Electronic Supplementary Information

Unravelling the origin of strong non-reciprocal chiroptical features in thin films of a chiral diketo-pyrrolo[3,4-*c*]pyrrole dye

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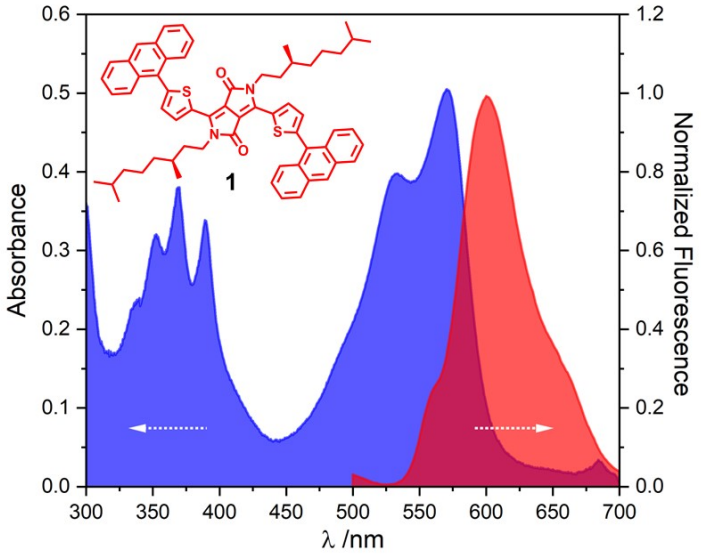


Figure S1.

Absorbance (blue line) and photoluminescence (red line) spectra of chiral DPP dye **1** in $CHCl_3$ solution. For absorbance measurements: cell length 1 cm; sample concentration 10^{-5} M. For photoluminescence measurements: sample concentration 10^{-6} M, excitation wavelength 365 nm.

