

Supplementary Materials (SM) for

Questions of mirror symmetry at the photoexcited and ground states of non-rigid luminophores raised by circularly polarized luminescence and circular dichroism spectroscopy. Part 1. Oligofluorenes, oligophenlenes, binaphthyls, and fused aromatics

Michiya Fujiki ^{1,*}, Julian R. Koe ^{2,*}, Takashi Mori ¹ and Yoshihiro Kimura ¹

¹ Division of Materials Science, Graduate School of Science and Technology, Nara Institute of Science and Technology (NAIST), 8916-5 Takayama, Ikoma, Nara 630-0036, Japan; mori@tri-osaka.jp (T.M.); yoshi19791024uk@gmail.com (Y.K.)

² Department of Natural Sciences, International Christian University (ICU), 3-10-2 Mitaka, Tokyo, 181-8585, Japan

* Correspondence: fujikim@ms.naist.jp (M.F.); koe@icu.ac.jp (J.R.K.); Tel.: +81-743-72-6040 (M.F.); +81-422-33-3249 (J.R.K.)

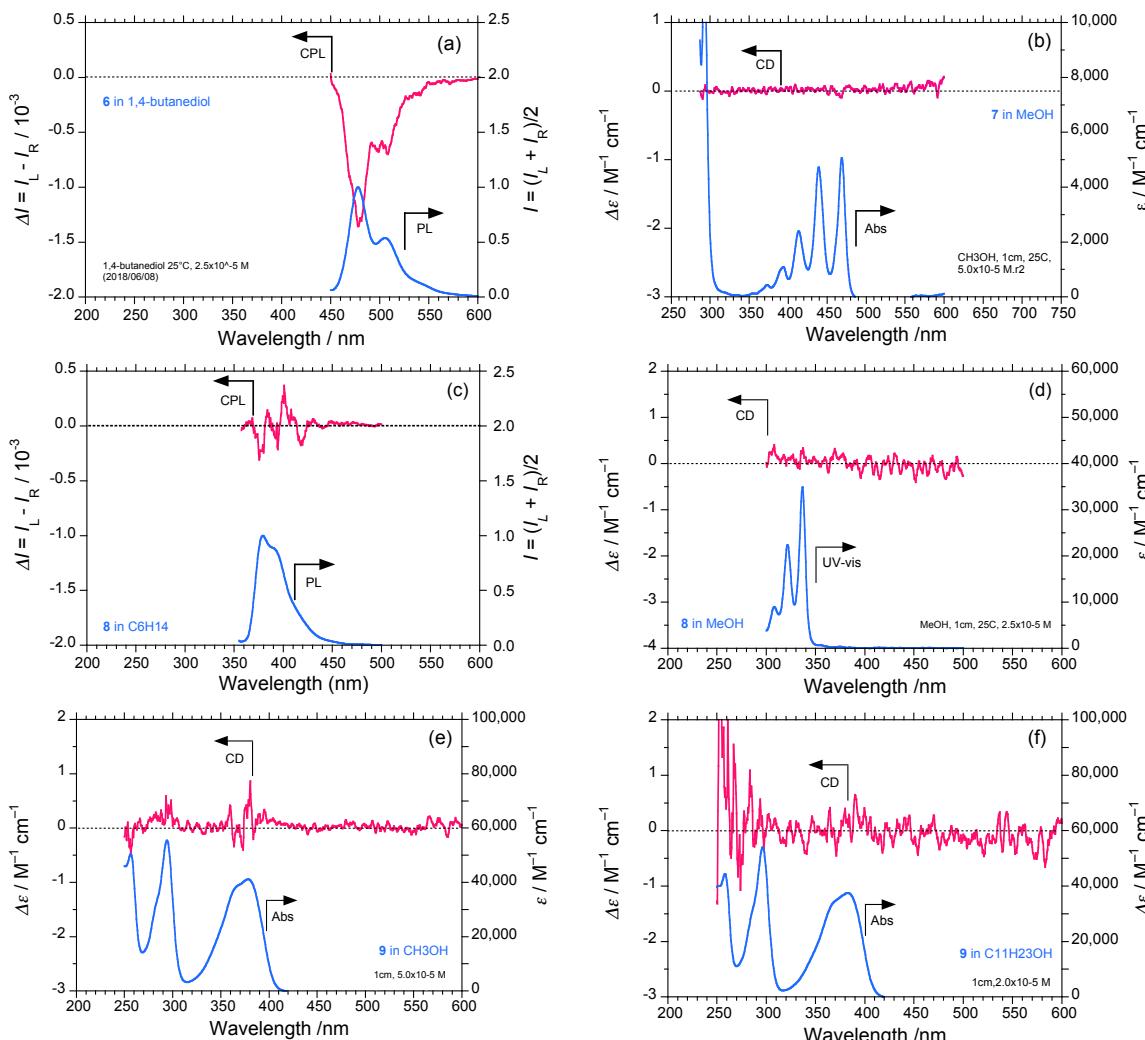


Figure S1. CPL/PL and CD/UV-vis spectral characteristics of pseudo- D_{2h} -symmetrical fused aromatics carrying multiple rotatable substituents in various liquids at room