0Electronic Supporting Information for

Circularly polarised luminescence from planar-chiral Phanephos/Tb(III)(hfa)₃ hybrid luminophores

Ayano Taniguchi,[a] Nobuyuki Hara,[a] Motohiro Shizuma,[b] Nobuo Tajima,[c] Michiya Fujiki[d] and Yoshitane Imai[a]*

[a] Department of Applied Chemistry, Faculty of Science and Engineering, Kindai University, 3-4-1 Kowakae, Higashi-Osaka, Osaka 577-8502, Japan.; E-mail: (Y.I.) y-imai@apch.kindai.ac.jp.
[b] Department of Biochemistry, Osaka Research Institute of Industrial Science and Technology, 1-6-50 Morinomiya, Joto-ku, Osaka 536-8553, Japan.
[c] Computational Materials Science Center, National Institute for Materials Science 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan.
[d] Graduate School of Materials Science, Nara Institute of Science and Technology, Takayama, Ikoma, Nara 630-0192, Japan.
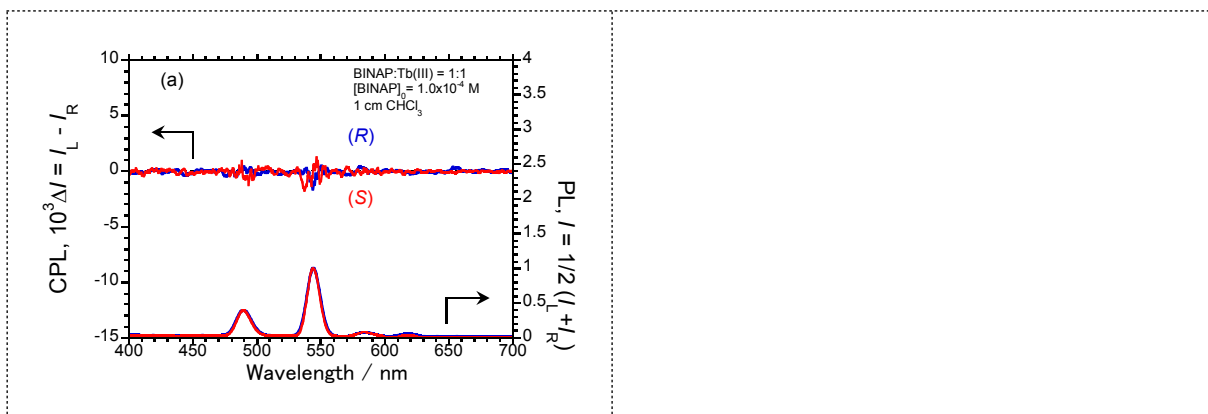
Table of Contents

Fig. S1. CPL and PL spectra of (*R*)- and (*S*)-BIANP : Tb(hfa)$_3$ = 1 to 1 molar ratio in EtOH-free chloroform. Path length 1.0 cm. λ_{ex} = 300 nm. [Tb(hfa)$_3$]$_0$ = 1.0 × 10^{-4} M. Bandwidth for emission 10 nm, bandwidth for excitation 10 nm, response time of PMT 8 sec, scanning rate 50 nm per min, and two scans.
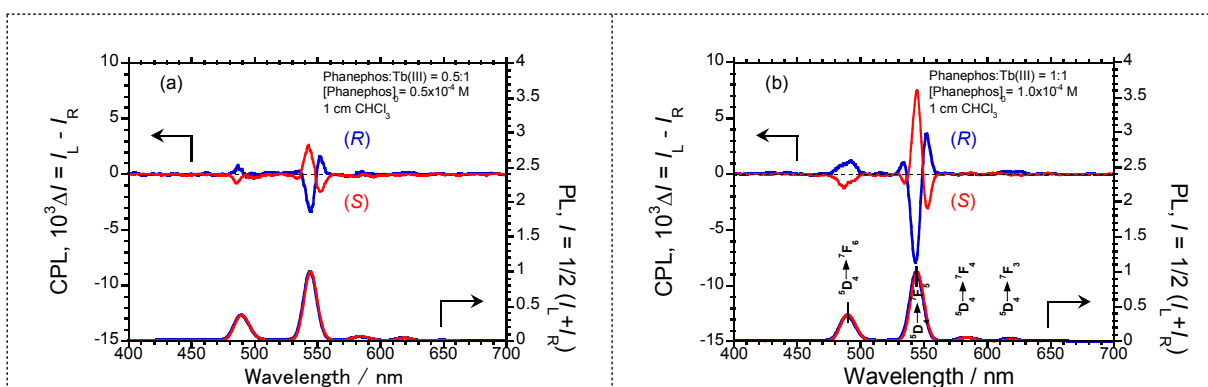

