

Supporting information

**Reproducible chiroptical activity from aggregated chiral thienopyrroledione–fluorene  $\pi$ -conjugated polymers.**

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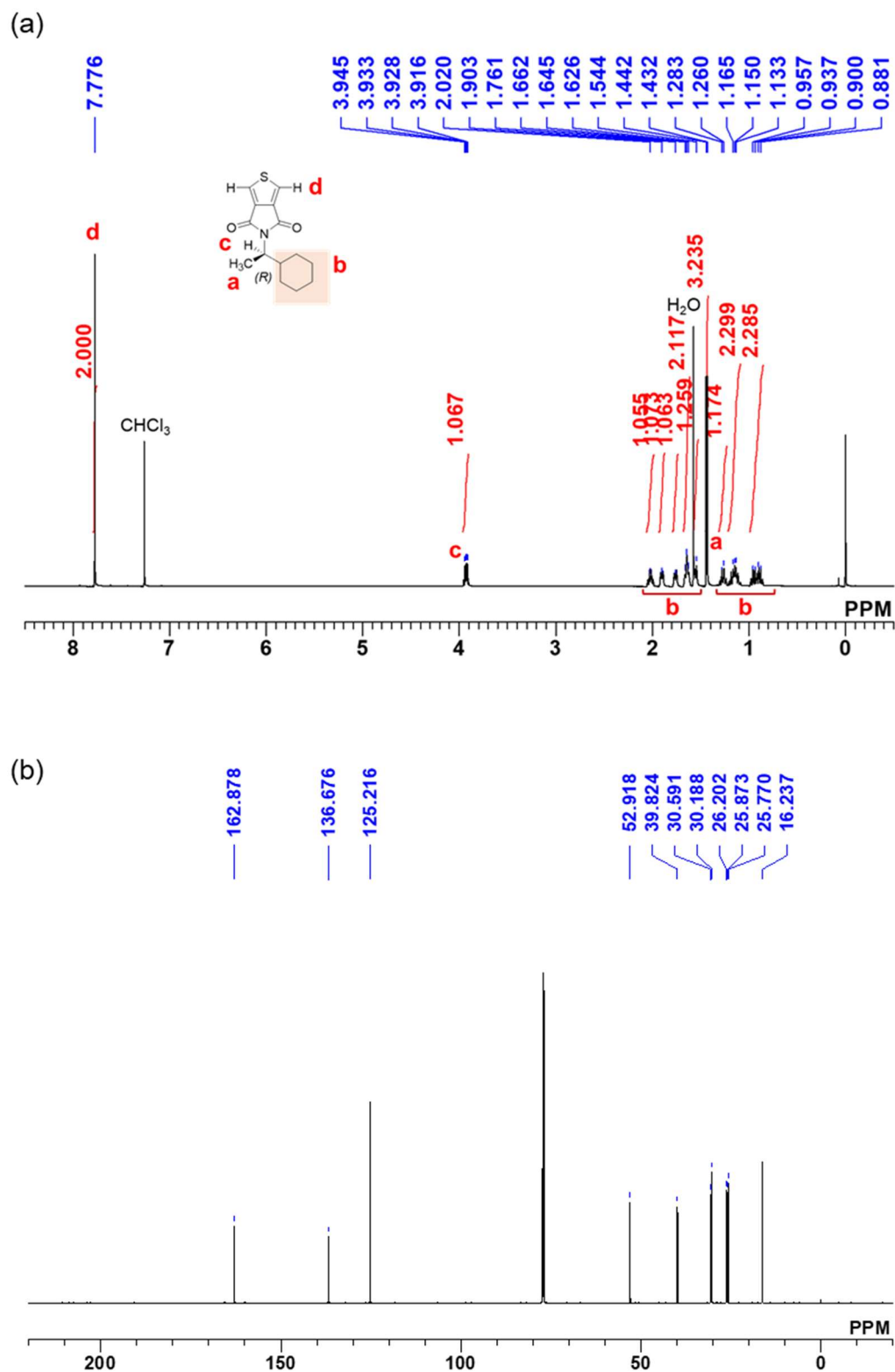


Figure S1. (a) <sup>1</sup>H NMR (CDCl<sub>3</sub>, 600 MHz, r.t.) and (b) <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of **(R)-TPD** (CDCl<sub>3</sub>, 150 MHz, r.t.).

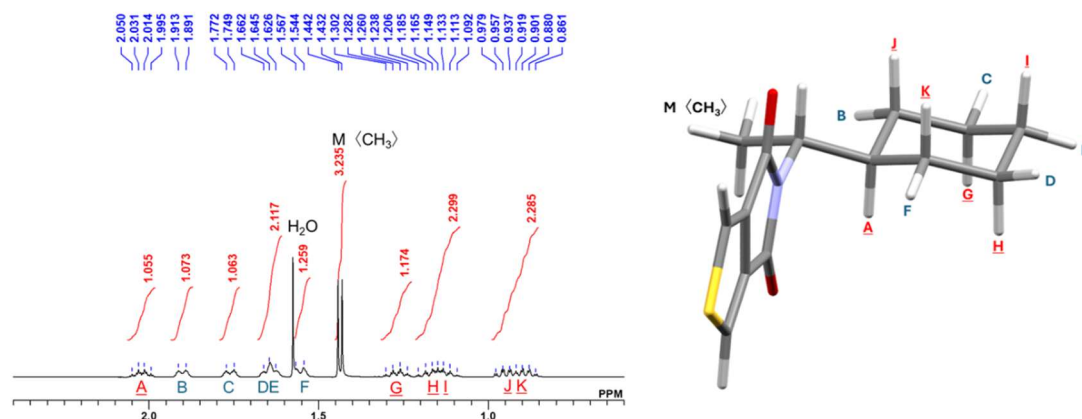


Figure S2.  $^1\text{H}$  NMR spectrum of (*R*)-TPD ( $\text{CDCl}_3$ , 600 MHz, r.t., 0.6–2.4 ppm)