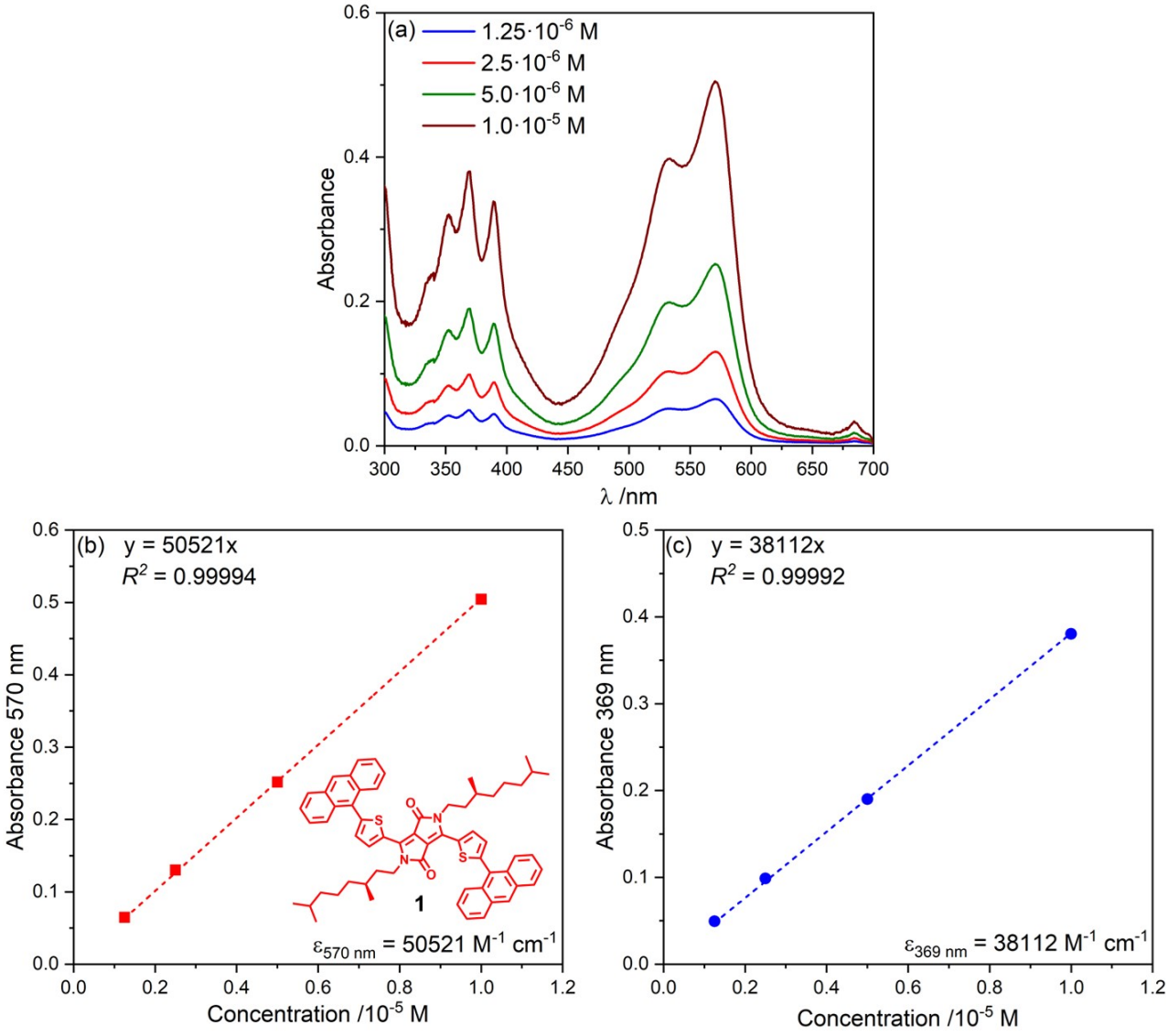


Figure S2.

Determination of molar extinction coefficients ε of chiral DPP dye **1** in $CHCl_3$ solution: (a) UV-Vis absorbance spectra at different concentrations (from $1.25 \cdot 10^{-6}$ M to $1.0 \cdot 10^{-5}$ M); (b) absorbance at 570 nm *vs.* concentration plot; (c) absorbance at 369 nm *vs.* concentration plot.

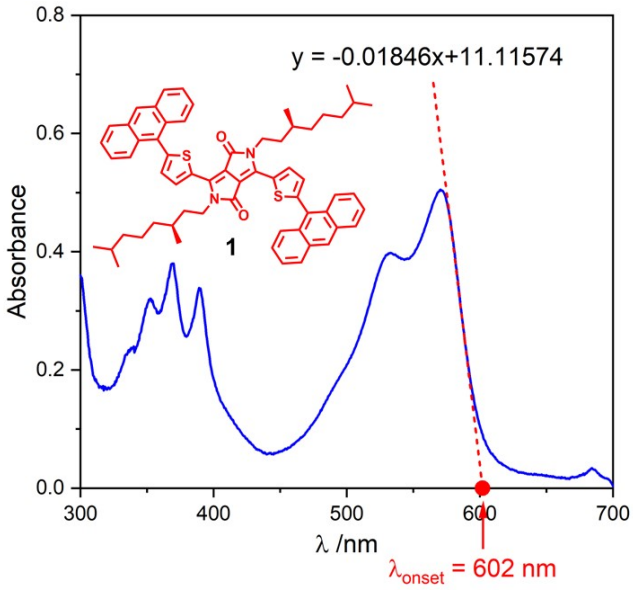


Figure S3.

Determination of UV-Vis absorption onset λ_{onset} of chiral DPP dye **1** in $CHCl_3$ solution, from the intercept of the red-side slope of the absorbance main band with the wavelength axis.