Fig. S2a. (*R*)- and (*S*)-Phanephos:Tb(hfa)$_3$ = 0.5:1.
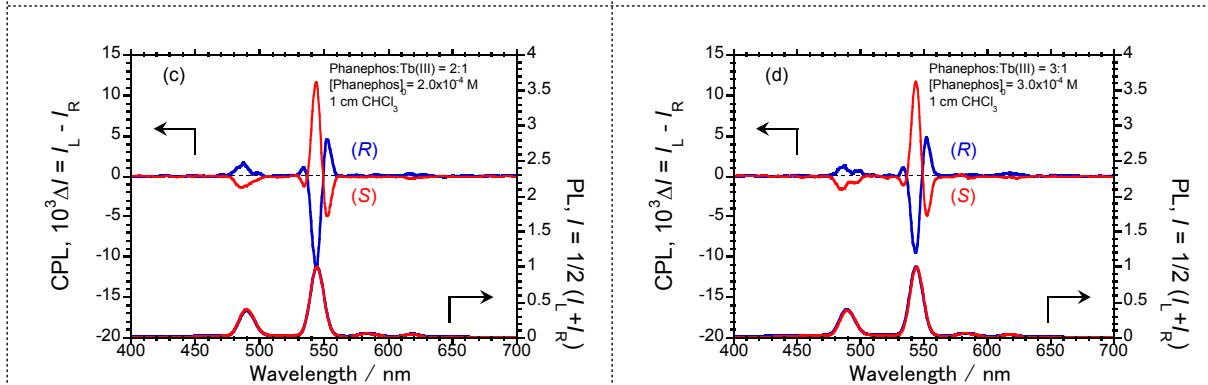

Fig. S2b. (*R*)- and (*S*)-Phanephos:Tb(hfa)$_3$ = 1:1

Fig. S2c. (*R*)- and (*S*)-Phanephos:Tb(hfa)$_3$ = 2:1.

Fig. S2d. (*R*)- and (*S*)-Phanephos:Tb(hfa)$_3$ = 3:1.

Fig. S2e. (*R*)- and (*S*)-Phanephos:Tb(hfa)$_3$ = 4:1.

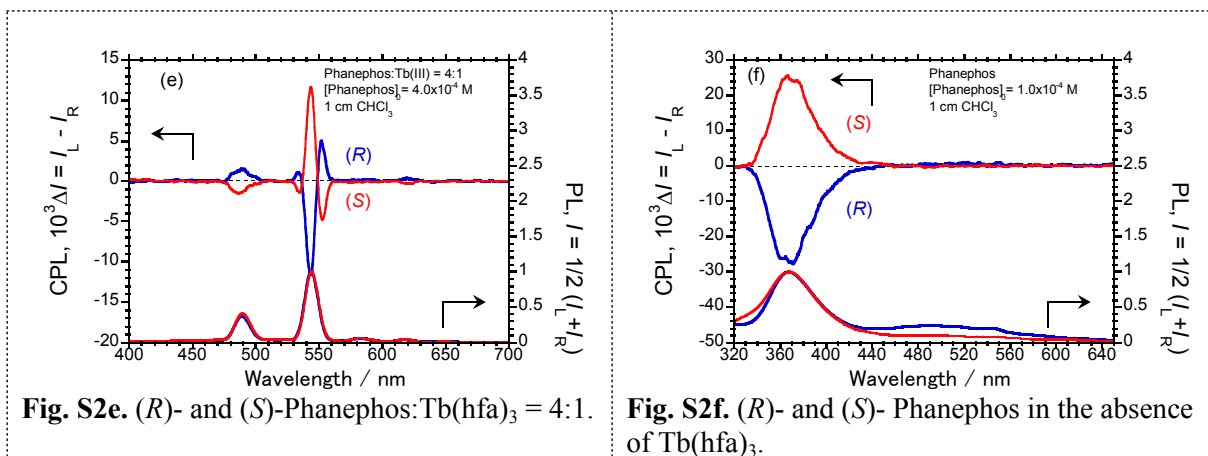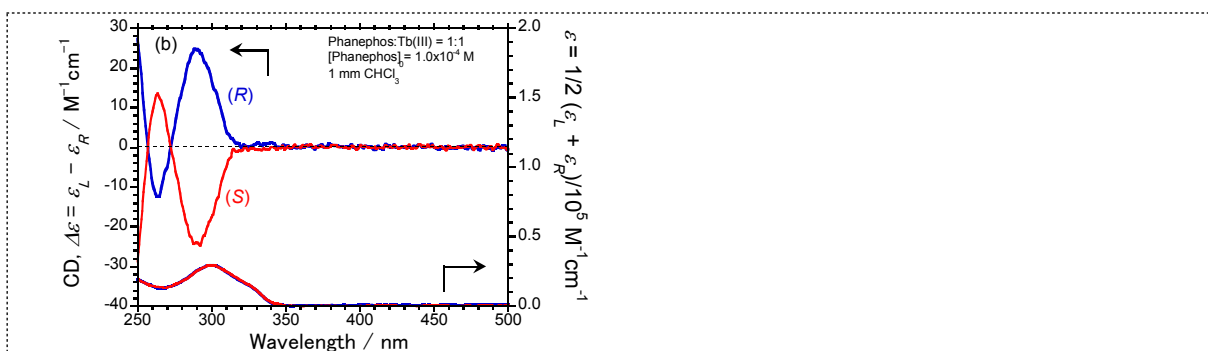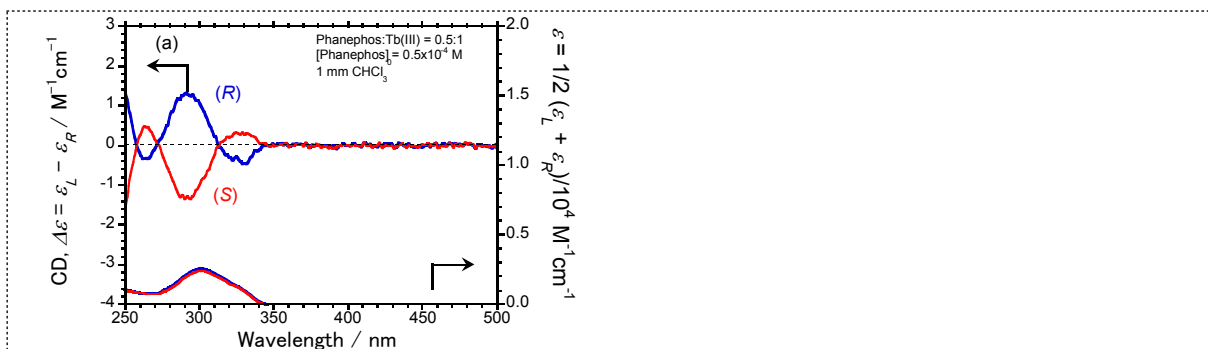**Fig. S2f.** (*R*)- and (*S*)- Phanephos in the absence of Tb(hfa)$_3$.