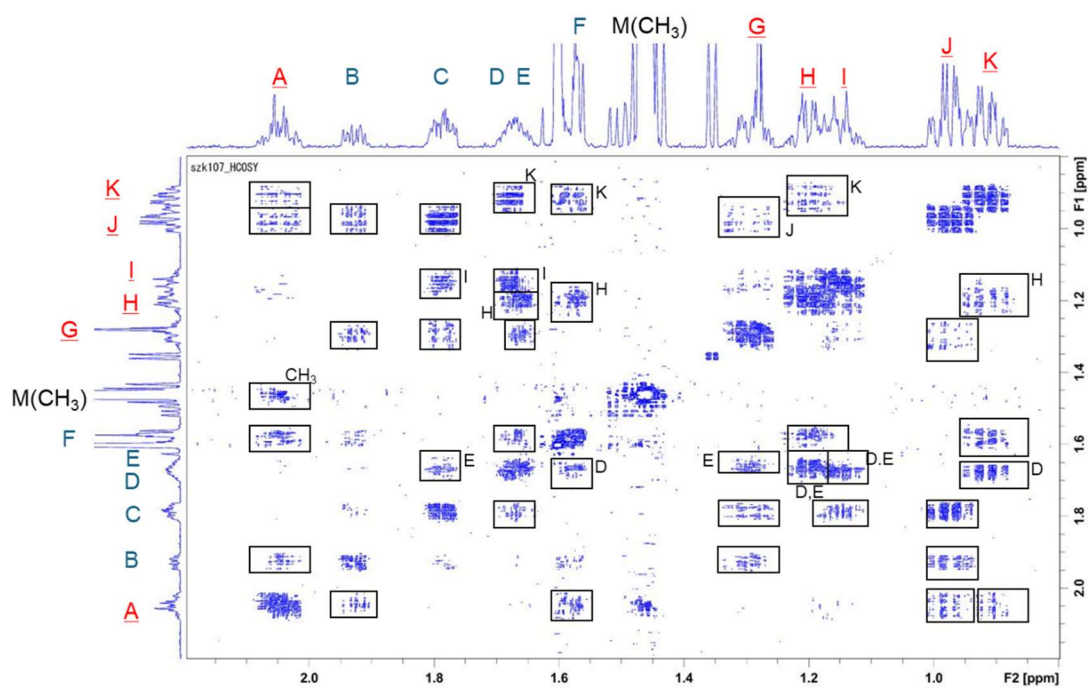


Figure S3.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of (*R*)-TPD ( $\text{CDCl}_3$ , 600 MHz, r.t., 0.6–2.4 ppm).

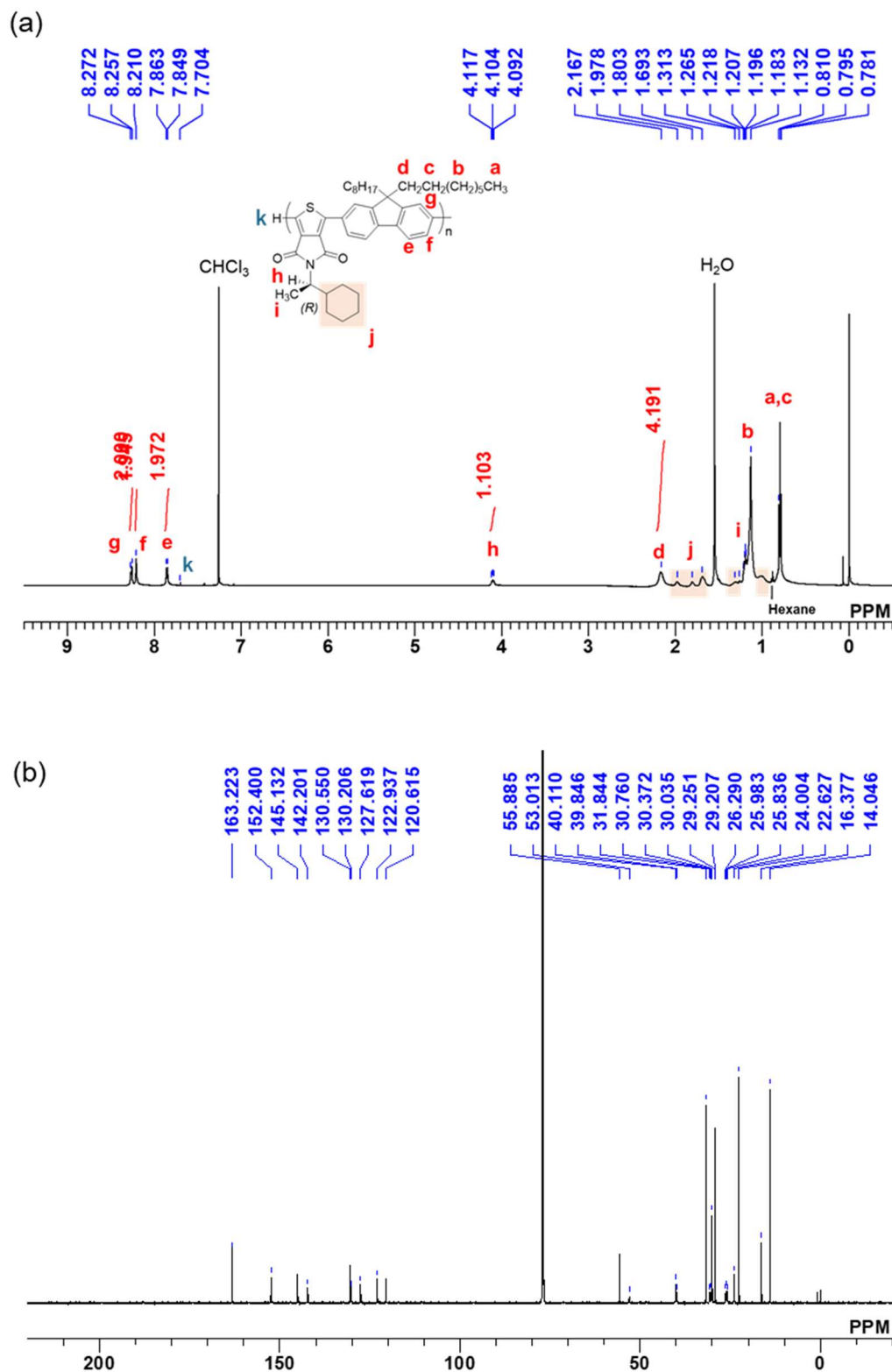
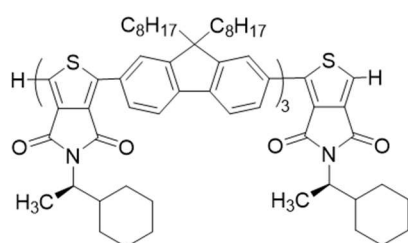
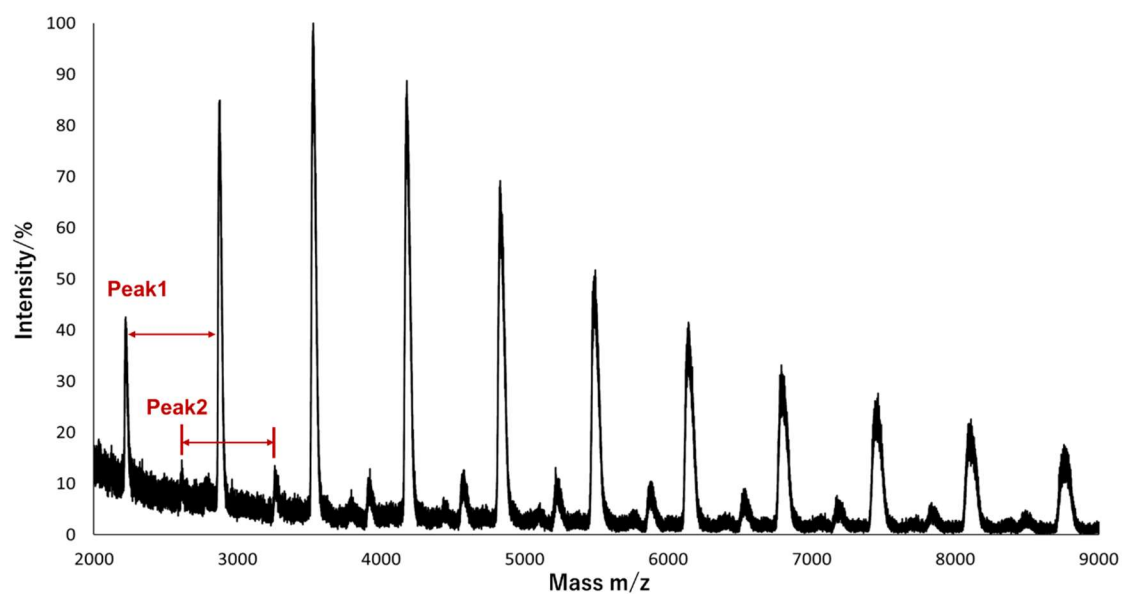
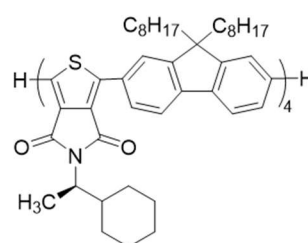