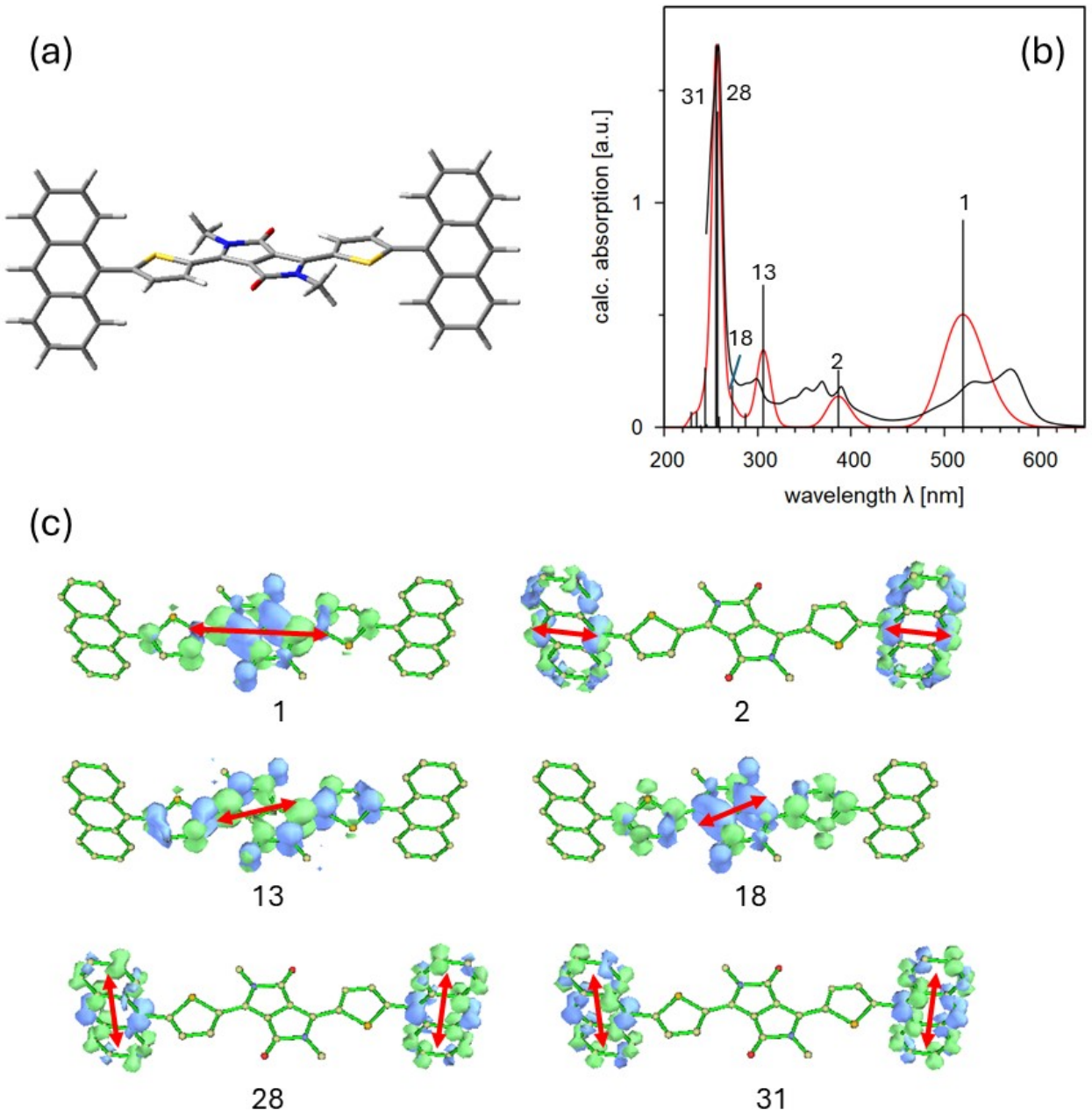


Figure S4.

(a) B3LYP-D3BJ/6-31+G(d,p) optimized structure of model **1'**. (b) CAM-B3LYP/def2-TZVP calculated UV-vis spectrum of **1'** (red trace) compared with the experimental solution spectrum of **1**. Vertical bars show oscillator strengths, while the numbers label the main transitions. Plotting parameters: σ= 0.16 eV, wavelength shift 20 nm. (c) Hole (blue)/electron (green) surfaces plotted for the main transitions of **1'**; isovalue 0.002. Red double arrows depict the orientation of electric transition dipole moments.

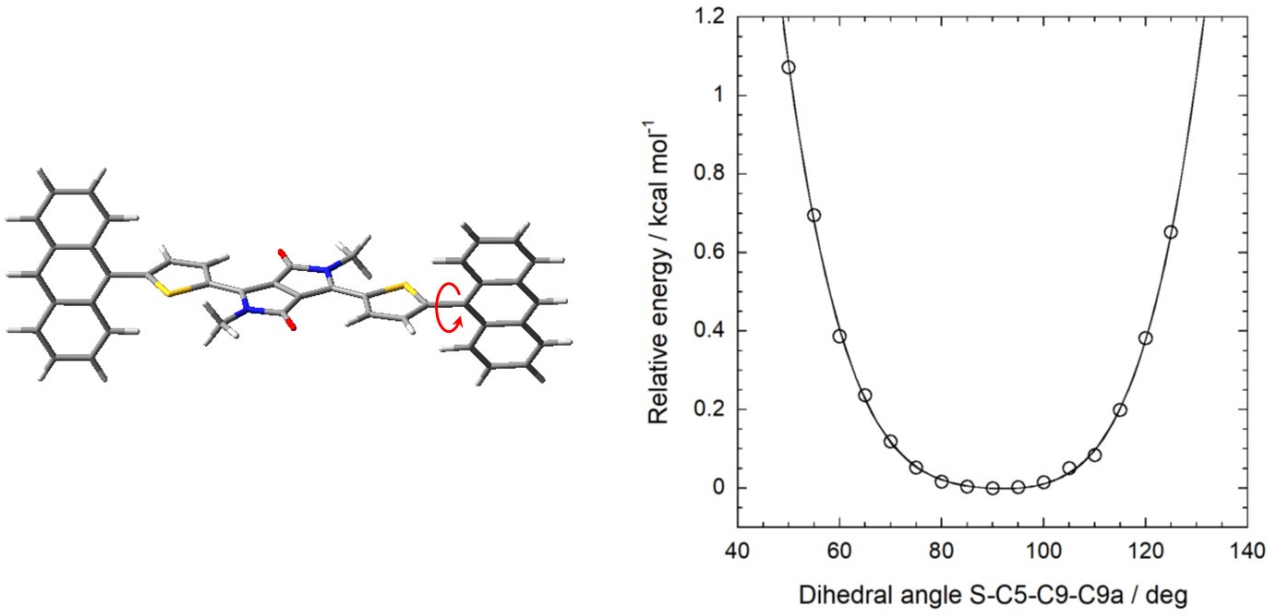


Figure S5.

Relaxed torsional energy scan run at B3LYP-D3BJ/6-31+G(d,p) level for the marked dihedral angle of model **1'**.

