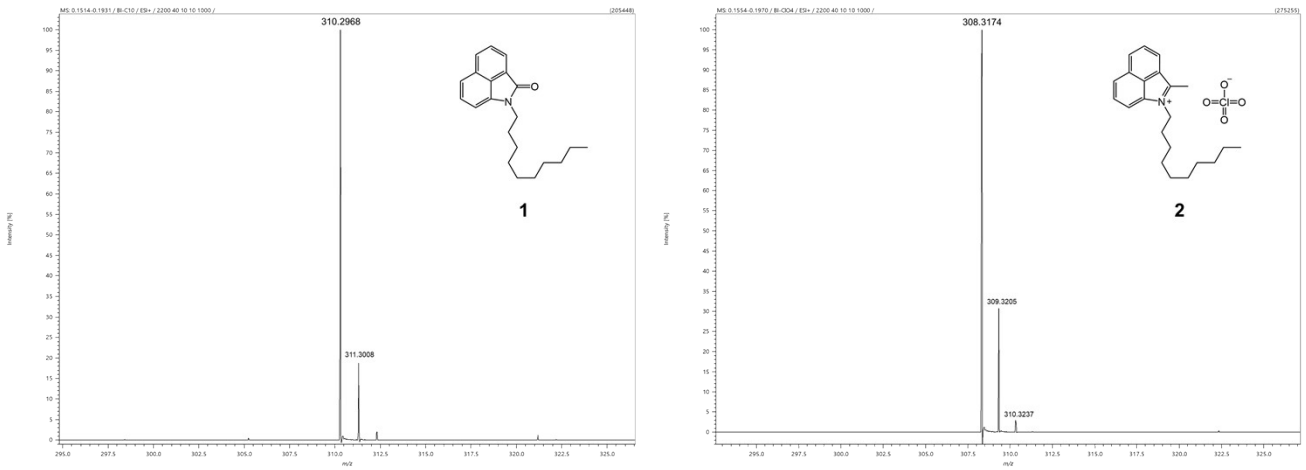
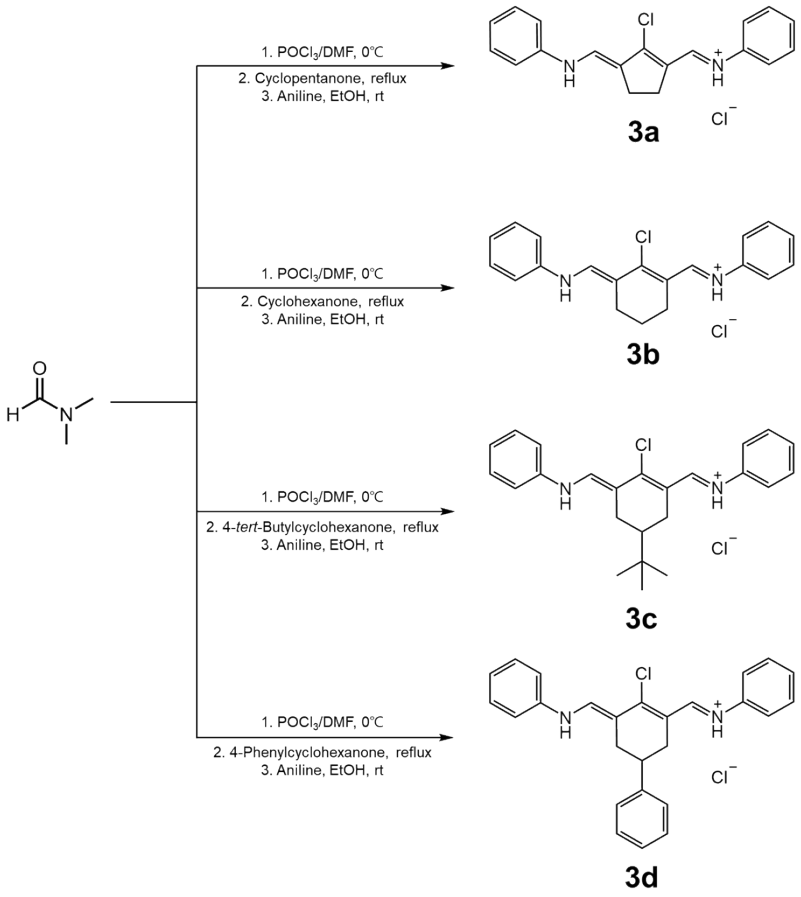


Fig. S9. LC/TOF-MS data of compounds **1** and **2**.

S2.1.3 Synthesis of anilinium salts

Anilinium salts **3a**–**3d** were synthesized following the general procedure described below. A 500 mL three-neck flask was equipped with a mechanical stirrer connected to a glass shaft with a PTFE blade. Anhydrous dimethylformamide 11.8 mL (152.6 mmol) was placed in the flask, and phosphoryl chloride 10 mL (106.9 mmol) was added dropwise while maintaining the reaction temperature below 5 ℃ using an ice bath. To the resulting opaque slurry, cycloketones or 4-substituted cyclohexenes (52.6 mmol) dissolved in 12 mL dichloromethane were added dropwise, respectively. The mixture was then heated to 100 ℃ and stirred for 2 hours. After cooling to room temperature, the flask was returned to the ice bath, and an aniline/ethanol mixture (16.4 ml, 1:1) was added dropwise.



Scheme S3. Synthesis of anilinium salts (**3a**–**3d**).

The resulting deep red solution was stirred at ambient temperature for 1 hour. Then, 100 mL of ice-cold 2M HCl solution was poured into the reaction flask and stirred overnight to give a dark wine-colored precipitate. The precipitate was filtered, washed with copious amounts of cold water, acetone, diethyl ether, and dichloromethane, and dried under a vacuum. The target products (**3a**–**3d**) were obtained as purple crystals and

used directly in the next reaction step without further purification. LC/TOF-MS (ESI+) of **3a** found: *m/z* 309.1929. Calcd for $C_{19}H_{18}ClN_2^+$: [M−Cl], 309.1153, **3b** found: *m/z* 323.1743. Calcd for $C_{20}H_{20}ClN_2^+$: [M−Cl], 323.1310, **3c** found: *m/z* 379.2897. Calcd for $C_{24}H_{28}ClN_2^+$: [M−Cl], 379.1936, **3d** found: *m/z* 399.2642. Calcd for $C_{26}H_{24}ClN_2^+$: [M−Cl], 399.1623.