Figure S4. (a) <sup>1</sup>H NMR (CDCl<sub>3</sub>, 600 MHz, r.t.) and (b) <sup>13</sup>C{<sup>1</sup>H} NMR spectra of **(R)-PFTPD** (CDCl<sub>3</sub>, 150 MHz, r.t.).



Peak 1



Peak 2

Figure S5. MALDI-TOF-MS spectrum of (*R*)-PFTPD.

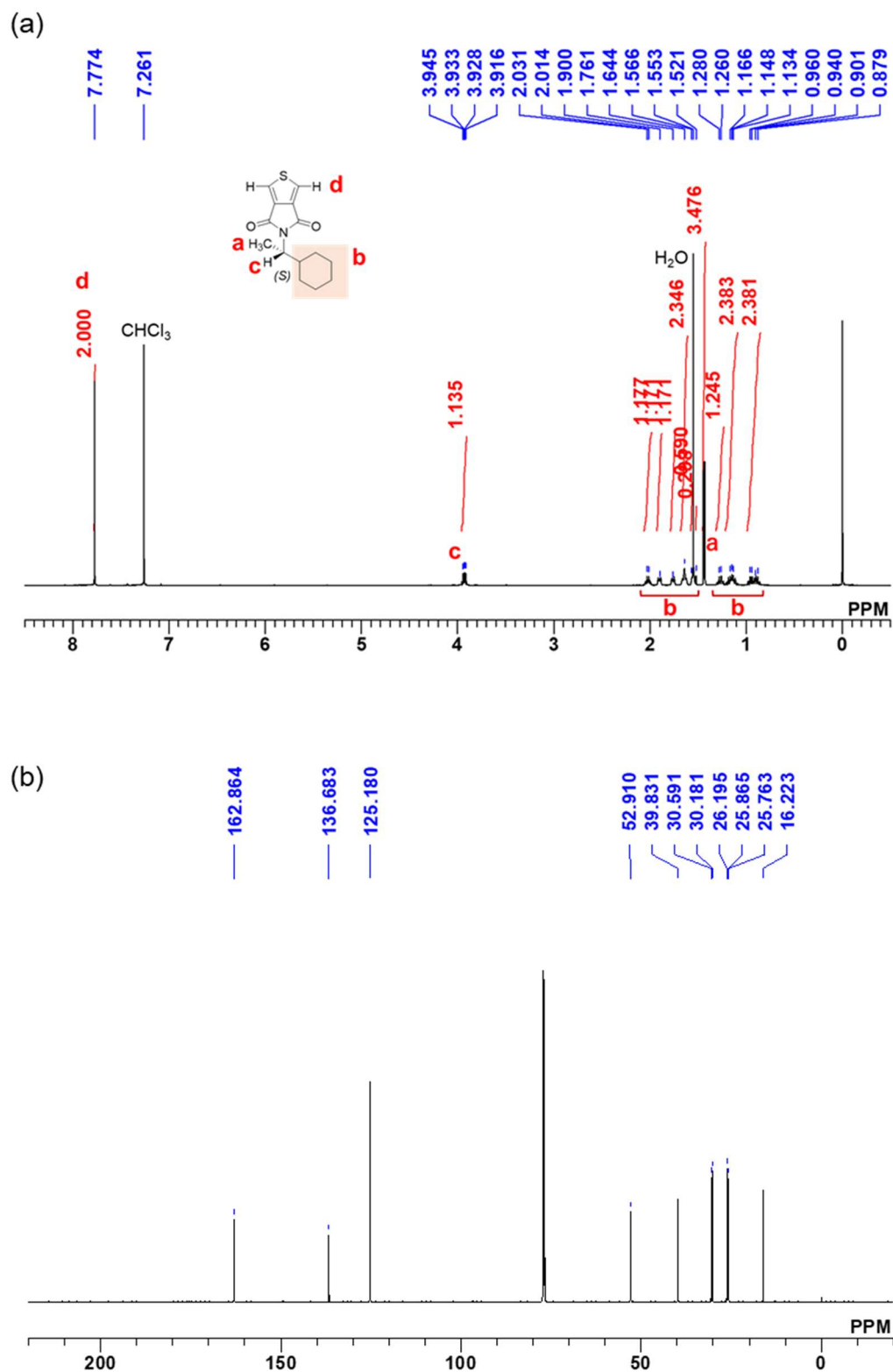


Figure S6. (a)  $^1\text{H}$  NMR (CDCl<sub>3</sub>, 600 MHz, r.t.) and (b)  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of *(S)*-TPD (CDCl<sub>3</sub>, 150 MHz, r.t.).