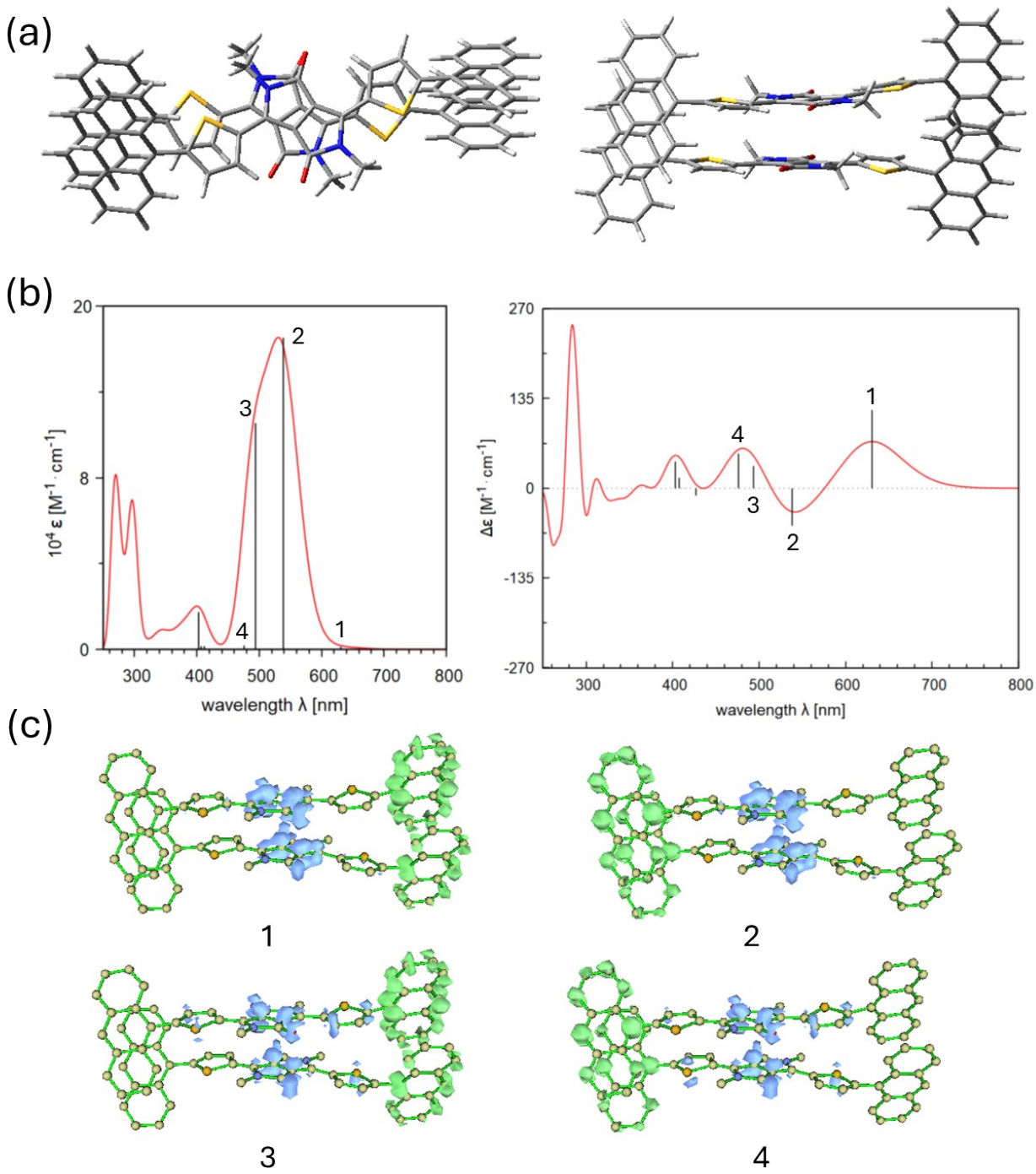


Figure S6.

(a) B3LYP-D3BJ/6-31G(d) optimized structure of dimer B, two views. (b) CAM-B3LYP/def2-TZVP calculated UV-vis and ECD spectra of dimer B. Vertical bars show oscillator and rotational strengths for the first 8 transitions, while the numbers label the first 4 transitions. Plotting parameters: σ = 0.16 eV. (c) Hole (blue)/electron (green) surfaces plotted for the first 4 transitions of dimer B; isovalue 0.002.