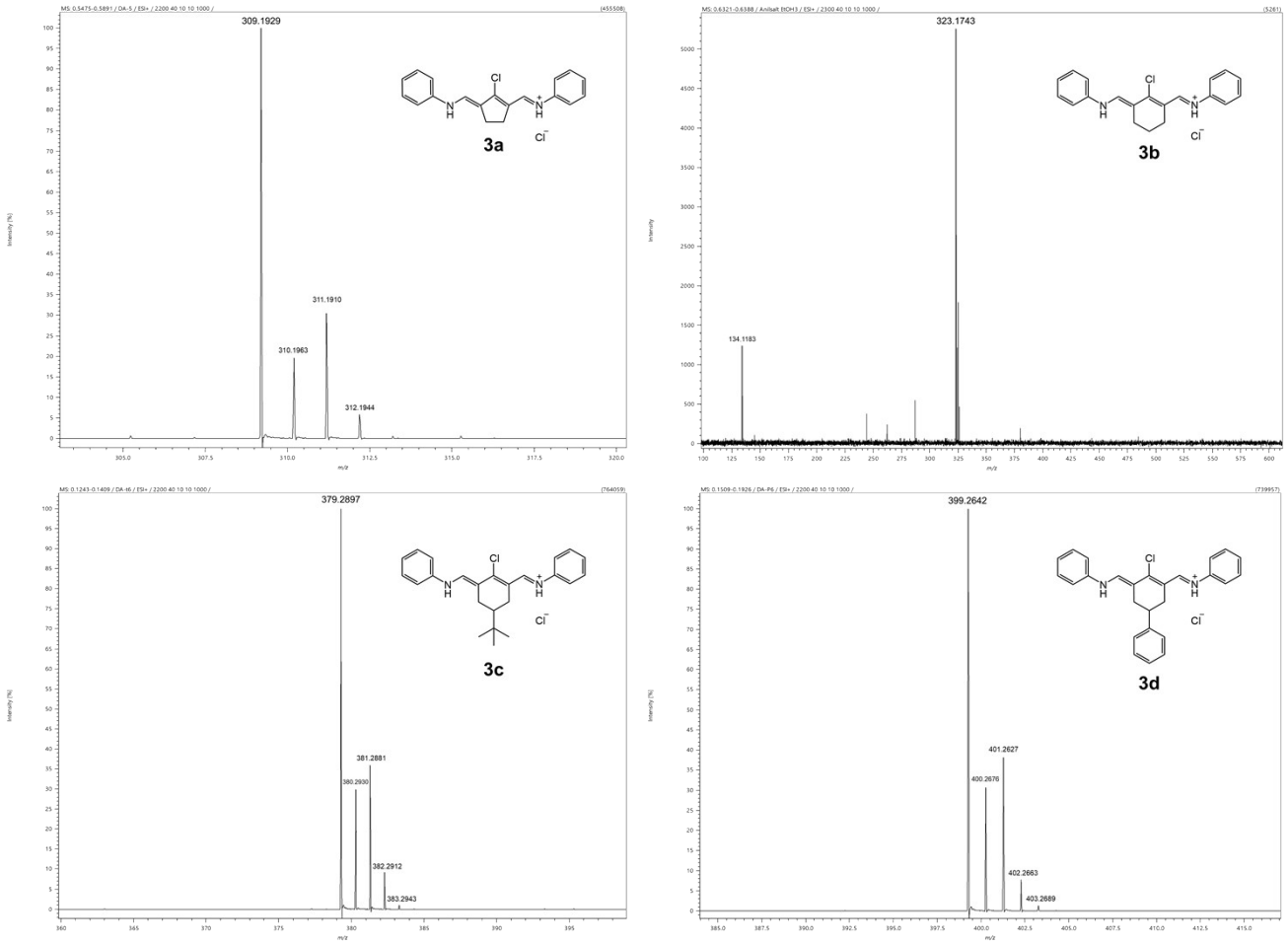


Fig. S10. LC/TOF-MS data of compound **3a**–**3d**.

S2.2. Synthesis of heptamethine cyanine dyes

Benzo[*cd*]indolenyl-substituted heptamethine cyanine dyes (Cy-5, Cy-6, Cy-t6, Cy-p6) were synthesized following the general procedure described below. A solution of benzo[*cd*]indolenyl derivative **2** (1.5 g, 3.68 mmol) and anilinium salt (**3a**–**3d**, 1.84 mmol) in acetic anhydride (40 mL) was added to a 120 mL amber vial. Then, the reaction mixture was treated with anhydrous sodium acetate (0.643 g, 7.84 mmol) and stirred overnight at room temperature. The crude product was dissolved in dichloromethane and filtered to remove sodium acetate. The filtrate was then evaporated, and the resulting residue was re-dissolved in a minimum

amount of dichloromethane (8 mL) and dropped into diethyl ether (500 mL) under sonication to obtain a dark brown precipitate. The precipitate was filtered, and the crude product was purified using column chromatography on silica gel with dichloromethane/methanol (50:1) as the eluent. For higher purity, the obtained products were dissolved in ethanol (70 mL) and recrystallized under sonication. The target compounds (Cy-5, Cy-6, Cy-t6, Cy-p6) were obtained as reddish-brown powders in moderate yields. (Yield: 43–68%).

S2.2.1. Characterization of 2-((*E*)-2-((*E*)-2-chloro-3-((*E*)-2-(1-decylbenzo[*cd*]indol-2(1*H*)-ylidene) ethyli-dene)cyclopent-1-en-1-yl)vinyl)-1-decylbenzo[*cd*]indol-1-ium perchlorate (Cy-5)

Yield: 55%, ^{1}H NMR of Cy-5 (850 MHz, $CDCl_3$): δ (ppm) 8.08–8.06 (br d, 2H), 7.87–7.84 (d, J=13.6 Hz, 2H), 7.79–7.75 (m, 4H), 7.28–7.25 (d, J=7.8 Hz, 2H), 7.18–7.15 (t, J=7.4 Hz, 2H), 6.67–6.64 (d, J=6.8 Hz, 2H), 6.19–6.15 (d, J=13.6 Hz, 2H), 3.73–3.68 (t, J=6.7 Hz, 4H), 3.03–2.98 (br s, 4H), 1.62–1.57 (p, J=7.3 Hz, 4H), 1.27–1.23 (p, J=7.3 Hz, 4H), 1.22–1.13 (m, 24H), 0.79–0.76 (t, J=7.2 Hz, 6H). GC/HRMS (FAB) found: *m/z* 737.4607. Calcd for $C_{51}H_{62}ClN_2^+$: M – ClO_4, 737.4596.