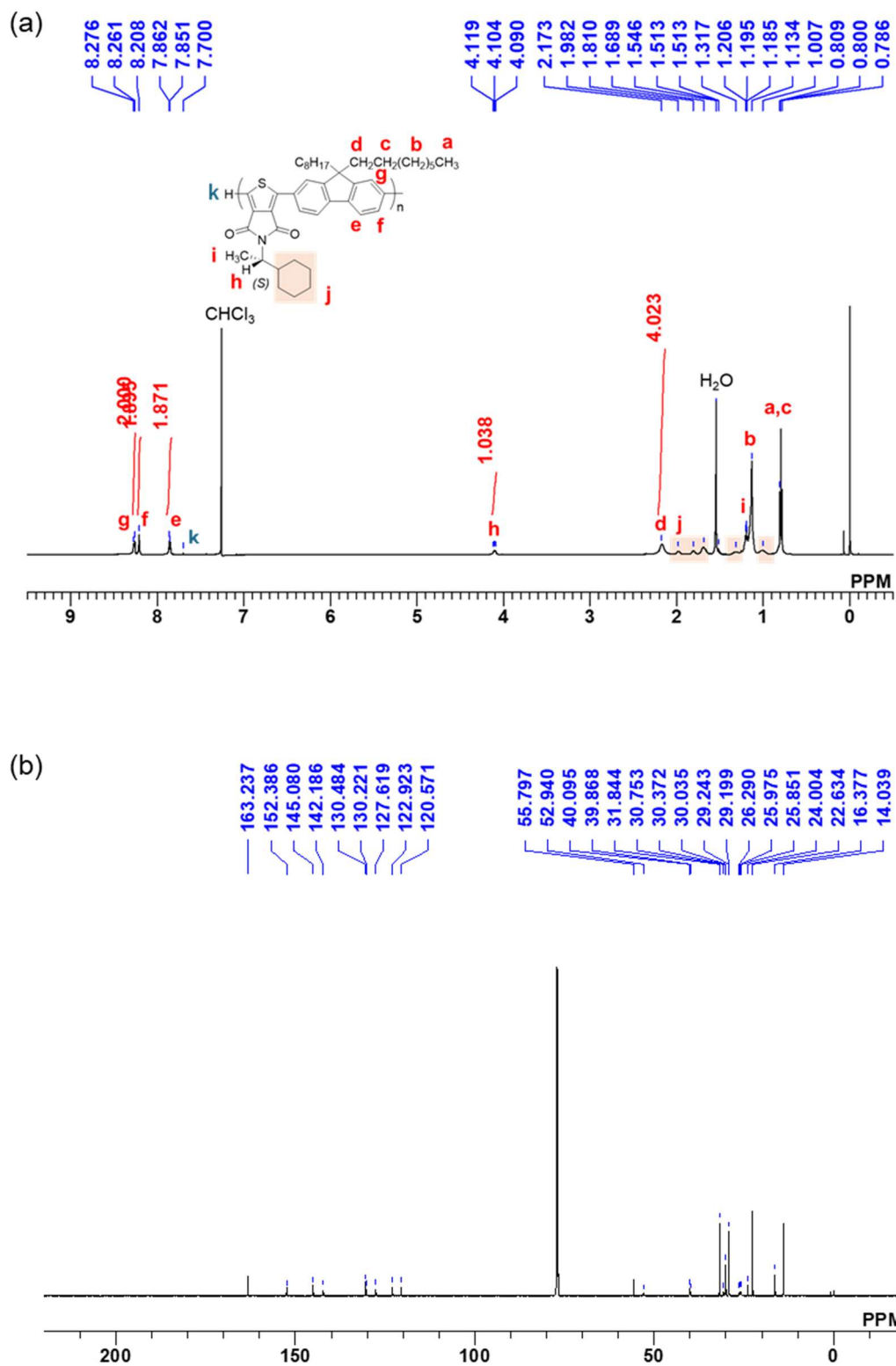
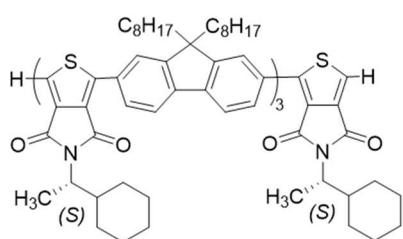
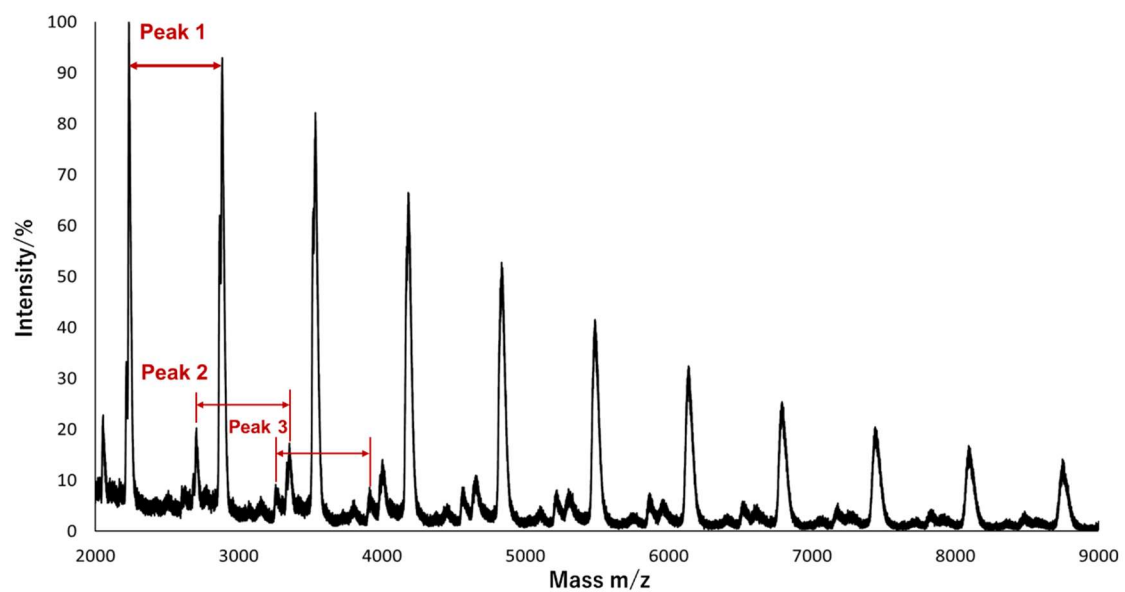
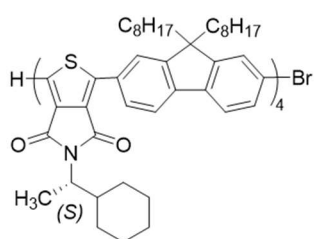


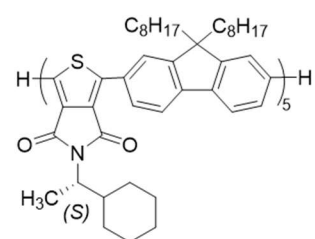
Figure S7. (a) <sup>1</sup>H NMR (CDCl<sub>3</sub>, 600 MHz, r.t.) and (b) <sup>13</sup>C{<sup>1</sup>H} NMR spectra of **(S)-PFTPD** (CDCl<sub>3</sub>, 150 MHz, r.t.).



**Peak 1**



**Peak 2**



**Peak 3**

Figure S8. MALDI-TOF-MS spectrum of **(S)-PFTPD**.



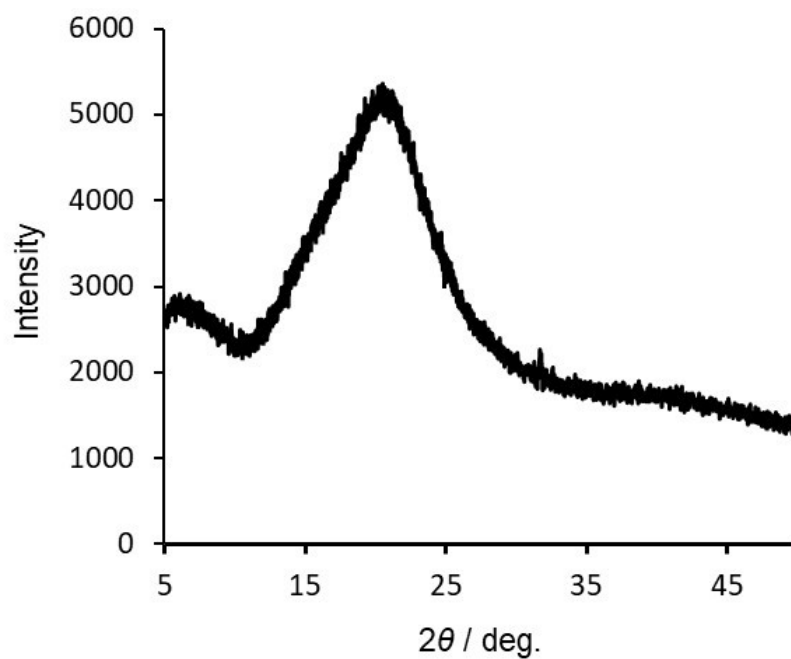


Figure S9. X-ray diffraction (XRD) patterns of a cast film of **(R)-PFTPD** measured using  $\text{CuK}\alpha$  radiation at room temperature.