temperature. (a) CPL/PL spectra of **6** excited at 320 nm in 1,4-butanediol. (b) CD/UV-vis spectra of **7** in methanol. (c) CPL/PL spectra of **8** excited at 325 nm in *n*-hexane. (d) CD/UV-vis spectra of **8** in methanol. CD/UV-vis spectra of **9** in (e) methanol and (f) *n*-undecanol. Measurement conditions: path length: 10 mm, cylindrical cuvette, conc.: $(2.5\text{--}5.0) \times 10^{-5}$ M at room temperature.

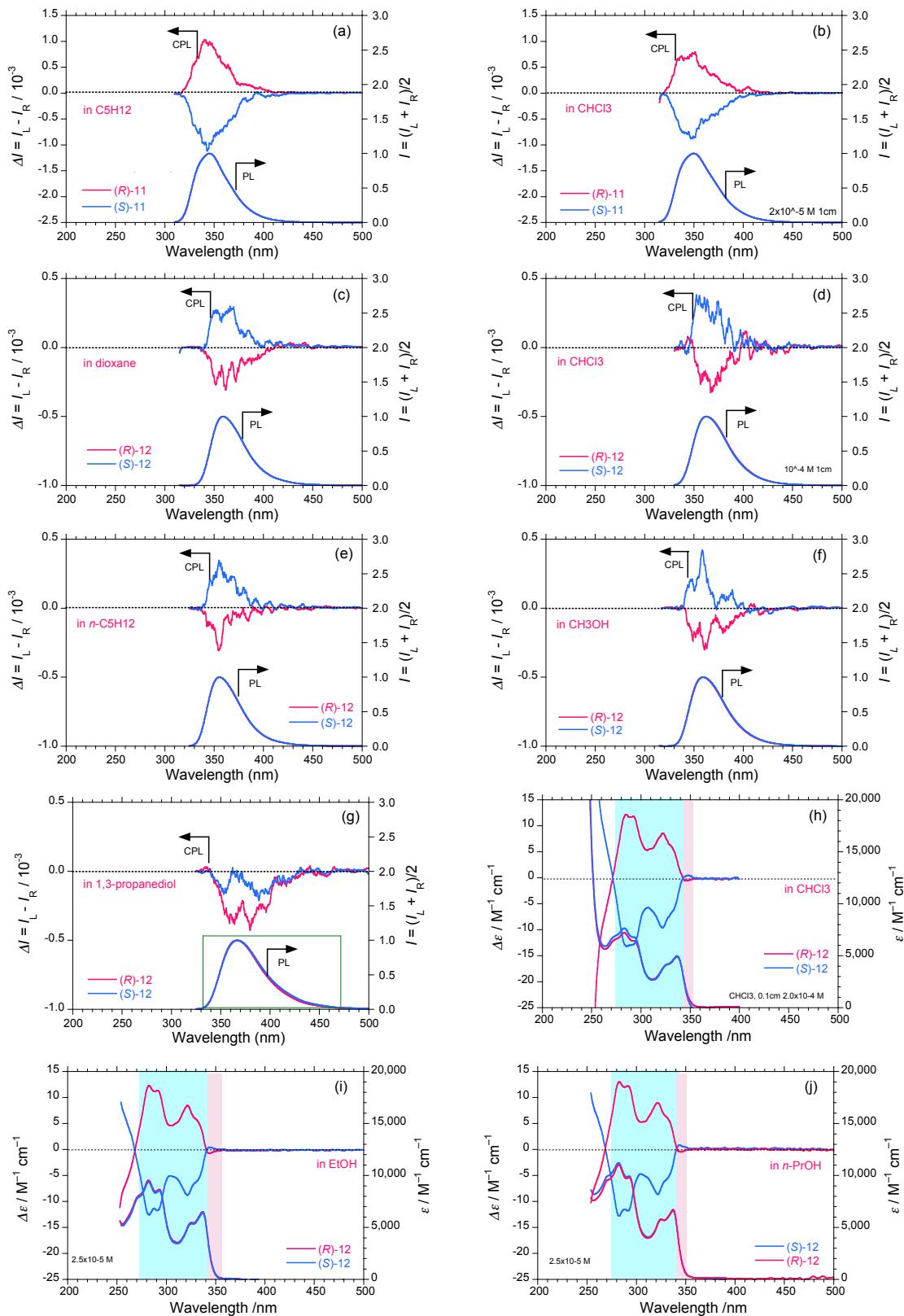


Figure S2. CD/UV-vis and CPL/PL spectra of rigid binaphthol derivatives and semirigid binaphthol derivatives allowing pivotal motion in various solvents at room temperature (path length: 10 mm, cylindrical cuvette, conc.: (2–5) × 10⁻⁴ M; CPL/PL spectra of **R**-11 and **S**-11 excited at 290 nm (a) in *n*-pentane and (b) in chloroform; CPL/PL spectra of **R**-12 and **S**-12 excited at 295 nm (c) in *p*-dioxane, (d) in chloroform, (e) in *n*-pentane, (f) in methanol, and (g) in 1,3-propanediol; CD/UV-vis spectra of **R**-12 and **S**-12 (h) in chloroform, (i) in ethanol, and (j) in *n*-propanol.