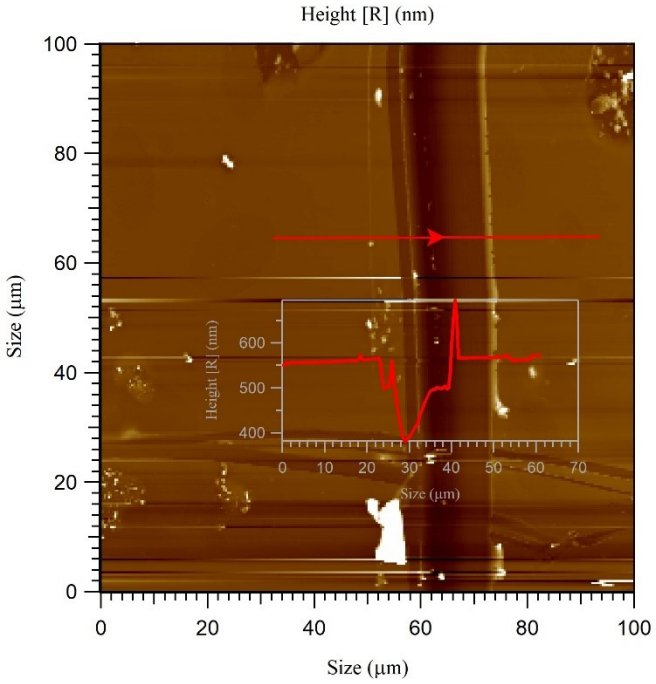


Figure S7.

AFM profilometry of a section perpendicular to a steel scalpel scratch for a thin film of chiral DPP dye **1** prepared by spin coating technique, used for the evaluation of thickness (about 40 nm).

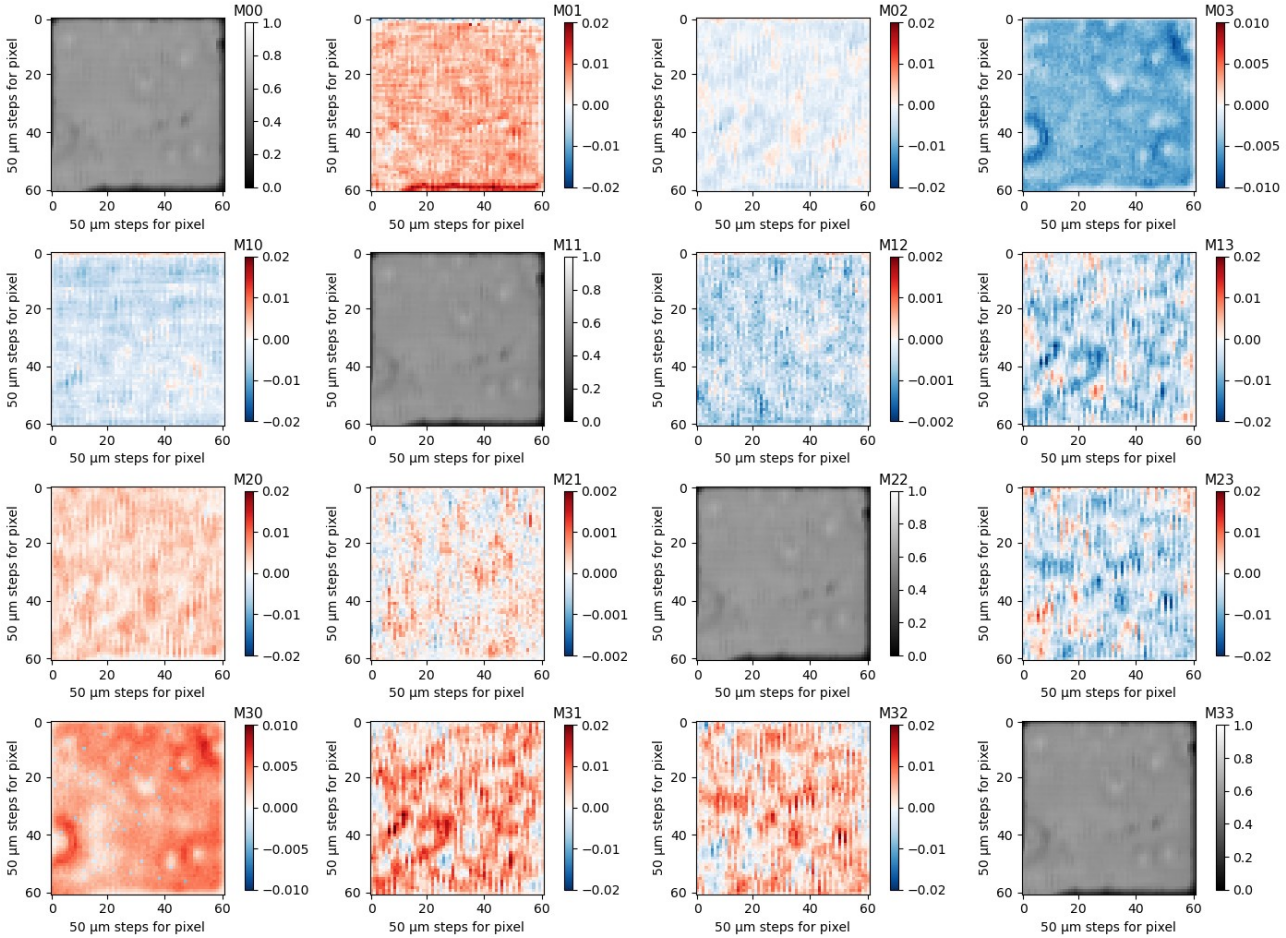


Figure S8.