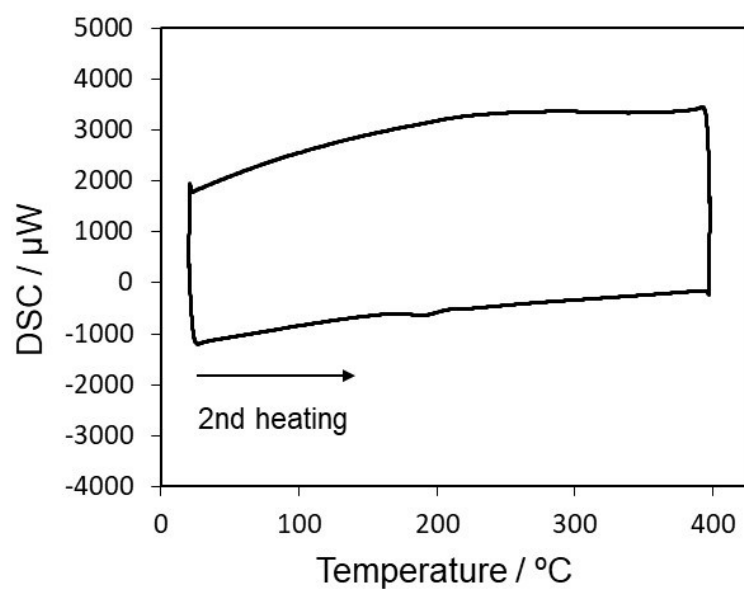


Figure S10. DSC thermograms of **(R)-PFTPD** measured under an Ar atmosphere at a heating rate of  $10 \text{ K min}^{-1}$  using a sample mass of 4.43 mg. The second heating scan after erasing the thermal history is shown.

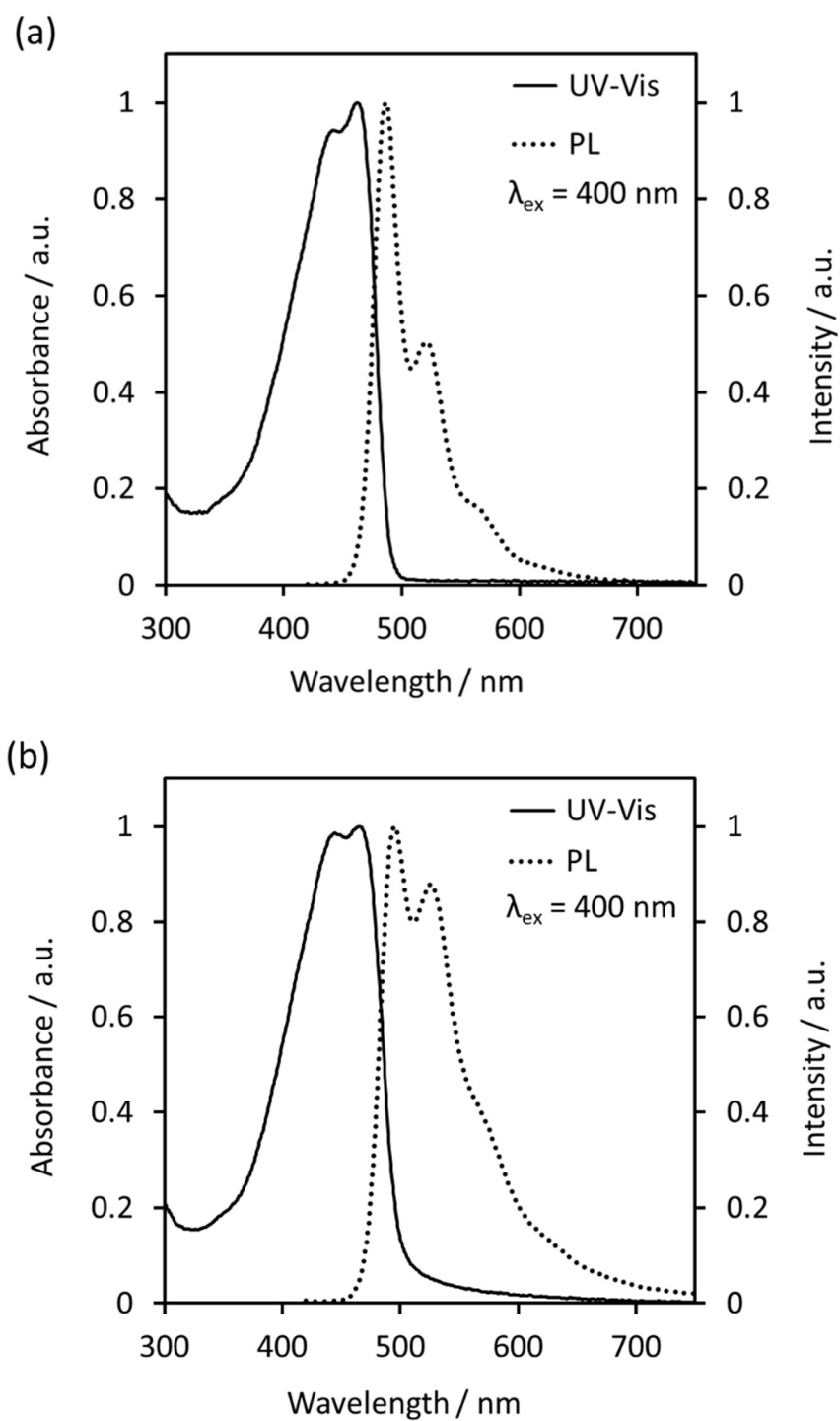


Figure S11. UV-Vis absorption and photoluminescence spectra of (*R*)-PFTPD (a) in solution state (CHCl<sub>3</sub>, 5.0 × 10<sup>-6</sup> M) and (b) in thin film state.