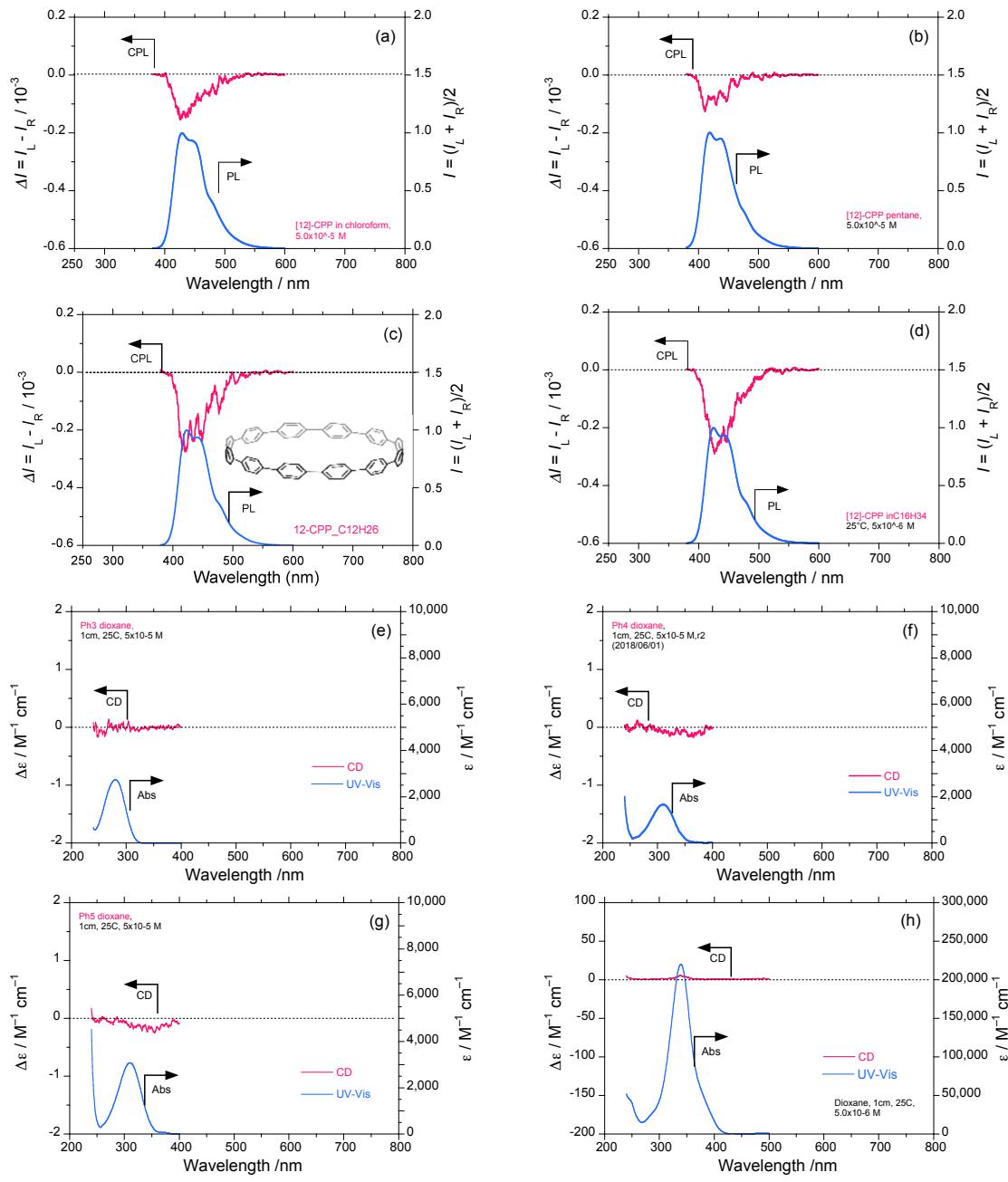


Figure S3. CPL/PL and CD/UV-Vis spectra of unsubstituted linear and cyclic oligo-*p*-phenyls in several solvents at room temperature (path length: 10 mm, cylindrical cuvette, conc.: $(0.5\text{--}5) \times 10^{-5}$ M). CPL/PL spectra of **12-CPP** excited at 350 nm (a) in chloroform, (b) in *n*-pentane, (c) in *n*-dodecane, and (d) in *n*-hexadecane; CD/UV-Vis spectra of (e) **Ph3**, (f) **Ph4**, (g) **Ph5**, and (h) **12-CPP** in *p*-dioxane.