Fig. S2. CPL and PL spectra as a function of (*R*)- and (*S*)-Phanephos : Tb(hfa)$_3$ ratio in EtOH-free chloroform. Path length 1.0 cm. λ_{ex} = 300 nm. [Tb(hfa)$_3$]$_0$ = 1.0 × 10^{-4} M. Bandwidth for emission 10 nm, bandwidth for excitation 10 nm, response time of PMT 8 sec, scanning rate 50 nm per min, and two scans.
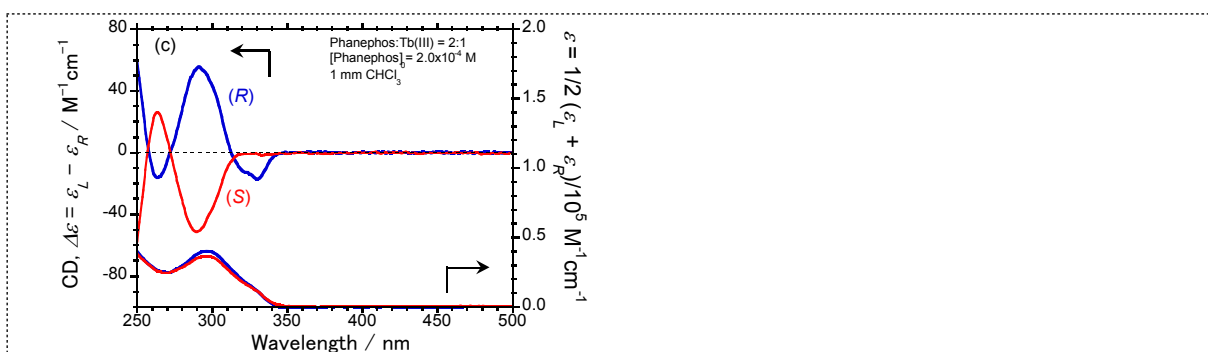

Fig. S3. (a) (*R*)- and (*S*)-Phanephos: Tb(hfa)$_3$ = 0.5:1. [Tb(hfa)$_3$]$_0$ = 1.0 x 10^{-4} M (final concentration), path length 1 mm.