SR-MMP*i* investigation for a thin film of chiral DPP dye **1** prepared by spin coating technique: 2D maps of the 16 Mueller matrix elements M_{ij} *vs.* x–y coordinate, scanned at 291 nm for the front face of the sample on a 60×60 grid array area at 50 µm steps with a beam-light diameter of 50 µm.

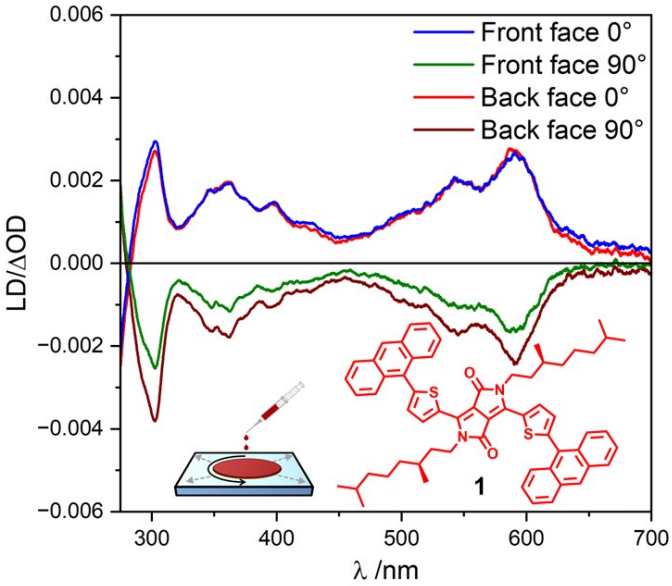
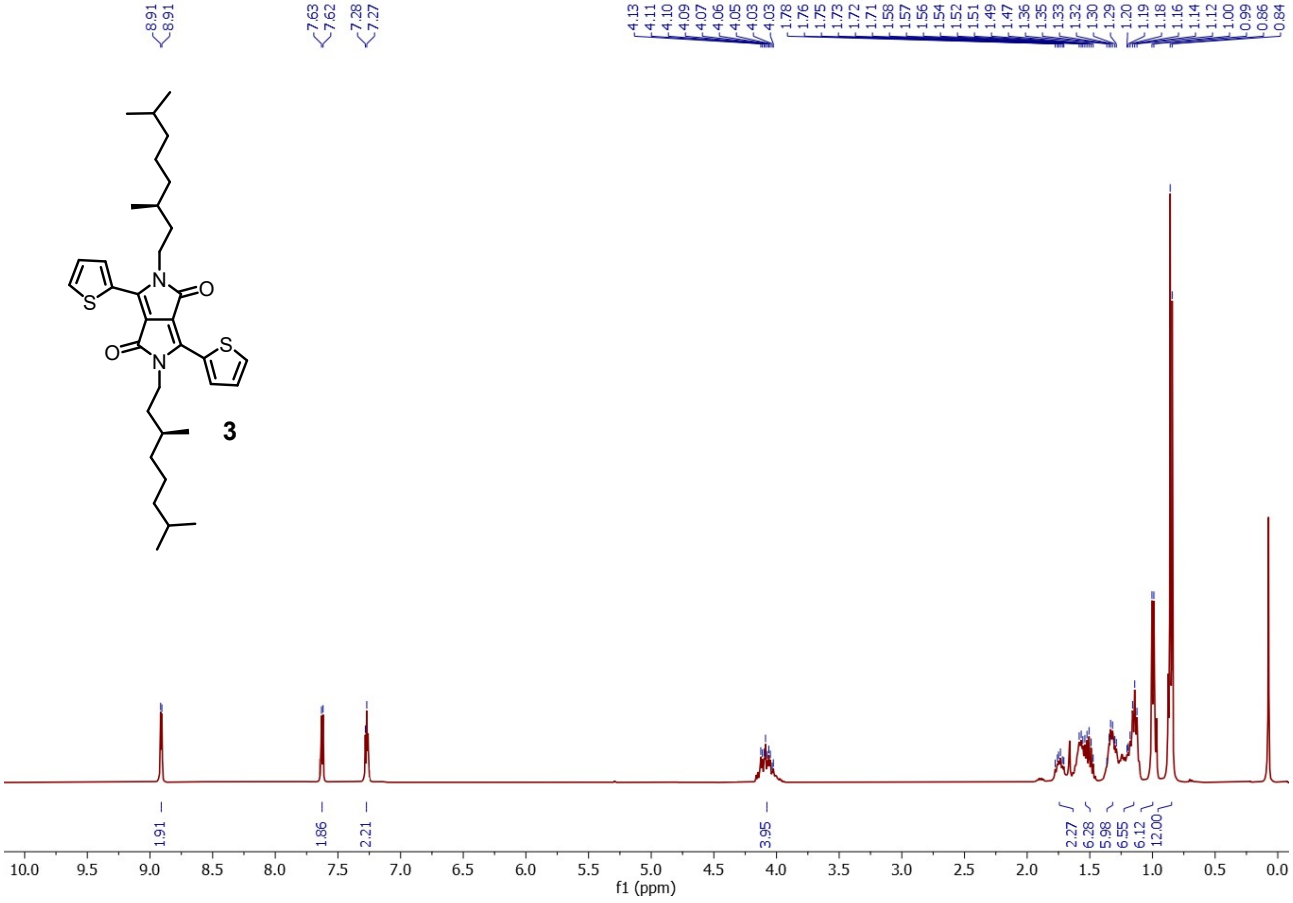