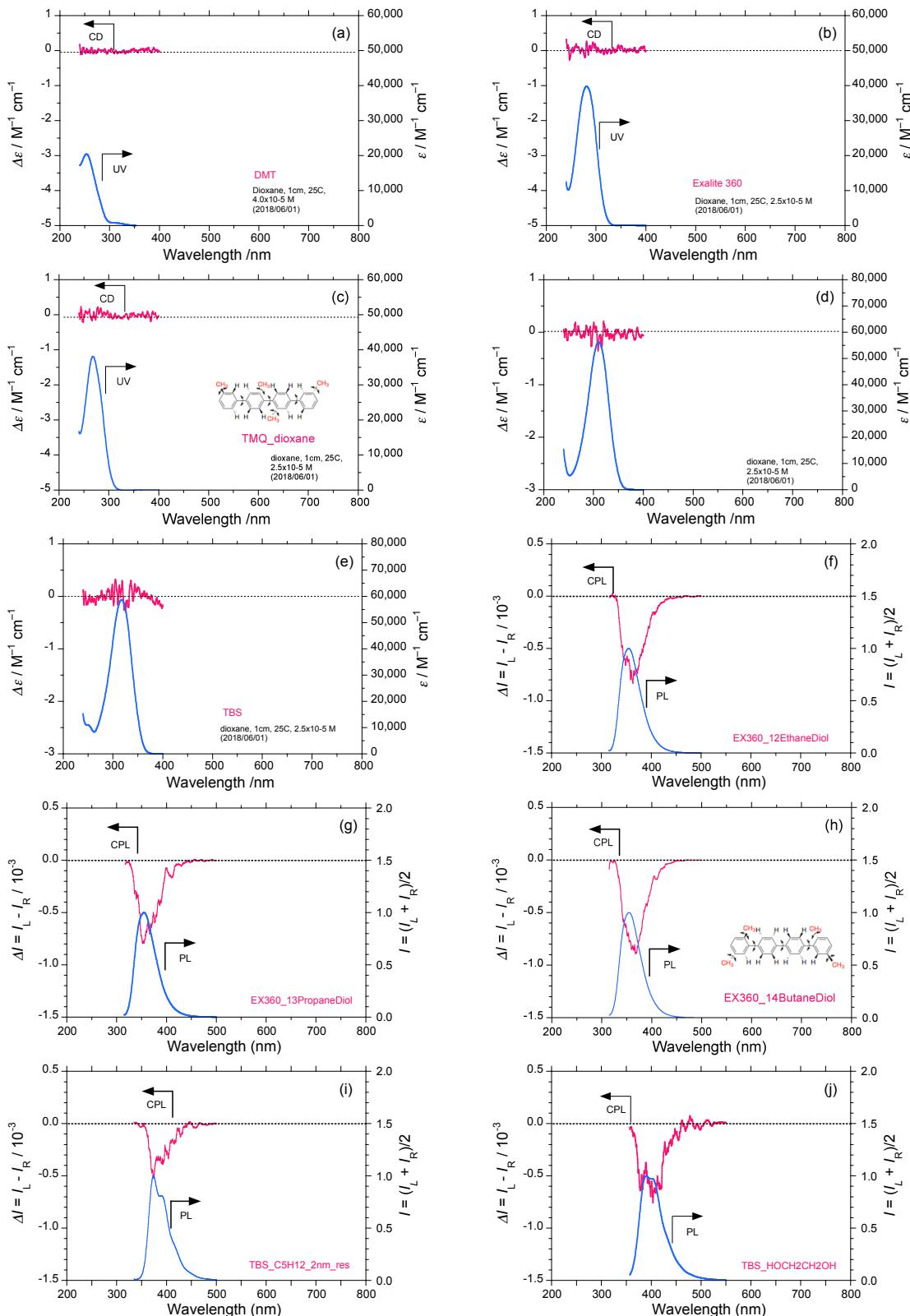


Figure S4. CD/UV-vis spectra of (a) DMT, (b) Exalite360, (c) TMQ, (d) QUI, and (e) TBS in *p*-dioxane. CPL/PL spectra of DMT excited at 315 nm. CPL/PL spectra of linear oligo-*p*-phenyls carrying methyl and *t*-butyl groups in *p*-dioxane and other solvents at room temperature; CPL/PL spectra of Exalite360 excited at 280 nm (f) in ethylene glycol, (g) in 1,3-propane diol, and (h) in 1,4-butane diol; CPL/PL spectra of Exalite360 excited at 280 nm (f) in ethylene glycol, (g) in 1,3-propane diol, and (h) in 1,4-butane diol; CPL/PL spectra of TBS excited at 315 nm (i) in *n*-pentane and (j) in ethylene glycol.