Fig. S3. (b) (*R*)- and (*S*)-Phanephos: Tb(hfa)$_3$ = 1:1. [Tb(hfa)$_3$]$_0$ = 1.0 x 10^{-4} M (final concentration), path length 1 mm

Fig. S3. (c) (*R*)- and (*S*)-Phanephos: Tb(hfa)$_3$ = 2:1. [Tb(hfa)$_3$]$_0$ = 1.0 x 10^{-4} M (final concentration), path length 1 mm

Fig. S3. (d) (*R*)- and (*S*)-Phanephos: Tb(hfa)$_3$ = 3:1. [Tb(hfa)$_3$]$_0$ = 1.0 x 10^{-4} M (final concentration), path length 1 mm

Fig. S3. (e) (*R*)- and (*S*)-Phanephos: Tb(hfa)$_3$ = 4:1. [Tb(hfa)$_3$]$_0$ = 1.0 x 10^{-4} M (final concentration), path length 1 mm

.

Fig. S3. (f) (*R*)- and (*S*)-Phanephos in the absence of Tb(hfa)$_3$ in CHCl$_3$. [Phanephos]$_0$ = 1.0 x 10^{-4} M (final concentration), path length 1 mm.
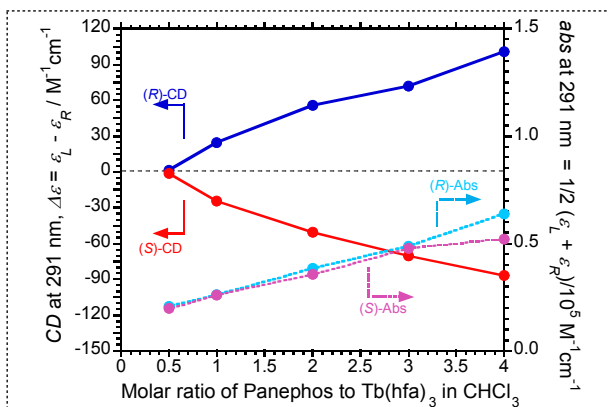
Fig. S3. (g) The CD amplitudes at 291 nm ($\Delta\Delta Abs$) (left ordinate) and UV absorbance (*Abs,* right ordinate) as a function of Phanphos-to-Tb molar ratio. All data were taken from **Fig. S3a–S3f.**

Fig. S3. CD and UV-vis spectra of (*R*)- and (*S*)-Phanephos : Tb(hfa)$_3$ in EtOH-free chloroform. [Tb(hfa)$_3$]$_0$ = 1.0 ×10^{-4} M (final concentration, fixed, path length 1 mm.).

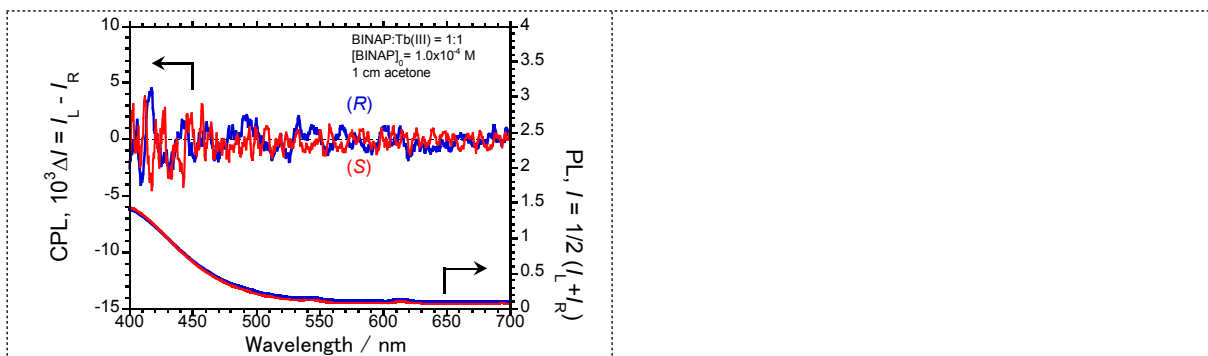**Fig. S4.** CPL and PL spectra as a function of (*R*)- and (*S*)-BIANP : Tb(hfa)$_3$ = 1 to 1 molar ratio in acetone. Path length 1.0 cm. λ_{ex} = 300 nm. [Tb(hfa)$_3$]$_0$ = 1.0 × 10^{-4} M. Bandwidth for emission 10 nm, bandwidth for excitation 10 nm, response time of PMT 8 sec, scanning rate 50 nm per min, and two scans.
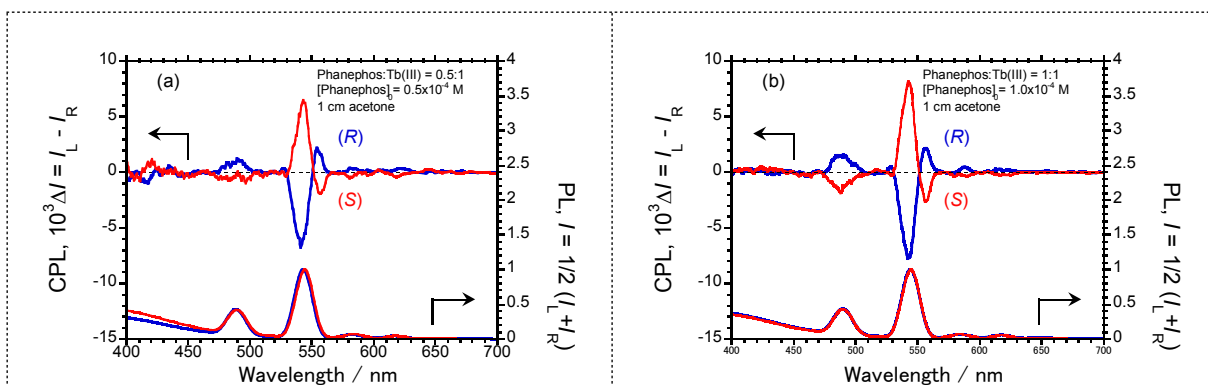