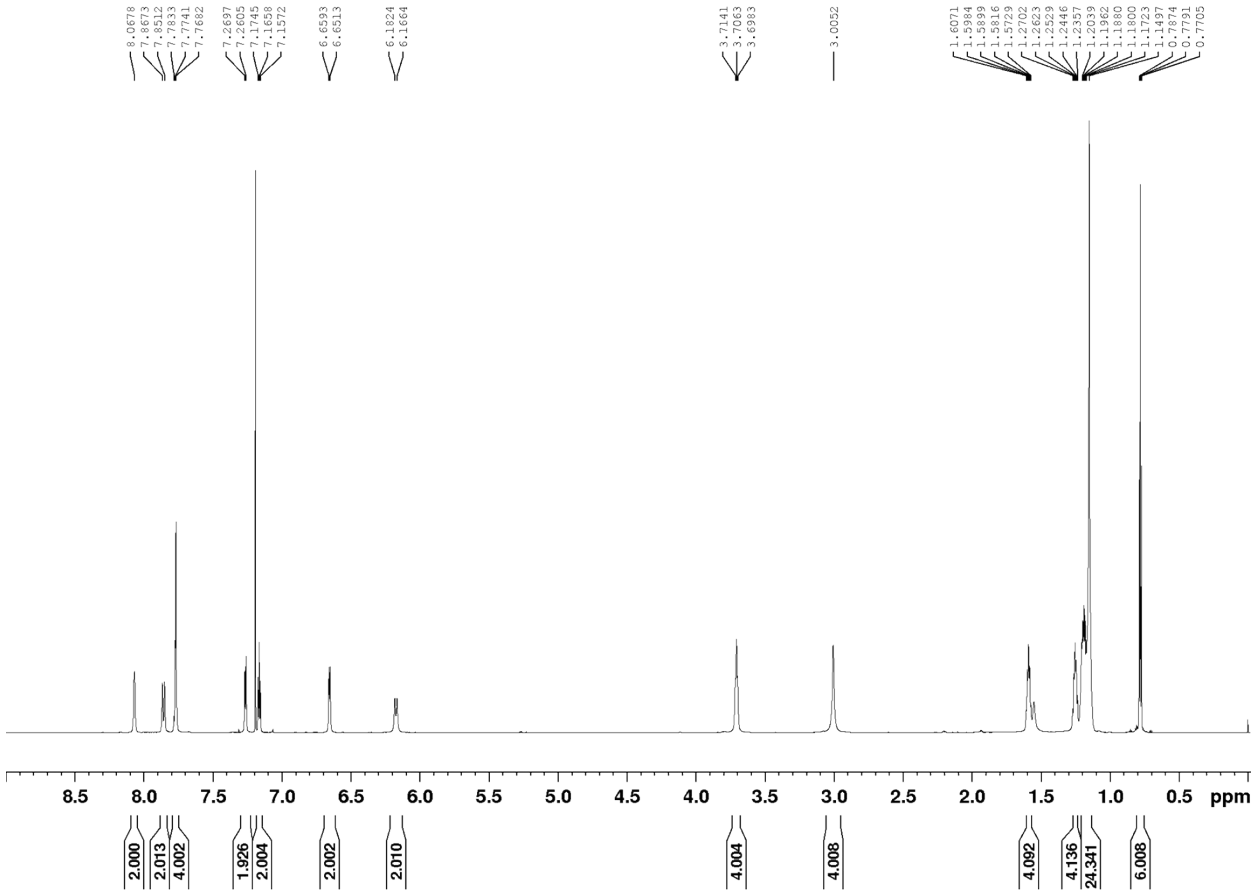


Fig. S11. ^{1}H NMR of Cy-5.

S2.2.2. Characterization of 2-((*E*)-2-((*E*)-2-chloro-3-((*E*)-2-(1-decylbenzo[*cd*]indol-2(1*H*)-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-1-decylbenzo[cd]indol-1-ium perchlorate (Cy-6)

Yield: 68%, ^{1}H NMR of Cy-6 (850 MHz, $CDCl_3$): δ (ppm) 8.70–8.50 (br s, 2H), 8.24–8.18 (br s, 2H), 7.98–7.94 (br s, 2H), 7.86–7.82 (t, J=7.1 Hz, 2H), 7.55–7.45 (br s, 2H), 7.45–7.40 (t, J=6.6 Hz, 2H), 7.10–6.92 (br s, 2H), 6.73–6.24 (br s, 2H), 4.07–3.91 (br s, 2H), 3.21–2.46 (br s, 4H), 2.08–2.04 (br t, 2H), 1.78–1.75 (p, J=7.3 Hz, 4H), 1.39–1.35 (p, J=7.3 Hz, 4H), 1.31–1.28 (p, J=7.1 Hz, 4H), 1.26–1.21 (m, 20H), 0.87–0.84 (t, J=7.2 Hz, 6H). GC/HRMS (FAB) found: *m/z* 751.4755. Calcd for $C_{52}H_{64}ClN_2^+$: M – ClO_4, 751.4753.

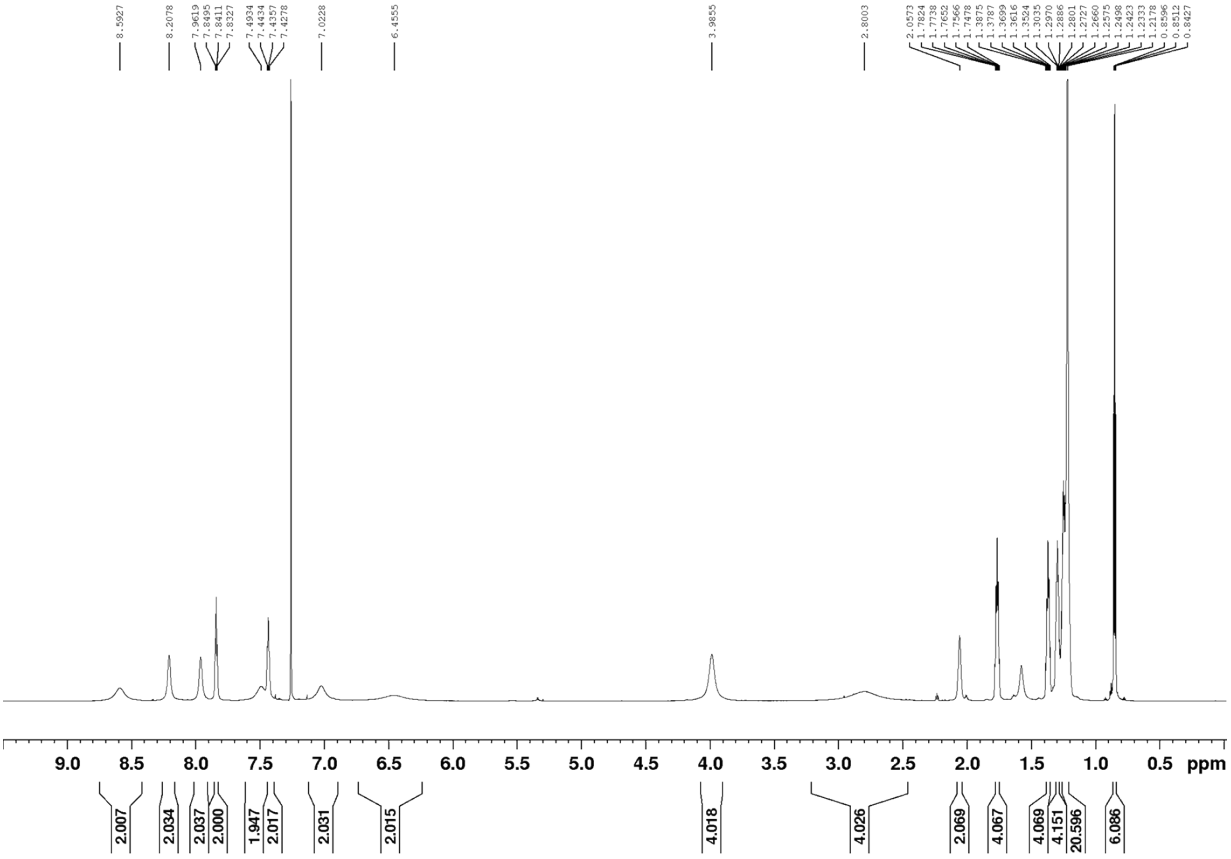


Fig. S12. ^{1}H NMR of Cy-6.