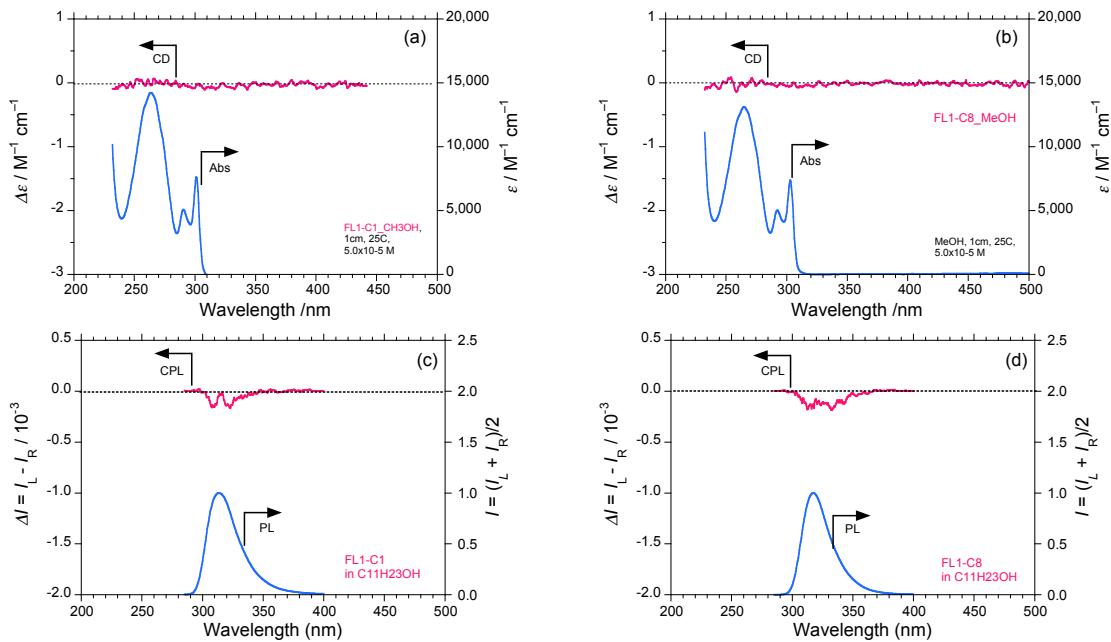


Figure S5. CD/UV-Vis spectra of (a) FL1-C₁ and (b) FL1-C₈ in methanol. CPL/PL spectra of (c) FL1-C₁ excited at 255 nm and (d) FL1-C₈ excited at 255 nm at room temperature in *n*-undecanol. Path length: 10 mm, cylindrical cuvette, conc.: 5 × 10⁻⁵ M.