Fig. S5a. (*R*)- and (*S*)- Phanephos: Tb(hfa)$_3$ = 0.5:1 in acetone.

Fig. S5b. (*R*)- and (*S*)- Phanephos: Tb(hfa)$_3$ = 1:1 in acetone.

Fig. S5c. (*R*)- and (*S*)- Phanephos: Tb(hfa)$_3$ = 2:1 in acetone.

Fig. S5d. (*R*)- and (*S*)- Phanephos: Tb(hfa)$_3$ = 3:1 in acetone.

Fig. S5e. (*R*)- and (*S*)- Phanephos: Tb(hfa)$_3$ = 4:1 in acetone.

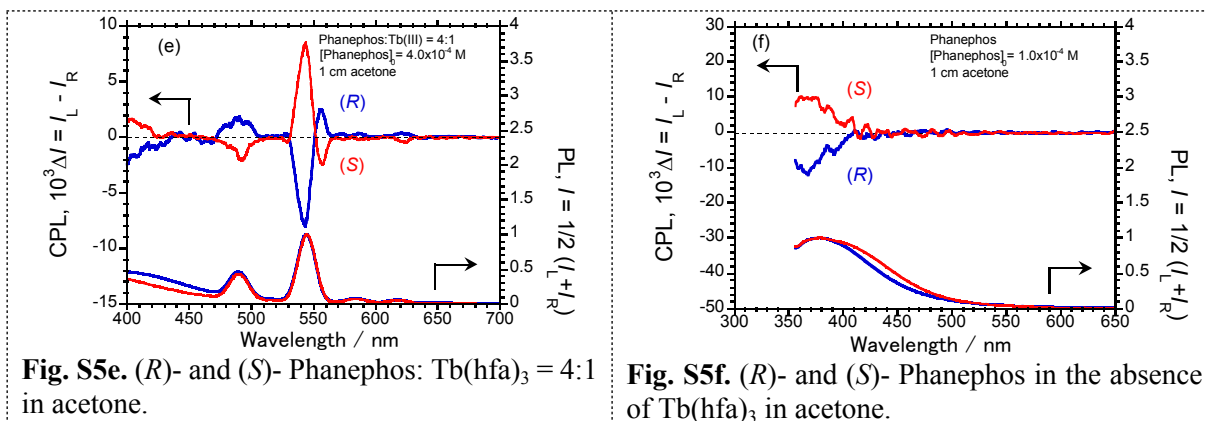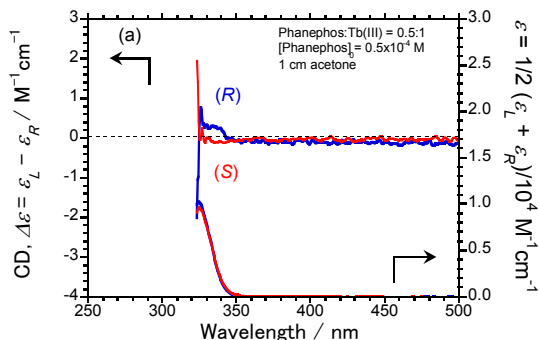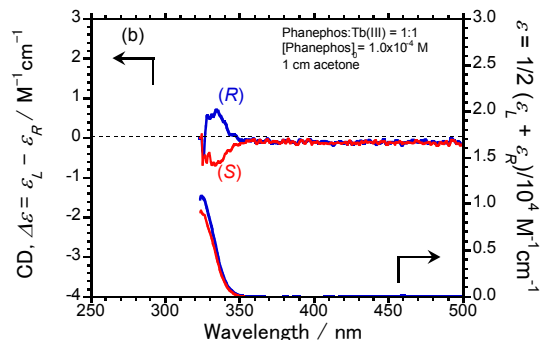**Fig. S5f.** (*R*)- and (*S*)- Phanephos in the absence of Tb(hfa)$_3$ in acetone.