S2.2.3. Characterization of 2-((*E*)-2-((*E*)-5-(tert-butyl)-2-chloro-3-((*E*)-2-(1-decylbenzo[*cd*]indol-2(1*H*)-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-1-decylbenzo[*cd*]indol-1-ium perchlorate (Cy-t6)

Yield: 60%, ^{1}H NMR of Cy-t6 (850 MHz, $CDCl_3$): δ (ppm) 8.51–8.47 (d, J=13.7 Hz, 2H), 8.14–8.12 (d, J=6.8 Hz, 2H), 7.88–7.86 (d, J=7.6 Hz, 2H), 7.76–7.73 (t, J=7.2 Hz, 2H), 7.42–7.39 (d, J=7.9 Hz, 2H), 7.37–7.34 (t,

J=7.4 Hz, 2H), 7.05–7.02 (d, J=6.8 Hz, 2H), 6.42–6.37 (d, J=13.7 Hz, 2H), 4.12–4.00 (m, 4H), 2.89–2.85 (d, J=13.0 Hz, 2H), 2.20–2.14 (t, J=12.2 Hz, 2H), 1.76–1.71 (p, J=7.4 Hz, 4H), 1.52–1.47 (tt, J_1=12.6 Hz, J_2=3.2 Hz, 1H), 1.35–1.31 (p, J=7.5 Hz, 4H), 1.26–1.22 (p, J=7.2 Hz, 4H), 1.19–1.13 (m, 20H), 1.06 (s, 9H), 0.79–0.77 (t, J=7.2 Hz, 6H). GC/HRMS (FAB) found: *m/z* 807.5379. Calcd for $C_{56}H_{72}ClN_2^+$: M – ClO_4, 807.5379.

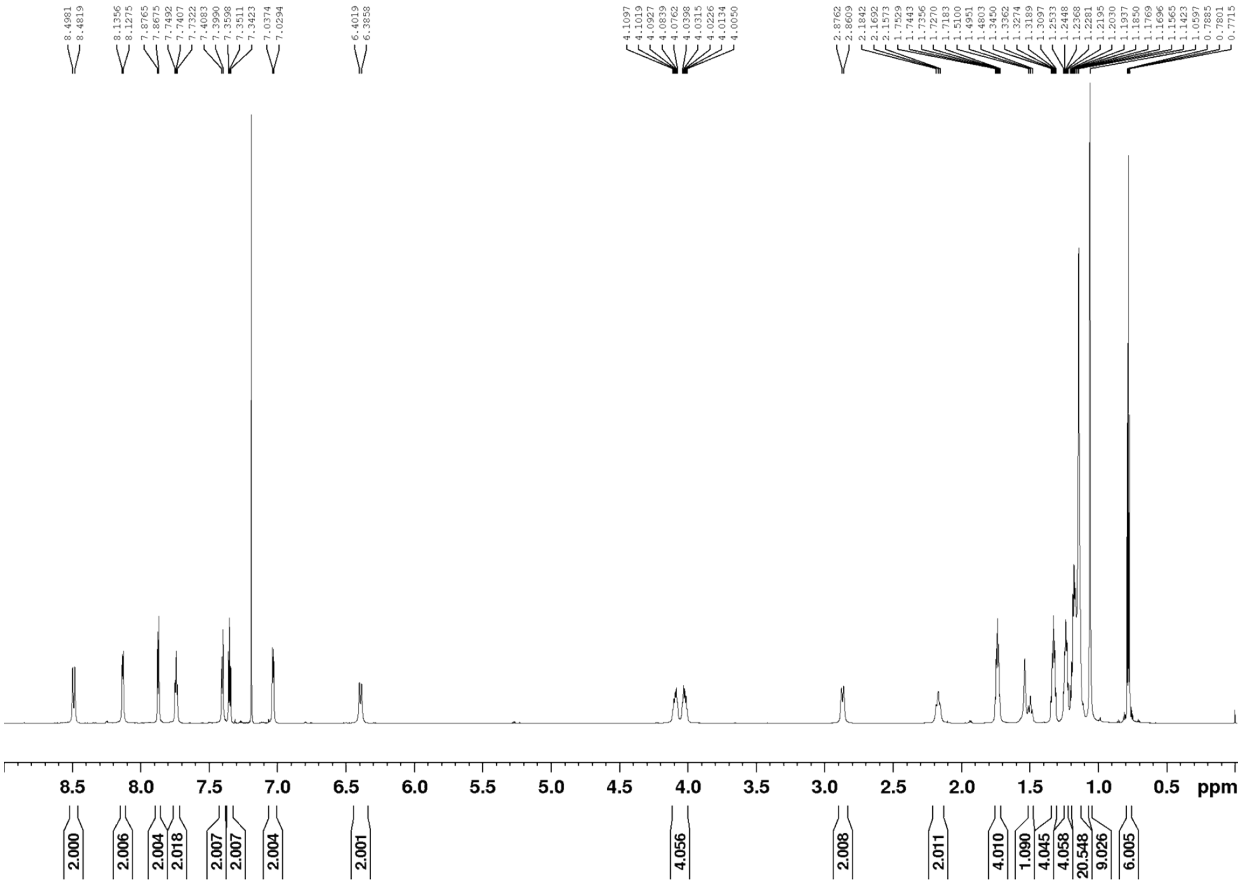


Fig. S13. ^{1}H NMR of Cy-t6.

S2.2.4. Characterization of 2-((*E*)-2-((*E*)-4-chloro-5-((*E*)-2-(1-decylbenzo[*cd*]indol-2(1*H*)-ylidene)ethylidene)-1,2,5,6-tetrahydro-[1,1'-biphenyl]-3-yl)vinyl)-1-decylbenzo[*cd*]indol-1-ium perchlorate (Cy-p6)

Yield: 43%, ^{1}H NMR of Cy-p6 (850 MHz, $CDCl_3$): δ (ppm) 8.66–8.62 (d, J=13.9 Hz, 2H), 8.23–8.20 (d, J=6.5 Hz, 2H), 7.92–7.90 (d, J=7.7 Hz, 2H), 7.79–7.75 (t, J=6.7 Hz, 2H), 7.48–7.45 (d, 7.9 Hz, 2H), 7.41–7.37 (m, 6H), 7.29–7.26 (t, 7.0 Hz, 1H), 7.06–7.03 (d, J=6.9 Hz, 2H), 6.36–6.33 (d, J=13.9 Hz, 2H), 4.01–3.92 (m, 4H), 3.15–3.10 (tt, J_1=11.3 Hz, J_2=3.2 Hz, 1H), 3.07–3.03 (d, J=14.0 Hz, 2H), 2.78–2.72 (t, J=13.0 Hz, 2H),

1.71–1.66 (p, J=7.3 Hz, 4H), 1.29–1.24 (p, J=7.4 Hz, 4H), 1.20–1.16 (m, 8H), 1.14–1.08 (m, 16H), 0.79–0.77 (t, J=7.3 Hz, 6H). HRMS (FAB) found: *m/z* 827.5067. Calcd for $C_{58}H_{68}ClN_2^+$: M – ClO_4, 827.5066.