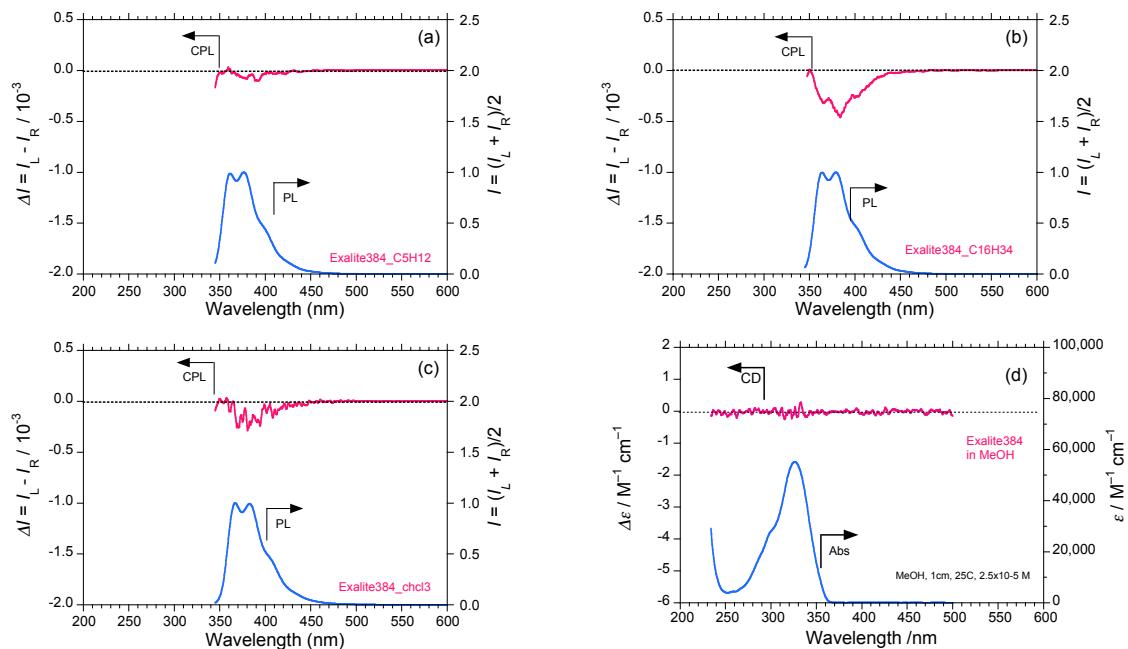


Figure S6. CPL/PL spectra of FL2-C₃ (Exalite 384, fluorene dimer) excited at 315 nm at room temperature (a) in *n*-pentane, (b) in *n*-hexadecane, and (c) in chloroform. (d) CD/UV-vis spectrum of FL2-C₃ (Exalite 384) in methanol. Path length: 10 mm, cylindrical cuvette, conc.: 1 × 10⁻⁵ M.

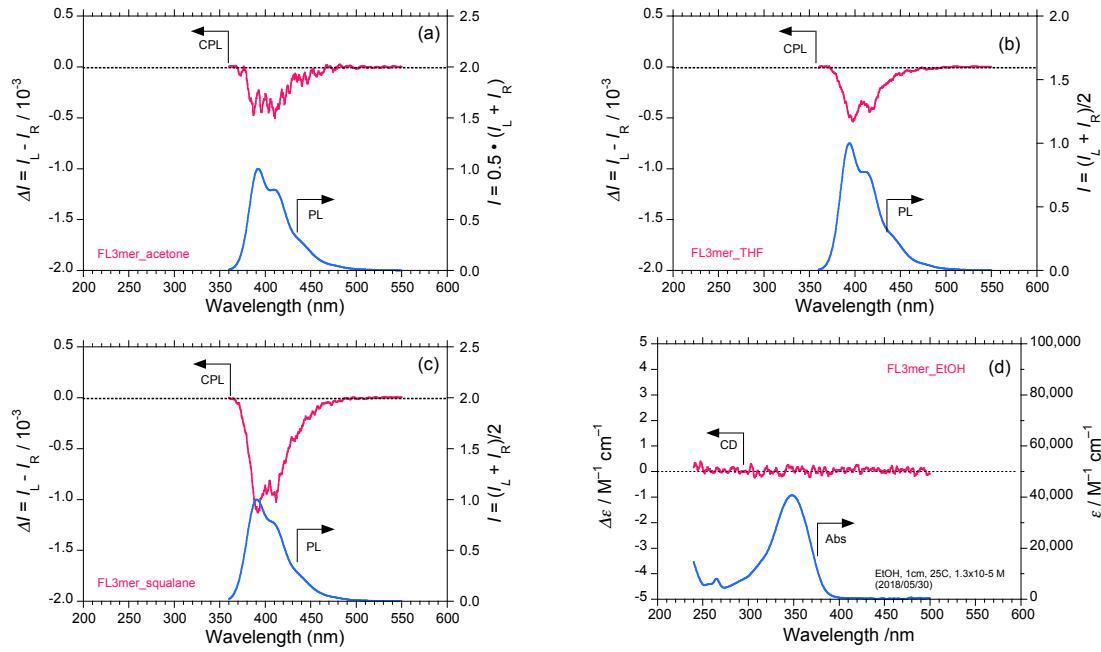


Figure S7. CPL/PL spectra of **FL3-C₆** (fluorene trimer) excited at 330 nm at room temperature (a) in acetone, (b) in tetrahydrofuran, and (c) in squalane; (d) CD/UV-vis spectrum of **FL3-C₆** in ethanol at room temperature. Path length: 10 mm, cylindrical cuvette, conc.: (1.3–2.0) × 10⁻⁵ M.