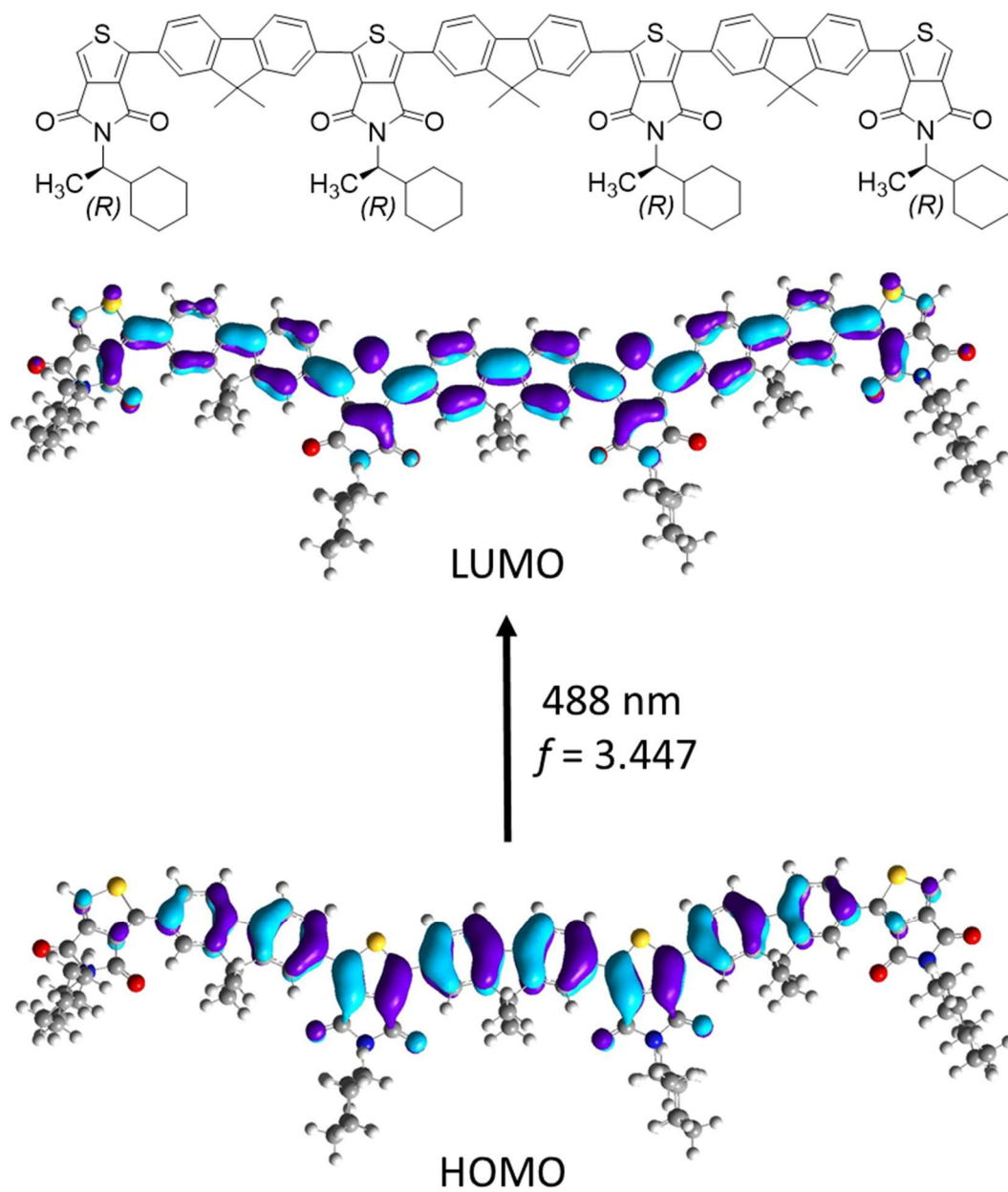


Figure S12. Frontier molecular orbitals (HOMO and LUMO), along with the predicted absorption wavelengths and corresponding oscillator strengths ( $f$ ) obtained from a TD-DFT calculation.

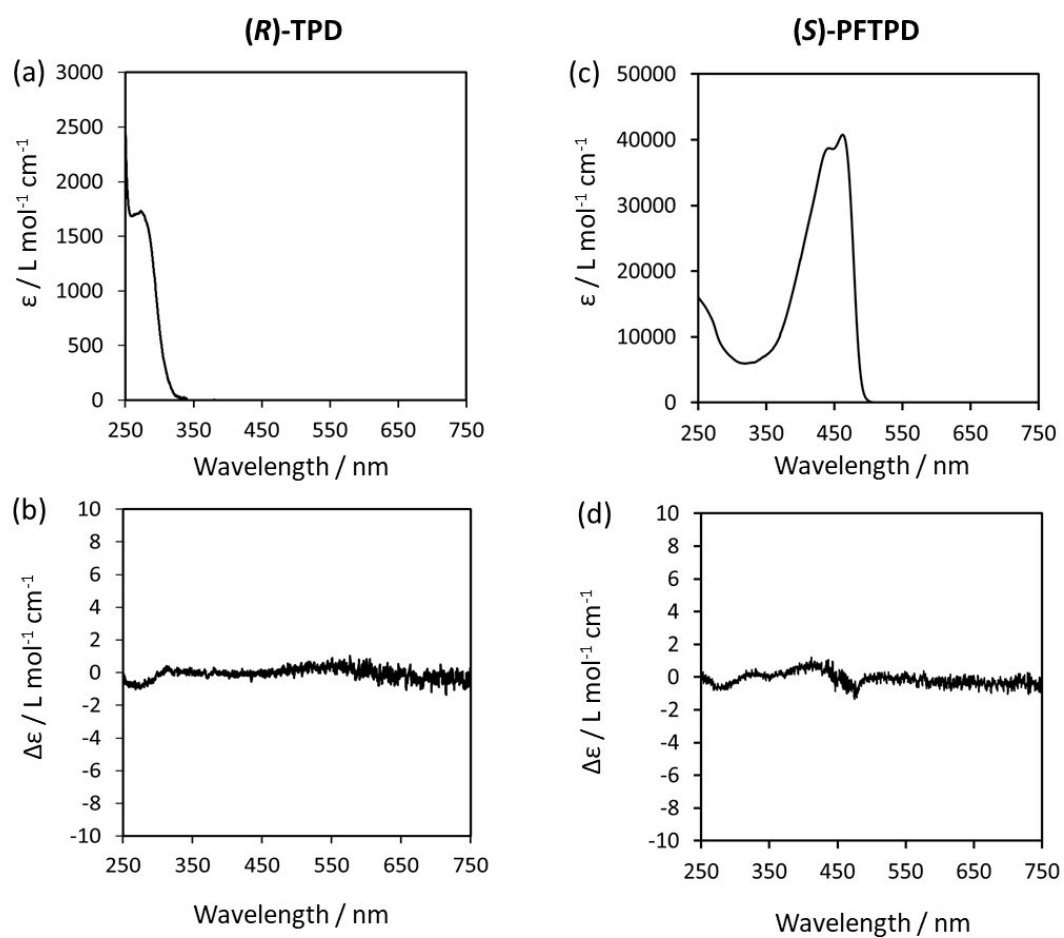


Figure S13. (a) UV-Vis absorption, (b) CD spectra of **(R)-TPD**, (c) UV-Vis absorption, and (d) CD spectra of **(S)-PFTPD** recorded in  $\text{CHCl}_3$  ( $3.0 \times 10^{-5} \text{ M}$ ).