Fig. S5. CPL and PL spectra as a function of (*R*)- and (*S*)-Phanephos : Tb(hfa)$_3$ ratio in acetone. Path length 1.0 cm. λ_{ex} = 325 nm. [Tb(hfa)$_3$]$_0$ = 1.0 × 10^{-4} M. Bandwidth for emission 10 nm, bandwidth for excitation 10 nm, response time of PMT 8 sec, scanning rate 50 nm per min, and two-time scans.

Fig. S6a. (*R*)- and (*S*)-Phanephos:Tb(hfa)$_3$= 0.5:1.

Fig. S6b. (*R*)- and (*S*)-Phanephos:Tb(hfa)$_3$ = 1:1.

Fig. S6c. (*R*)- and (*S*)-Phanephos:Tb(hfa)$_3$= 2:1.

Fig. S6d. (*R*)- and (*S*)- Phanephos:Tb(hfa)$_3$= 3:1.
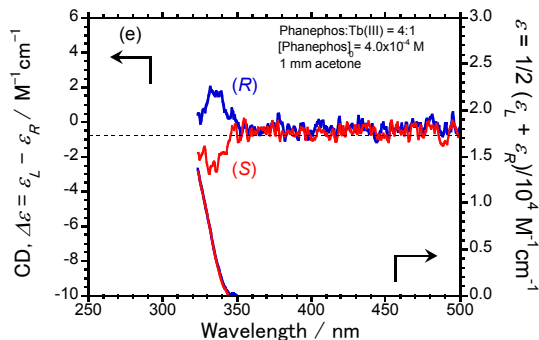

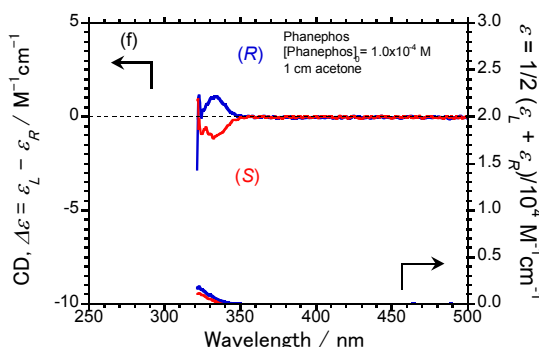**Fig. S6e.** (*R*)- and (*S*)-Phanephos:Tb(hfa)$_3$=4:1.

Fig. S6f. (*R*)- and (*S*)-Phanephos in the absence of Tb(hfa)$_3$ in acetone. [Phanephos]$_0$ = 1.0 x 10^{-4} M (final concentration), path length 1 mm.
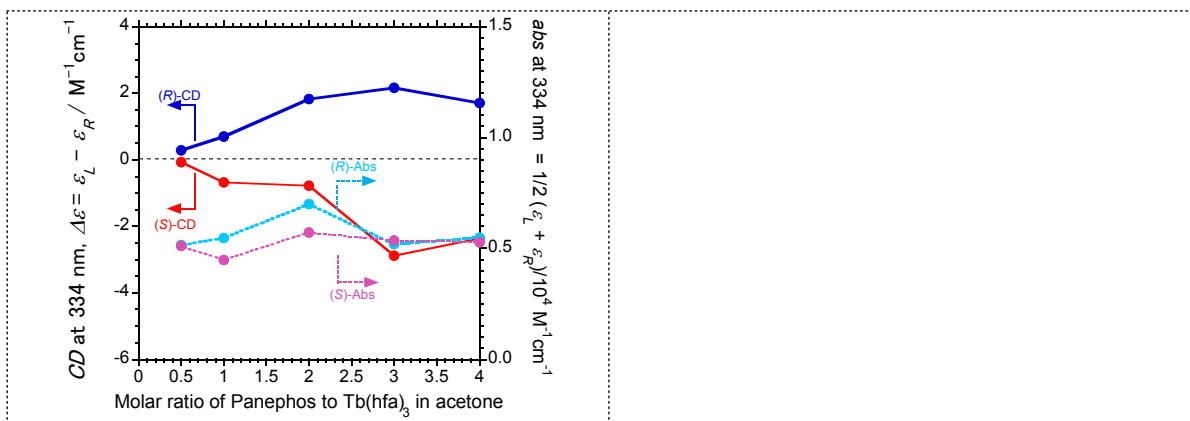
Fig. S6g. The CD amplitudes at 334 nm (*ΔΔbs*) (left ordinate) and UV absorbance at 334 nm (*Abs,* right ordinate) as a function of Phanphos-to-Tb molar ratio.