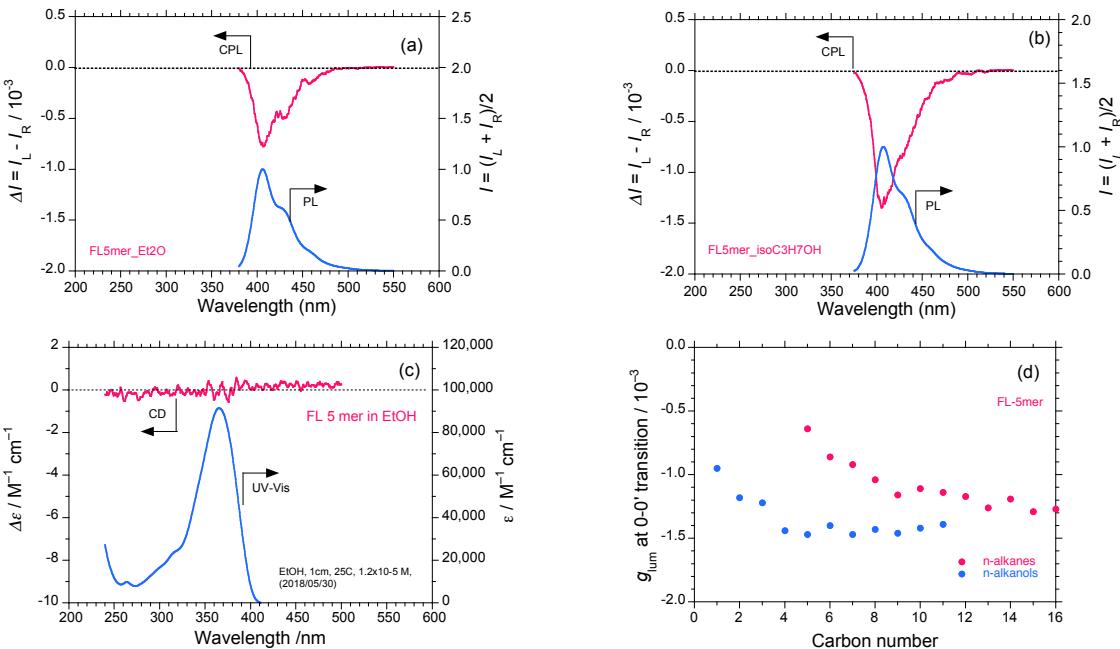


Figure S8 CPL/PL spectra of **FL5-C₆** (fluorene pentamer) excited at 340 nm at room temperature (a) in diethylether and (b) in isopropanol; (c) CD/UV-vis spectrum of **FL5-C₆** in ethanol at room temperature; (d) the g_{lum} value at 0-0' band of **FL5-C₆** as a function of carbon numbers in two series of *n*-alkanes and *n*-alkanol including methanol and ethanol. Path length: 10 mm, cylindrical cuvette, conc.: 5 × 10⁻⁶ M.