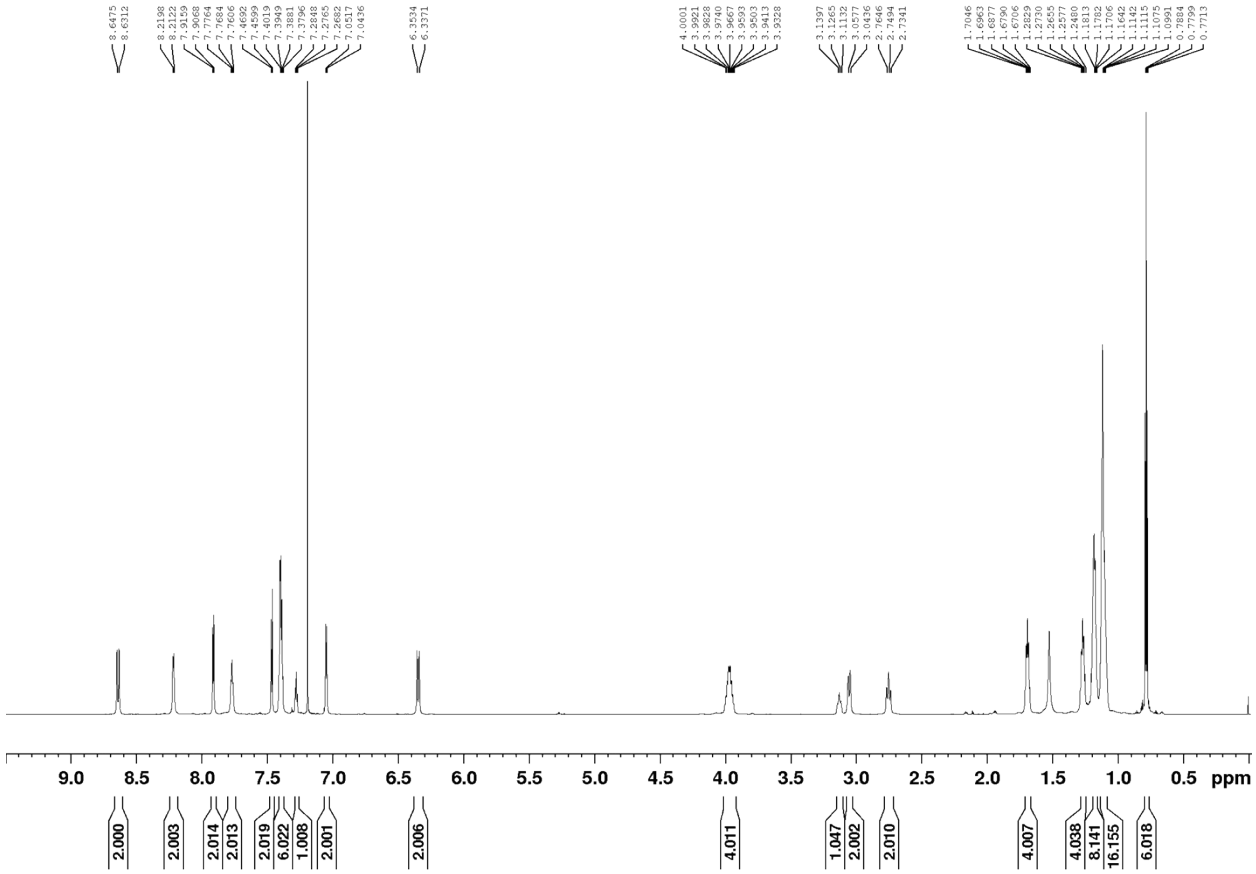


Fig. S14. [1]H NMR of Cy-p6.

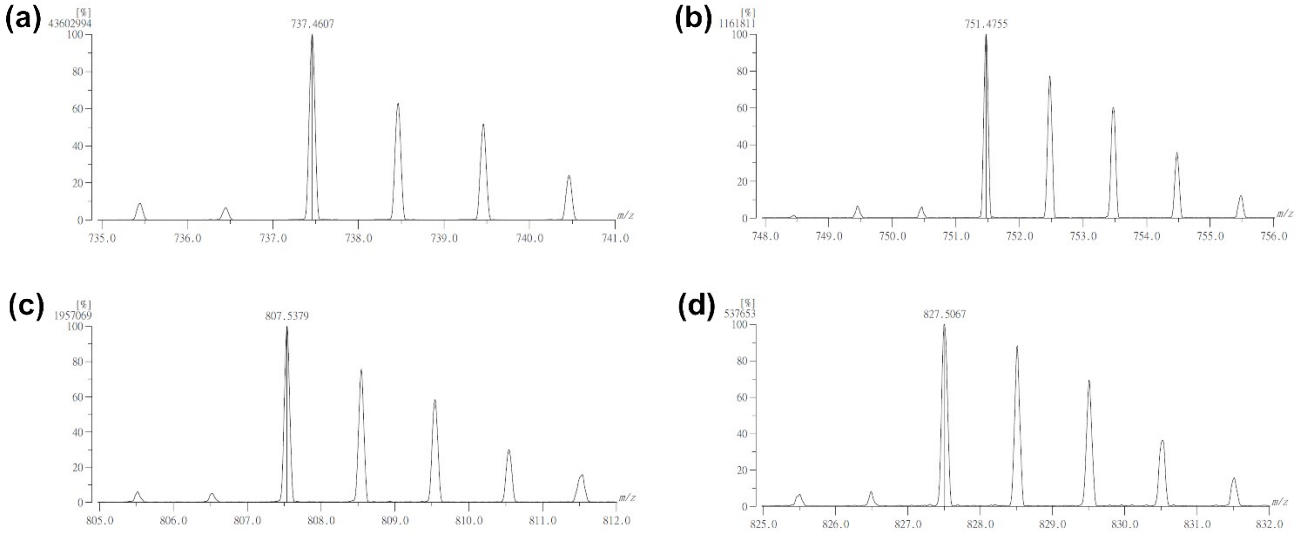
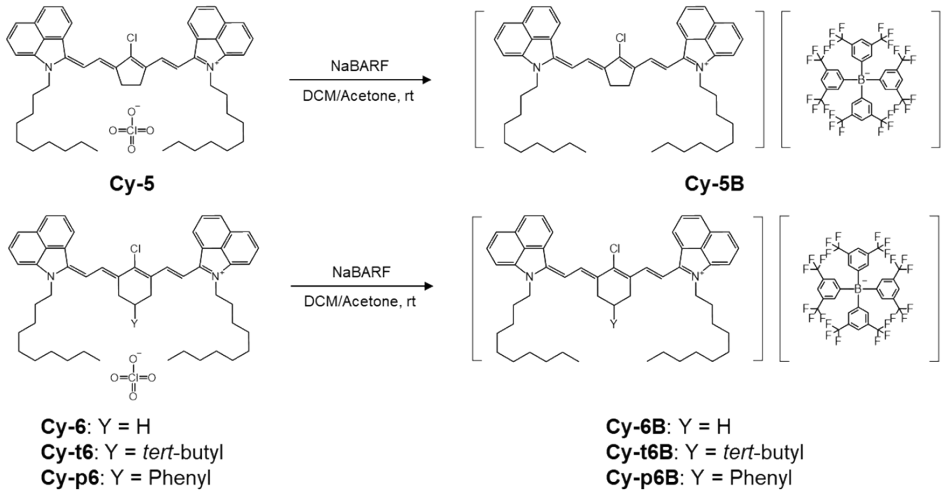


Fig. S15. HR-GC/MS data of synthesized cyanine dyes. (a) Cy-5, (b) Cy-6, (c) Cy-t6, (d) Cy-p6.