Figure S9.

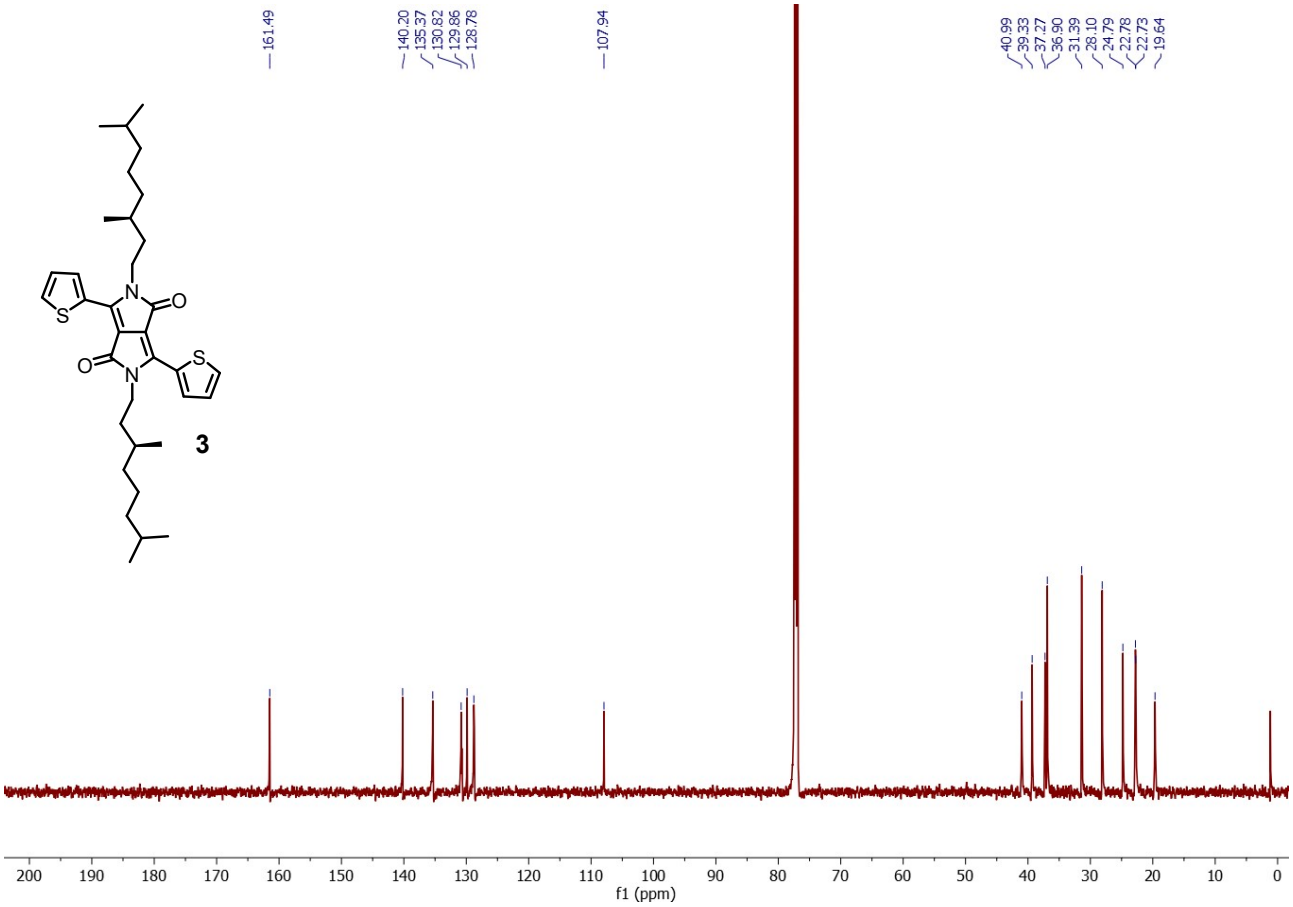
Linear dichroism (LD) spectra for thin films of chiral DPP dye **1** prepared by spin coating technique, recorded for the front face (blue line) and the back face (red line) at two different rotation angles (0° and 90°) around the optical axis.