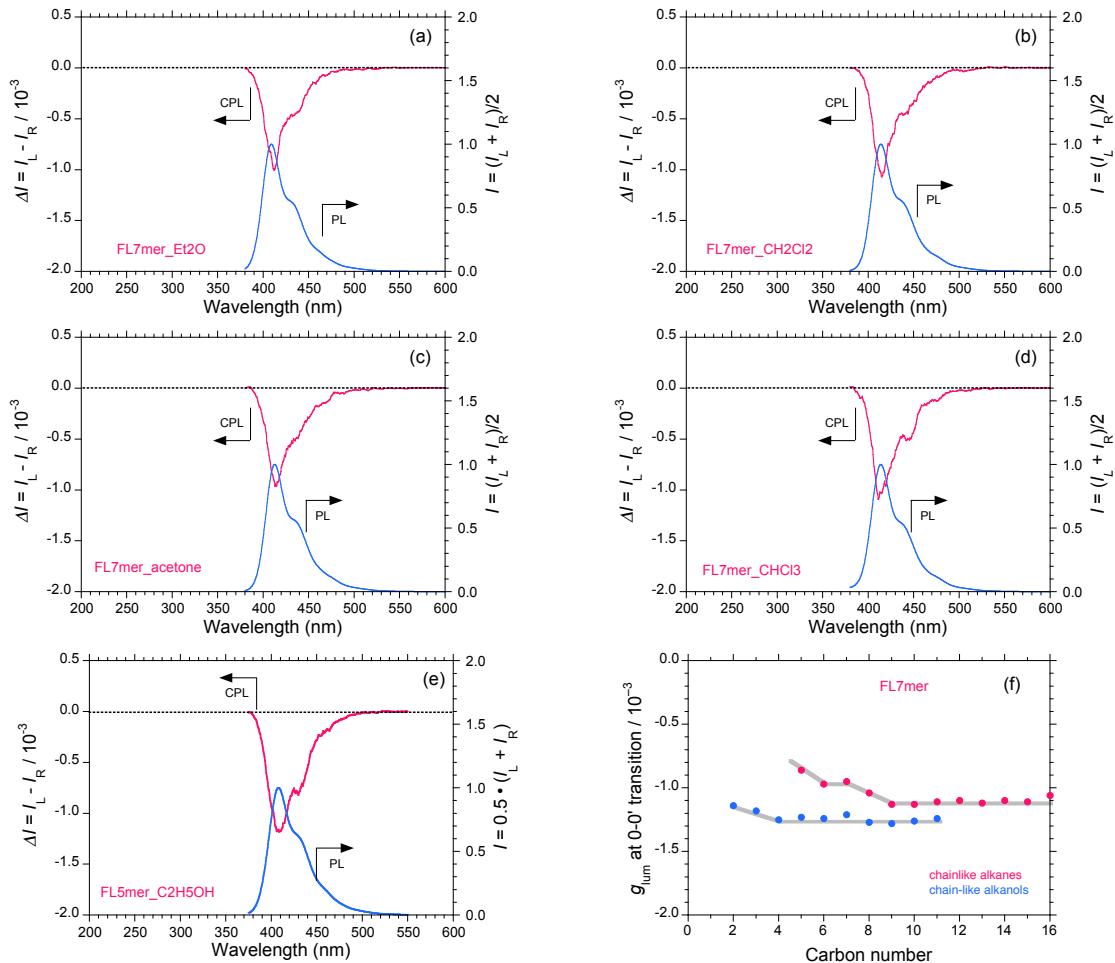


Figure S9. CPL/PL spectra of FL7-C₆ (fluorene heptamer) excited at 350 nm at room temperature (a) in diethylether, (b) in dichloromethane, (c) in acetone, and (d) in chloroform. (e) CD/UV-vis spectra of FL7-C₆ in ethanol at room temperature. (f) The g_{lum} value at 0-0' band of FL7-C₆ as a function of carbon numbers in two series of *n*-alkanes and *n*-alkanol including ethanol. Path length: 10 mm, cylindrical cuvette, conc.: 5×10^{-6} M.

Fig.1 アントラセン

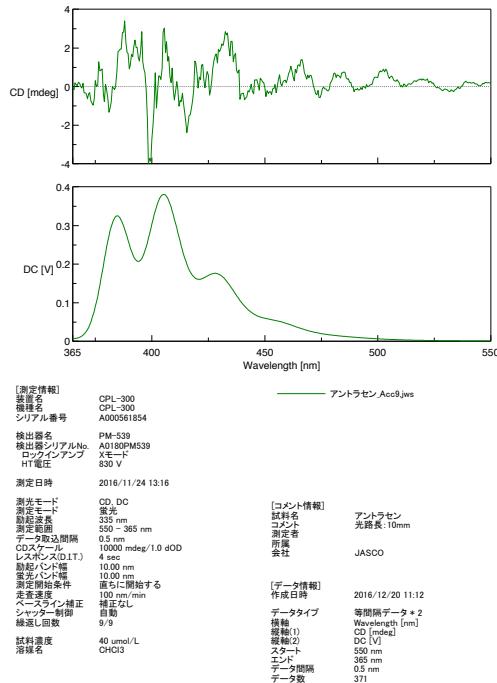


Fig.2 R- 及び S-Binaphthyl

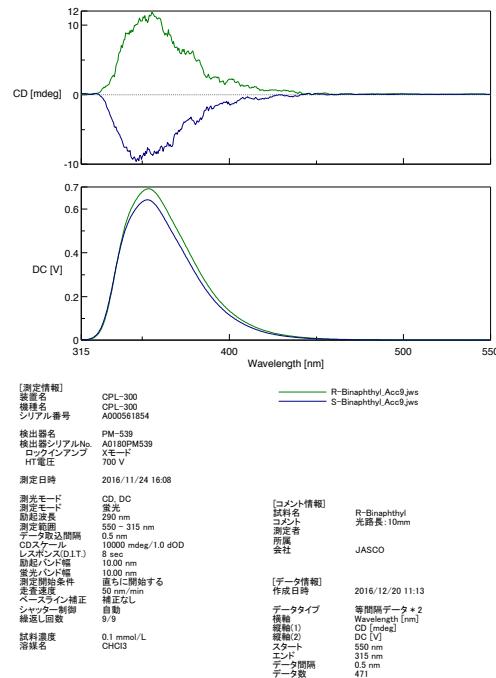


Fig.3 Exalite428

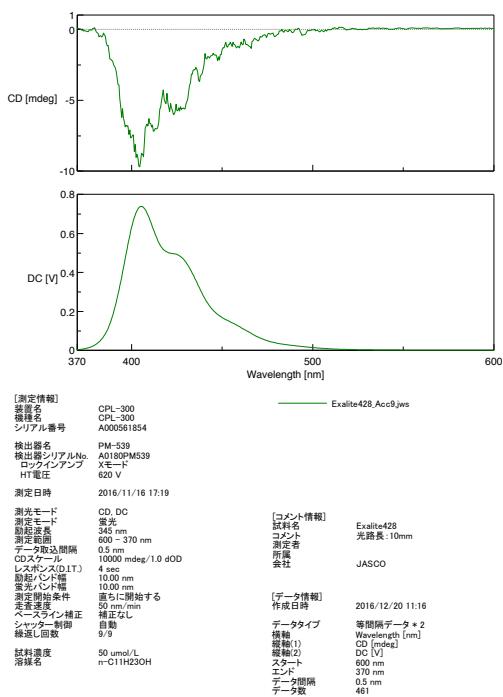


Figure S10. Raw CPL/PL spectra of **2** in chloroform, **R-11** and **S-11** in chloroform, and **Exalite 428** in *n*-undecanol at ambient temperature that were obtained independently by JASCO company using CPL-300 spectrofluoropolarimeter that is a newly designed model based on our CPL-200 spectrofluoropolarimeter (measured on 16 Nov 2018 and 24 Nov 2018).