S2.3. Synthesis of BARF-substituted heptamethine cyanine dyes



Scheme S4. Substitution of BARF anion.

BARF-substituted cyanine dyes (Cy-5B, Cy-6B, Cy-t6B, Cy-p6B) were synthesized through a simple ion-exchange reaction with sodium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (NaBARF). In a 150 ml amber vial, 0.2 mmol of cyanine dyes (Cy-5, Cy-6, Cy-t6, Cy-p6) and NaBARF (0.24 mmol, 0.213 g) were dissolved in a 100 ml solution of acetone/dichloromethane (1:1) and stirred at room temperature for 3 hours. The mixture solution was then evaporated under reduced pressure, and the resulting solid was dissolved in dichloromethane extracted with water (3 x 15 mL). The organic extracts were dried over anhydrous magnesium sulfate, and the solvent was removed using a rotary evaporator. The residue was purified by column chromatography on silica gel using dichloromethane as the eluent. The isolated products were dissolved in 5 mL of dichloromethane and dropped into 200 mL of hexane under sonication, and the precipitated solid was collected by filtration. Cy-5B was obtained as a dark blue powder (0.291 g, 91% yield), Cy-6B (0.284 g, 88% yield), and Cy-t6B (0.314 g, 94% yield) were obtained as dark olive green powders. In the case of Cy-p6B, the desired product failed to precipitate in hexane despite repeated column chromatography. Instead, the target product (Cy-p6B) was obtained as a dark green solid (0.247 g, 73%) through vacuum drying in an oven.

S2.3.1. Characterization of 2-((*E*)-2-((*E*)-2-chloro-3-((*E*)-2-(1-decylbenzo[*cd*]indol-2(1*H*)-ylidene) ethyli-dene)cyclopent-1-en-1-yl)vinyl)-1-decylbenzo[*cd*]indol-1-ium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (Cy-5B)

^{1}H NMR of Cy-5B (850 MHz, $CDCl_3$): δ (ppm) 8.31–8.28 (d, J=6.6 Hz, 2H), 8.28–8.24 (d, J=13.3 Hz, 2H), 8.04–8.00 (d, J=7.5 Hz, 2H), 7.77–7.74 (t, J=7.6 Hz, 2H), 7.65 (br s, 8H), 7.64–7.59 (br d, 2H), 7.53–7.50 (t, J=7.6 Hz, 2H), 7.44–7.42 (br s, 4H), 7.16–7.08 (br s, 2H), 6.35–6.28 (br d, J=10.4 Hz, 2H), 4.08 (br s, 4H), 2.94 (br s, 4H), 1.84–1.79 (p, J=7.4 Hz, 4H), 1.39–1.35 (p, J=7.4 Hz, 4H), 1.31–1.27 (p, J=7.4 Hz, 4H), 1.21–1.15 (m, 20H), 0.80–0.77 (t, J=7.1 Hz, 6H).

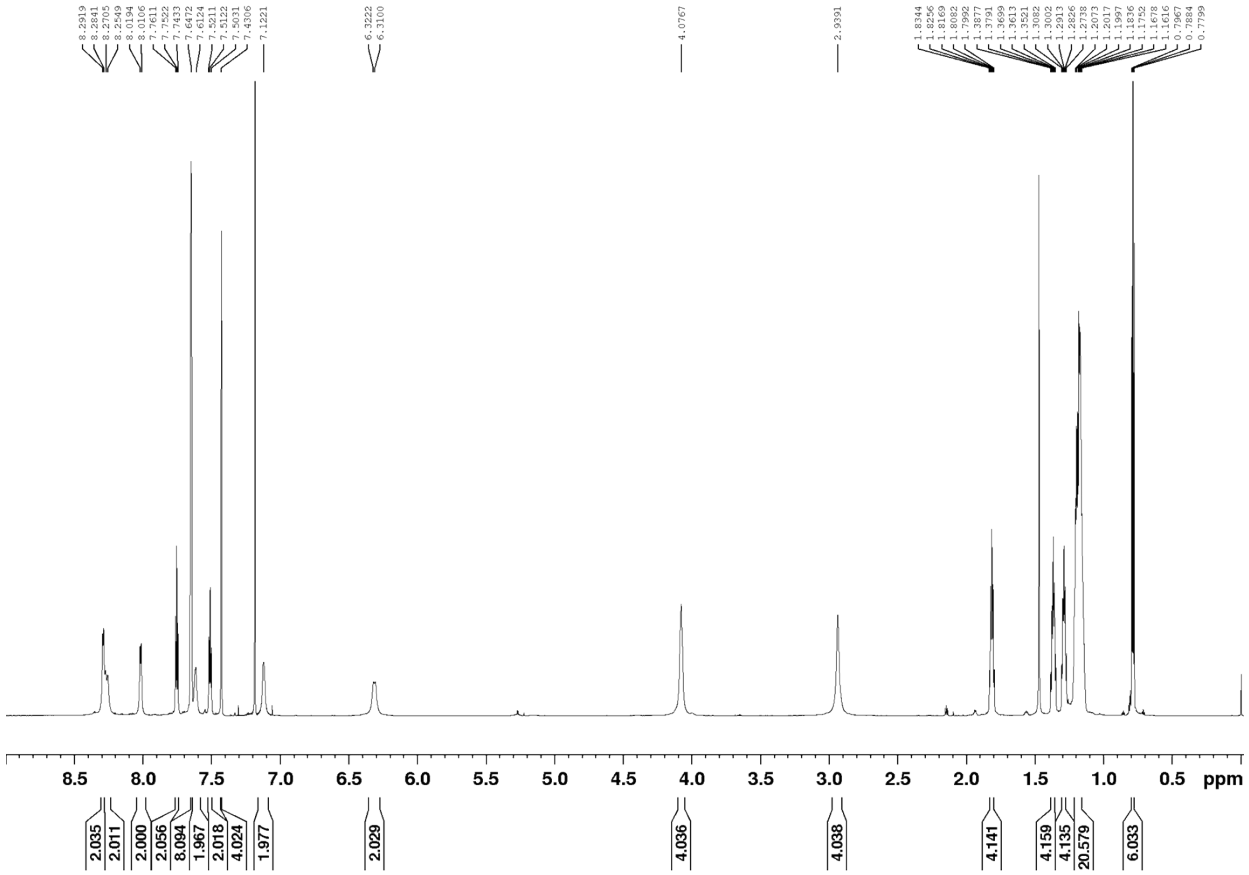


Fig. S16. ^{1}H NMR of Cy-5B.

S2.3.2. Characterization of 2-((*E*)-2-((*E*)-2-chloro-3-((*E*)-2-(1-decylbenzo[*cd*]indol-2(1*H*)-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-1-decylbenzo[cd]indol-1-ium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (Cy-6B)

^{1}H NMR of Cy-6B (850 MHz, $CDCl_3$): δ (ppm) 8.90–8.88 (d, J=13.7 Hz, 2H), 8.42–8.40 (d, J=7.1 Hz, 2H), 8.12–8.10 (d, J=7.8 Hz, 2H), 7.85–7.82 (t, J=7.6 Hz, 2H), 7.71 (br s, 8H), 7.71–7.70 (overlapped, 2H), 7.61–7.59 (t, J=7.6 Hz, 2H), 7.51 (br s, 4H), 7.24–7.21 (d, J=6.9 Hz, 2H), 6.58–6.55 (d, J=13.7Hz, 2H),

4.20–4.17 (t, J=6.7 Hz, 4H), 2.78–2.76 (br t, 4H), 1.99–1.95 (p, J=5.7 Hz, 2H), 1.93–1.89 (p, J=7.4 Hz, 4H), 1.48–1.44 (p, J=7.4 Hz, 4H), 1.40–1.36 (p, J=7.4 Hz, 4H), 1.30–1.23 (m, 20H), 0.87–0.85 (t, J=7.1 Hz, 6H).