^{1}H-NMR and ^{13}C-NMR spectra

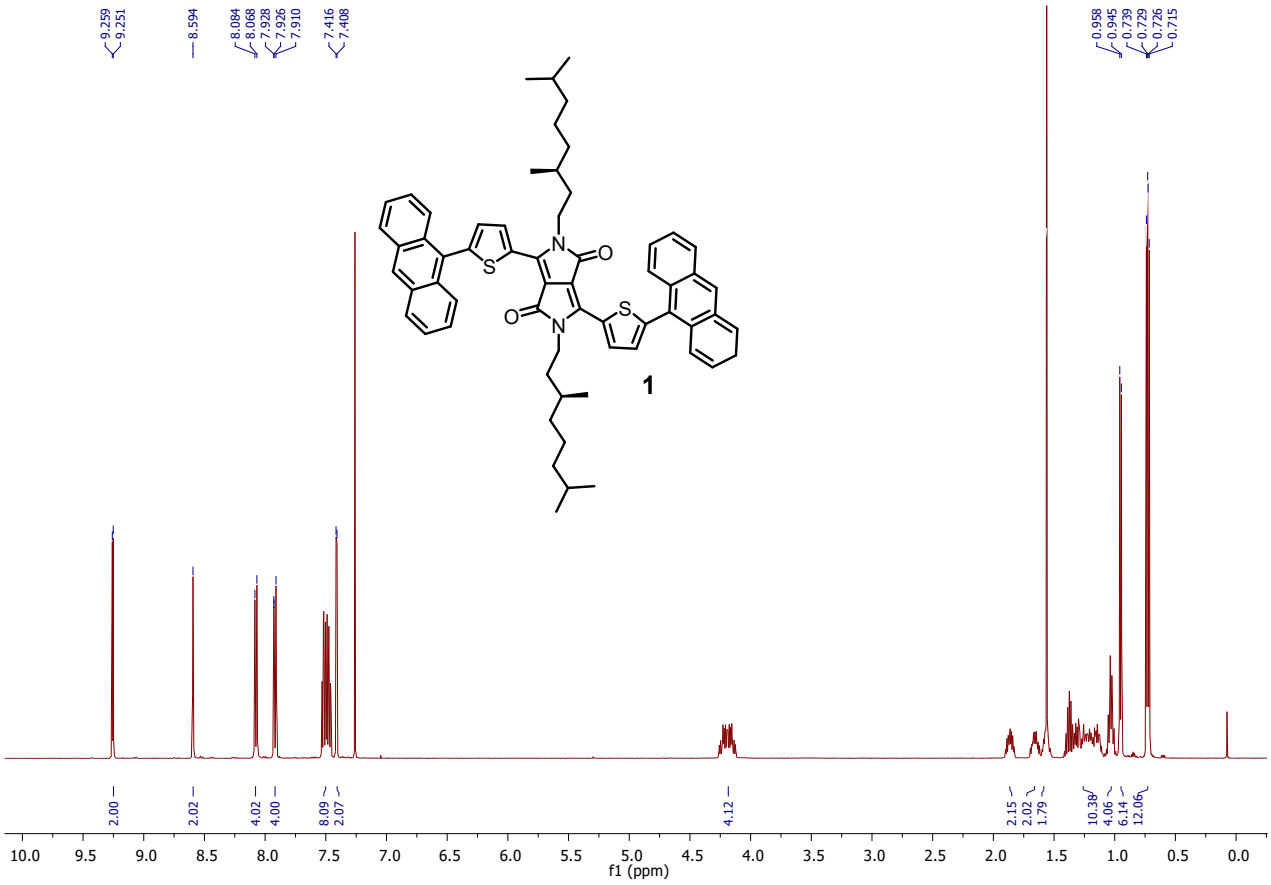
2,5-Bis((*S*)-3,7-dimethyloctyl)-3,6-di(thiophen-2-yl)pyrrolo[3,4-*c*]pyrrole-1,4(2*H*,5*H*)-dione (3): ^{1}H-NMR (500 MHz, $CDCl_3$)



2,5-Bis((*S*)-3,7-dimethyloctyl)-3,6-di(thiophen-2-yl)pyrrolo[3,4-*c*]pyrrole-1,4(2*H*,5*H*)-dione (3): ^{13}C-NMR (125 MHz, $CDCl_3$)



3,6-Bis(5-(anthracen-9-yl)thiophen-2-yl)-2,5-bis((*S*)-3,7-dimethyloctyl)-2,5-dihydropyrrolo[3,4-*c*]pyrrole-1,4-dione (1): ^{1}H-NMR (500 MHz, $CDCl_3$)



3,6-Bis(5-(anthracen-9-yl)thiophen-2-yl)-2,5-bis((*S*)-3,7-dimethyloctyl)-2,5-dihydropyrrolo[3,4-*c*]pyrrole-1,4-dione (1): ^{13}C-NMR (125 MHz, $CDCl_3$)