Fig. S6. CD and UV-vis spectra of (*R*)- and (*S*)-Phanephos:Tb(hfa)$_3$ in acetone. [Tb(hfa)$_3$]$_0$ = 1.0 × 10^{-4} M (final concentration (fixed). UV-vis/CD spectra shorter than 320 nm are not valid because of cut-off wavelength from strong *n-π** band of solvent acetone.
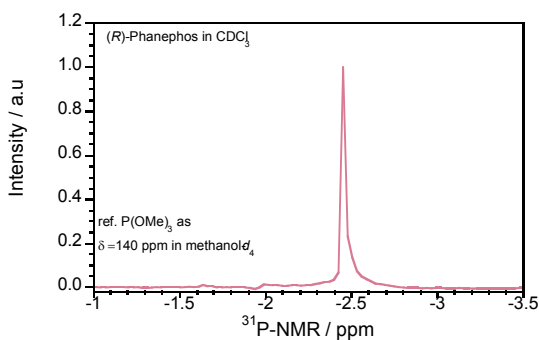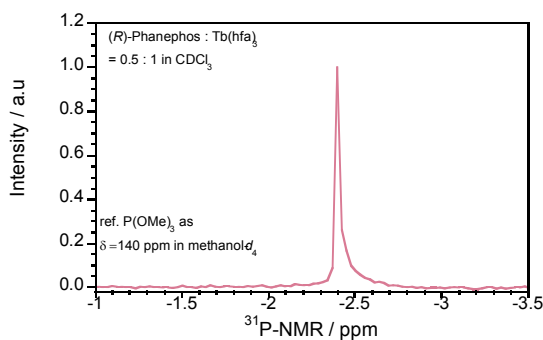
Fig. S7-a. (*R*)-Phanephos : Tb(hfa)$_3$ (1:0).

Fig. S7-b. *R*)-Phanephos : Tb(hfa)$_3$ (0.5:1).
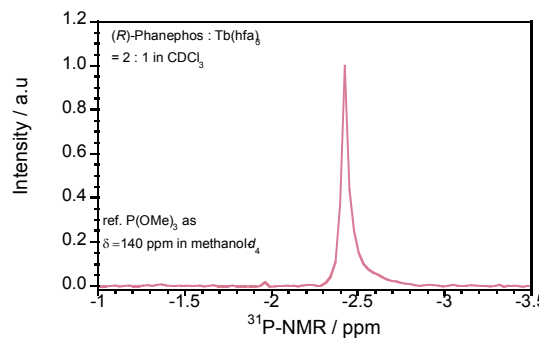
Fig. S7-c. (*R*)-Phanephos : Tb(hfa)$_3$ (1:1).

Fig. S7-d. (*R*)-Phanephos : Tb(hfa)$_3$ (2:1).
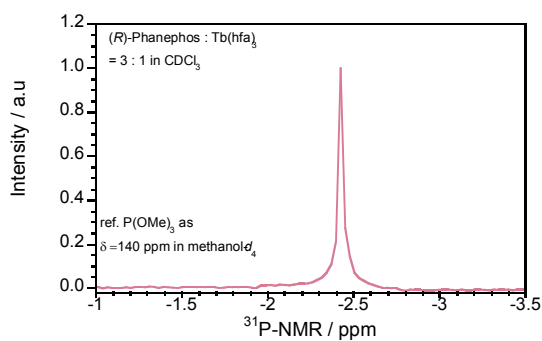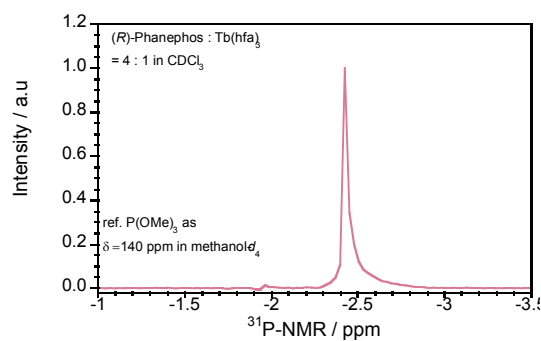
Fig. S7-e. (*R*)-Phanephos : Tb(hfa)$_3$ (3:1).

Fig. S7-f. (*R*)-Phanephos : Tb(hfa)$_3$ (4:1).