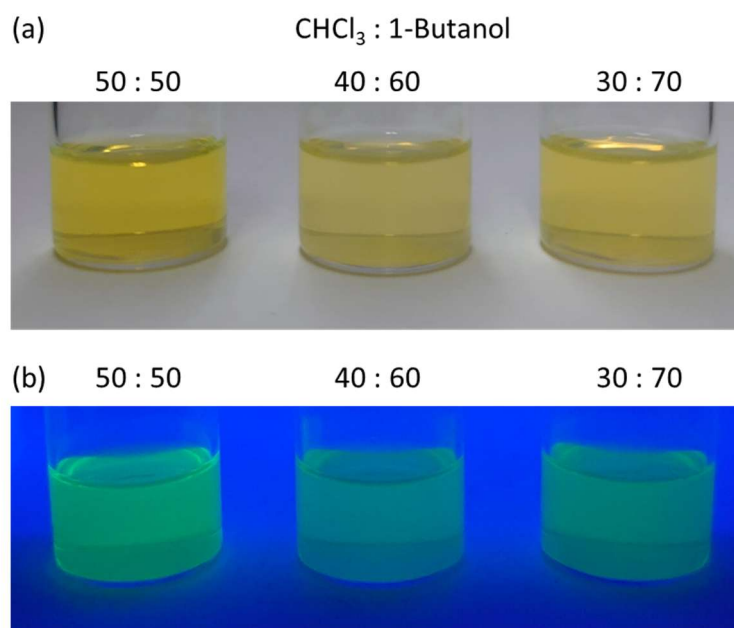


Figure S14. Photographs of **(R)-PFTPd** in the different solvent mixtures under natural light and under UV light (365 nm) illumination.

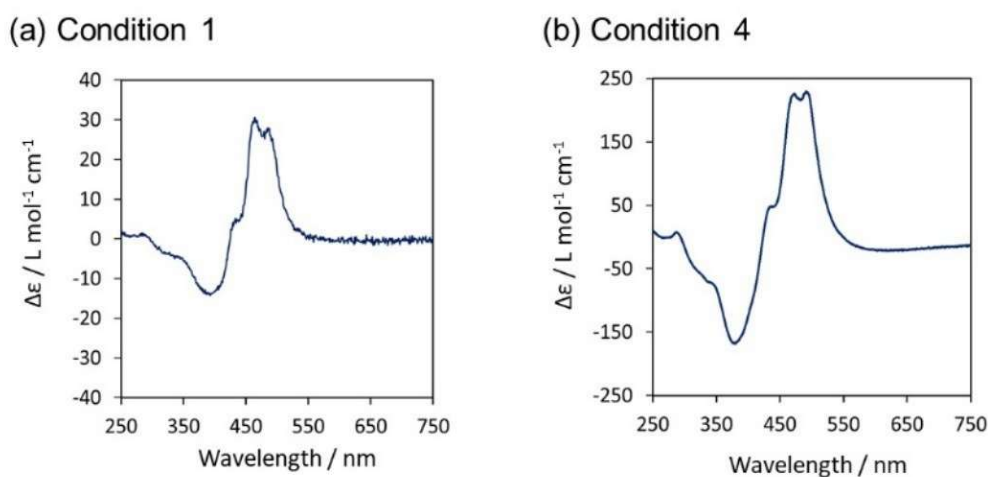


Figure S15. CD spectra of **(S)-PFTPd** aggregates prepared under different mixing conditions: (a) Condition 1 and (b) Condition 4. Figure (a) corresponds to the sample listed as Entry 2 in Table S1, while figure (b) corresponds to the sample listed as Entry 30 in Table S1. The spectra were recorded for samples of **(S)-PFTPd** in  $\text{CHCl}_3$ /1-butanol mixtures with a volume ratio of 40:60 ( $3.0 \times 10^{-5}$  M).

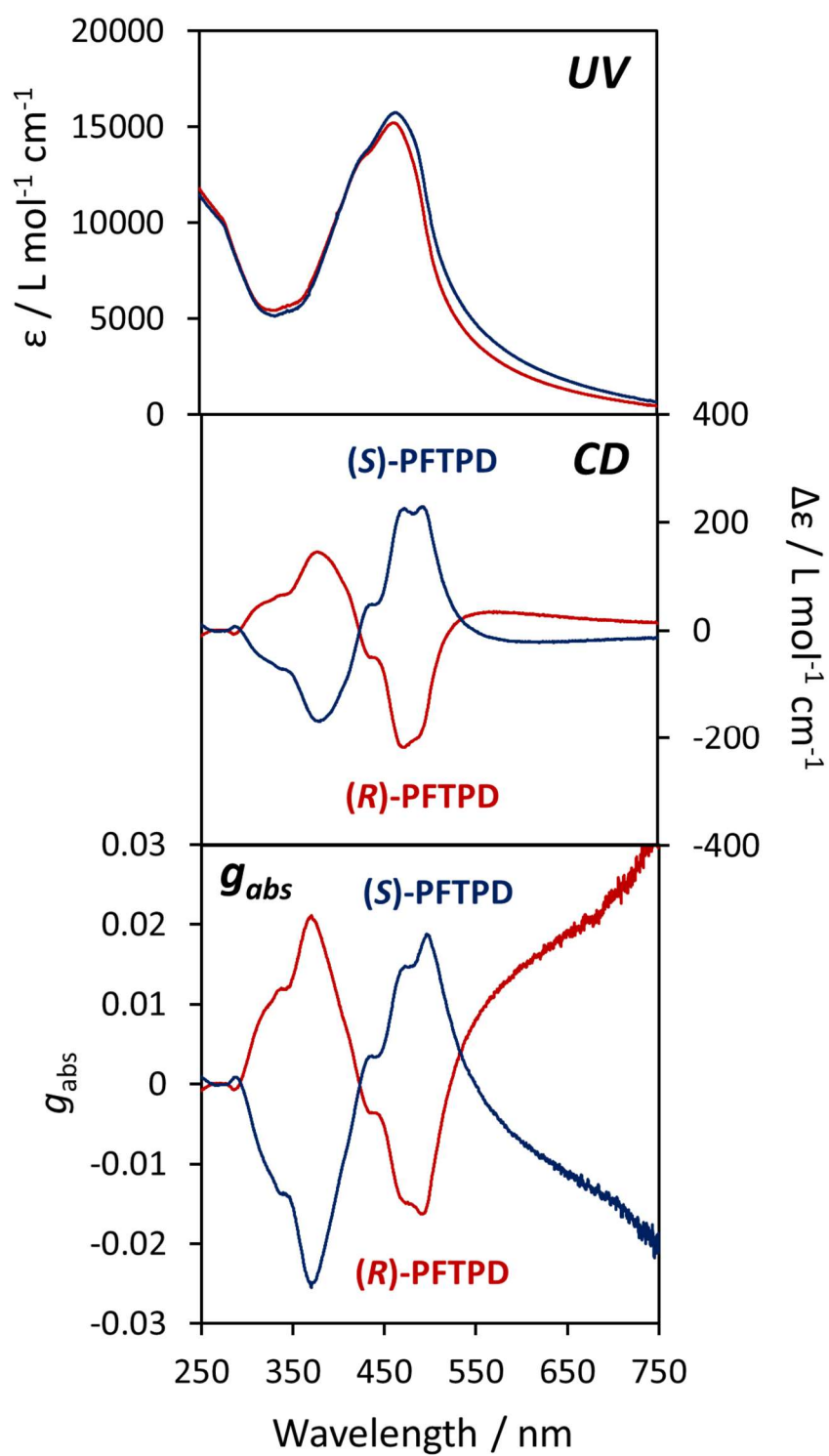


Figure S16. UV-Vis absorption spectra, CD spectra, and  $g_{\text{abs}}$  factors of (*R*)-PFTPD (red) and (*S*)-PFTPD (blue) recorded in  $\text{CHCl}_3$ /1-butanol mixtures with volume ratios of 40:60 ( $3.0 \times 10^{-5}$  M).