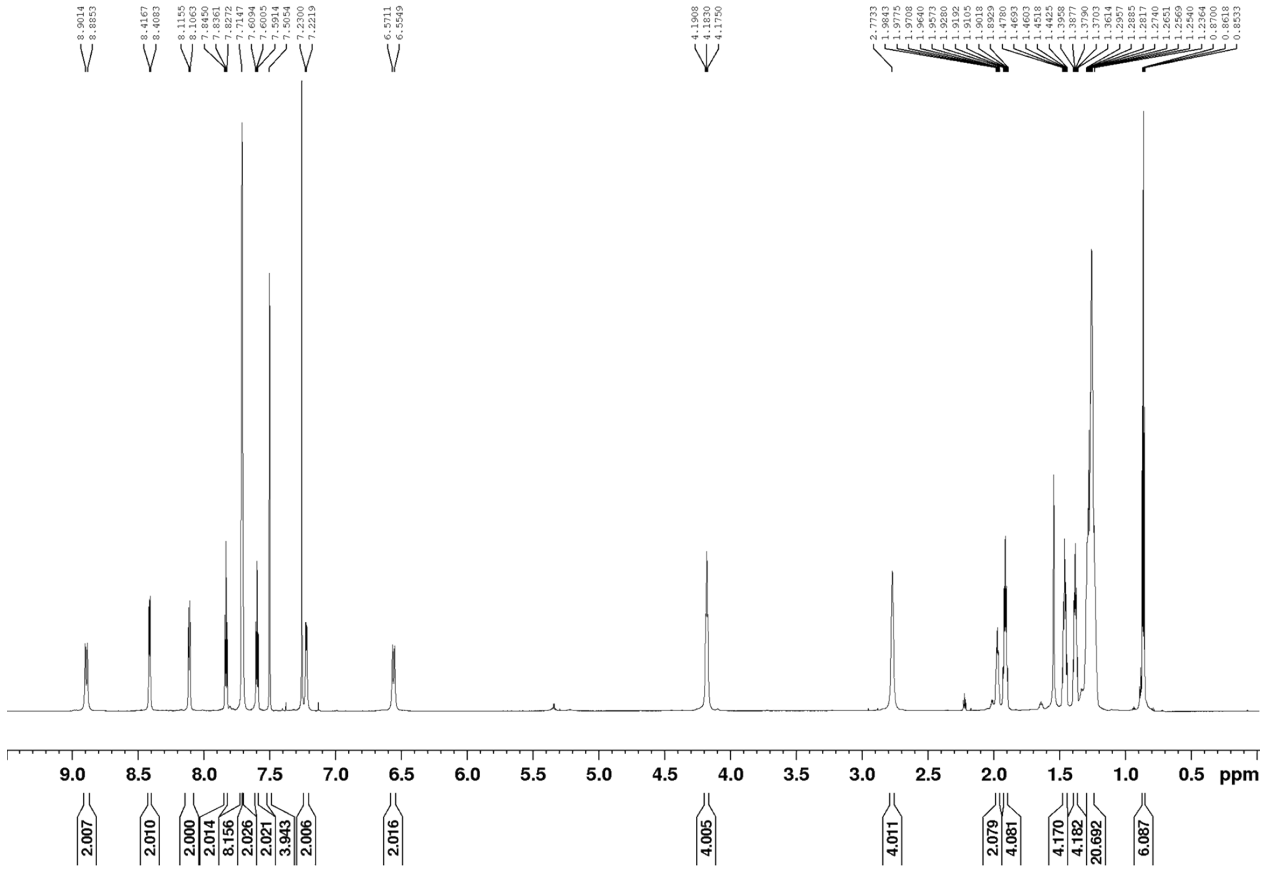


Fig. S17. ^{1}H NMR of Cy-6B.

S2.3.3. Characterization of 2-((*E*)-2-((*E*)-5-(tert-butyl)-2-chloro-3-((*E*)-2-(1-decylbenzo[*cd*]indol-2(1*H*)-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-1-decylbenzo[*cd*]indol-1-ium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (Cy-t6B)

^{1}H NMR of Cy-t6B (850 MHz, $CDCl_3$): δ (ppm) 8.84–8.80 (d, J=13.8 Hz, 2H), 8.35–8.33 (d, J=7.3 Hz, 2H), 8.05–8.03 (d, J=8.0 Hz, 2H), 7.78–7.75 (t, J=7.6 Hz, 2H), 7.65–7.62 (m, 10H), 7.54–7.51 (t, J=7.7 Hz, 2H), 7.42 (br s, 4H), 7.16–7.14 (d, J=7.2 Hz, 2H), 6.51–6.48 (d, J=13.8 Hz, 2H), 4.15–4.12 (t, J=7.5 Hz, 4H), 2.98–2.94 (dd, J_1=14.7 Hz, J_2=3.2 Hz, 2H), 2.29–2.25 (t, J=13.5 Hz, 2H), 1.88–1.83 (p, J=7.4 Hz, 4H), 1.67–1.62 (tt, J_1=12.5 Hz, J_2=3.7 Hz, 1H), 1.43–1.37 (p, J=7.4 Hz, 4H), 1.34–1.30 (p, J=7.4 Hz, 4H), 1.23–1.15 (m, 20H), 1.02 (s, 9H), 0.80–0.78 (t, J=7.1 Hz, 6H).

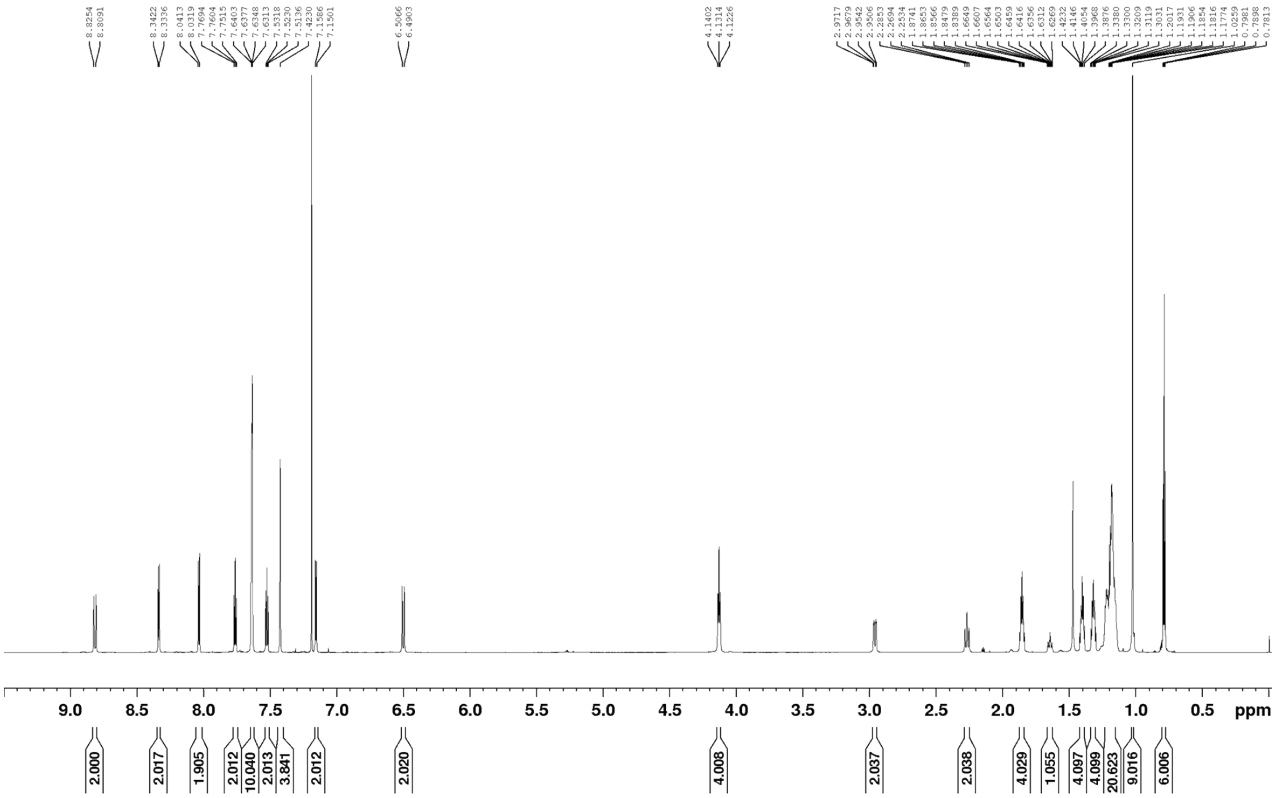


Fig. S18. ^{1}H NMR of Cy-t6B.

S2.3.4. Characterization of 2-((*E*)-2-((*E*)-4-chloro-5-((*E*)-2-(1-decylbenzo[*cd*]indol-2(1*H*)-ylidene)ethylidene)-1,2,5,6-tetrahydro-[1,1'-biphenyl]-3-yl)vinyl)-1-decylbenzo[*cd*]indol-1-ium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (Cy-p6B)

^{1}H NMR of Cy-p6B (850 MHz, $CDCl_3$): δ (ppm) 8.90–8.87 (d, J=13.9 Hz, 2H), 8.38–8.36 (d, J=7.3 Hz, 2H), 8.05–8.03 (d, J=8.0 Hz, 2H), 7.78–7.75 (t, J=7.6 Hz, 2H), 7.65–7.64 (d overlapped, 2H), 7.64–7.62 (br s, 8H), 7.53–7.50 (t, J=7.6 Hz, 2H), 7.41 (br s, 4H), 7.40–7.38 (t, J=7.6 Hz, 2H), 7.35–7.33 (d, J=7.6 Hz, 2H), 7.33–7.30 (t, J=7.5 Hz, 1H), 7.16–7.14 (d, J=7.2 Hz, 2H), 6.47–6.44 (d, J=13.9 Hz, 2H), 4.10–4.06 (t, J=7.4 Hz, 4H), 3.16–3.10 (m, 3H), 2.80–2.76 (t, J=13.0 Hz, 2H), 1.82–1.77 (p, J=7.4 Hz, 4H), 1.36–1.32 (p, J=7.5 Hz, 4H), 1.27–1.23 (p, J=7.4 Hz, 4H), 1.20–1.10 (m, 20H), 0.80–0.77 (t, J=7.2 Hz, 6H).

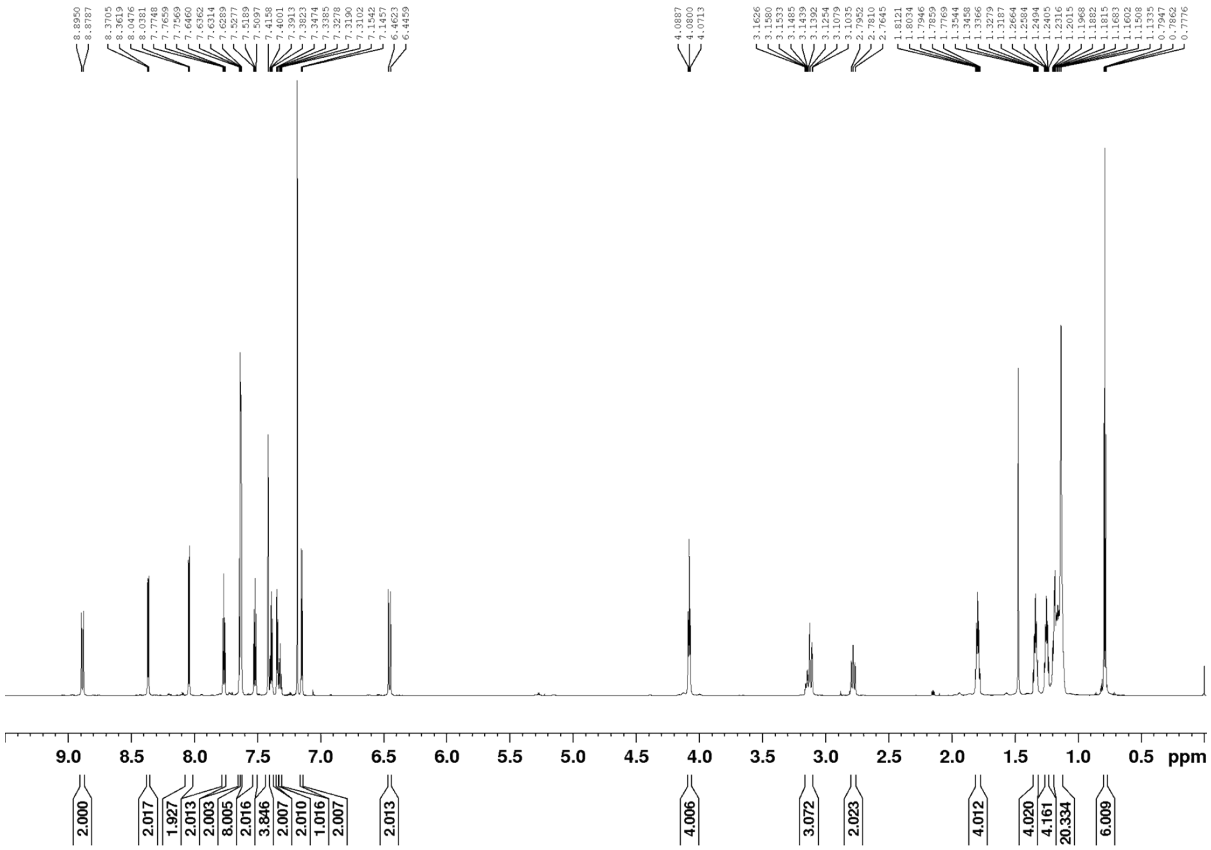


Fig. S19. ^{1}H NMR of Cy-p6B.