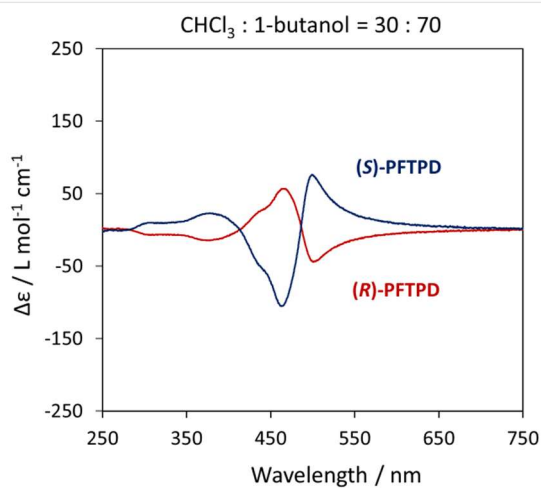
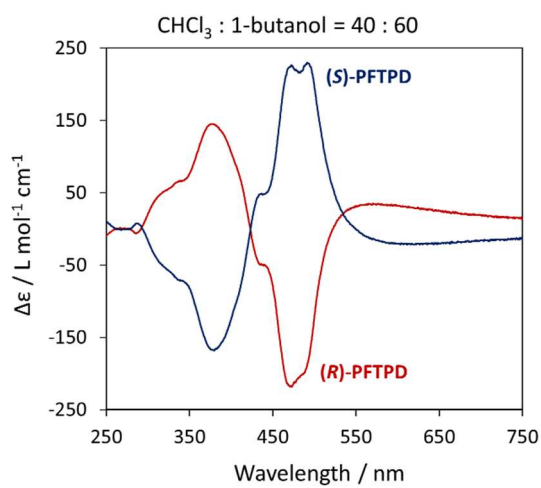
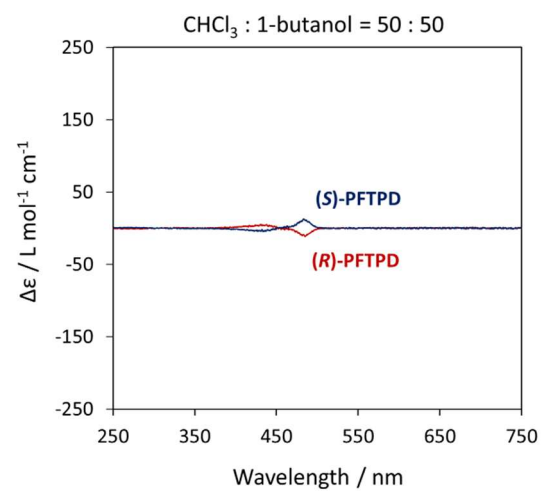


Figure S17. CD spectra of (*R*)-PFTPD (red) and (*S*)-PFTPD (blue) recorded in CHCl<sub>3</sub>/1-butanol mixtures with volume ratios of 50:50, 40:60, and 30:70 ( $3.0 \times 10^{-5}$  M).

Table S1. Original  $g_{\text{abs}}$  values corresponding to the preparation conditions. <sup>a</sup>

Entry	Condition	$R$ or $S$	$g_{\text{abs}}^f$
1	1 <sup>b</sup>	$S$	0.0000874
2		$S$	0.00266
3	2 <sup>c</sup>	$S$	0.00595
4		$S$	0.00231
5		$S$	0.0165
6		$S$	0.0128
7		$S$	0.00343
8		$R$	−0.00513
9		$R$	−0.00349
10	3 <sup>d</sup>	$S$	0.0186
11		$S$	0.0173
12		$S$	0.0127
13		$S$	0.0151
14		$S$	0.0277
15		$S$	0.0202
16		$S$	0.0234
17		$S$	0.0158
18		$S$	0.00935
19		$R$	−0.00540
20		$R$	−0.00770
21		$R$	−0.0188
22		$R$	−0.0152
23		$R$	−0.0127
24		$R$	−0.0100
25		$R$	−0.0118
26	4 <sup>e</sup>	$S$	0.0114
27		$S$	0.0116
28		$S$	0.0132
29		$S$	0.0142
30		$S$	0.0181
31		$R$	−0.0150
32		$R$	−0.0190
33		$R$	−0.0153
34		$R$	−0.0175



<sup>a</sup> 1-BuOH (6 mL) was added to a 75  $\mu$ M solution of (*R*)-PFTPD or (*S*)-PFTPD in CHCl<sub>3</sub> (4 mL). The conditions are shown in Table 2.

<sup>b</sup> 1-Butanol was slowly poured into the polymer solution in CHCl<sub>3</sub>, allowing the two solvents to diffuse gradually into each other.

<sup>c</sup> 1-Butanol was added all at once to the polymer solution in CHCl<sub>3</sub>, followed by manual shaking to promote immediate mixing.

<sup>d</sup> 1-Butanol was added dropwise to the polymer solution in CHCl<sub>3</sub> under stirring.

<sup>e</sup> 1-Butanol was added dropwise to the polymer solution in CHCl<sub>3</sub> under stirring (450 rpm).

<sup>f</sup>  $g_{\text{abs}}$  values at the peak wavelengths around 480 nm.

Table S2. Representative  $g_{\text{abs}}$  values of (*R*)-PFTPD. <sup>a</sup>

Solvent ratio CHCl <sub>3</sub> : 1-butanol	$g_{\text{abs}}$	Wavelength
100 : 0	$\sim 0$	-
50 : 50	$-4.2 \times 10^{-4}$	485
40 : 60	$-1.6 \times 10^{-2}$	491
30 : 70	$-6.8 \times 10^{-3}$	513

<sup>a</sup>  $g_{\text{abs}}$  values calculated from the data shown in Figures 3 and S11.

Table S3. Original  $g_{\text{lum}}$  values. <sup>a</sup>

<i>R</i> or <i>S</i>	$g_{\text{lum}}$
<i>S</i>	0.0239
<i>S</i>	0.0190
<i>S</i>	0.0127
<i>R</i>	-0.0256
<i>R</i>	-0.0168
<i>R</i>	-0.0158

<sup>a</sup>  $g_{\text{lum}}$  values (*R*)-PFTPD and (*S*)-PFTPD recorded in CHCl<sub>3</sub>/1-butanol mixtures with volume ratios of 40:60 ( $3 \times 10^{-5}$  M,  $\lambda_{\text{ex}} = 400$  nm).