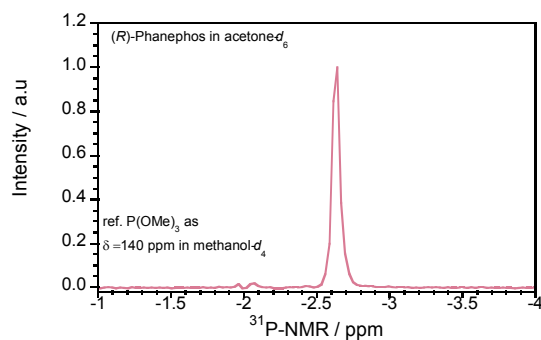**Fig. S7.** ^{31}P-NMR spectra of (*R*)-Phanephos as a function of (*R*)-Phanephos-to-Tb(hfa)$_3$ ratio in CDCl$_3$.

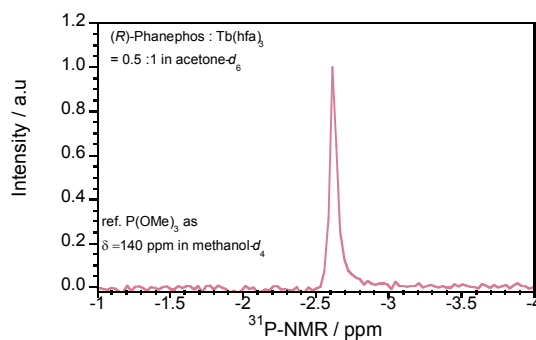**Fig. S8-a.** (*R*)-Phanephos : Tb(hfa)$_3$ (1:0).
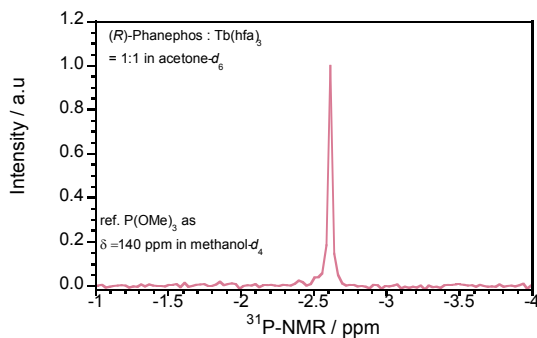

Fig. S8-b. (*R*)-Phanephos : Tb(hfa)$_3$ (0.5:1).
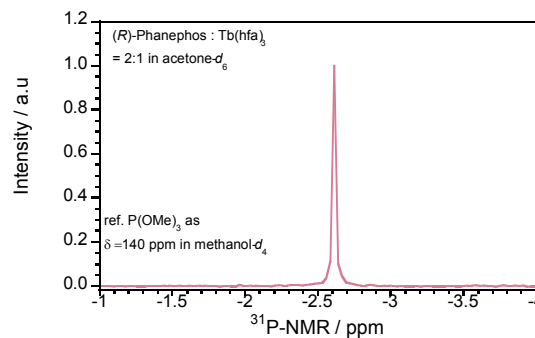

Fig. S8-c. (*R*)-Phanephos : Tb(hfa)$_3$ (1:1).
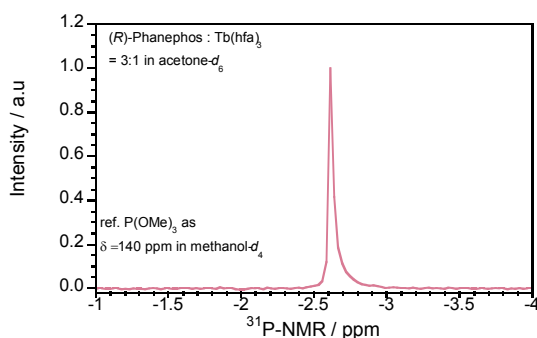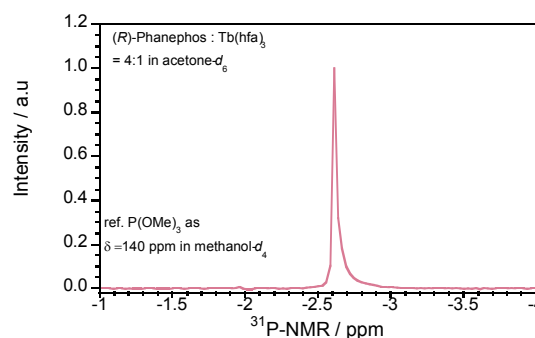

Fig. S8-d. (*R*)-Phanephos : Tb(hfa)$_3$ (2:1).

Fig. S8-e. (*R*)-Phanephos : Tb(hfa)$_3$ (3:1).

Fig. S8-f. (*R*)-Phanephos : Tb(hfa)$_3$ (4:1).

Fig. S8. ^{31}P-NMR spectra of (*R*)-Phanephos as a function of (*R*)-Phanephos-to-Tb(hfa)$_3$ ratio in acetone-d_6.
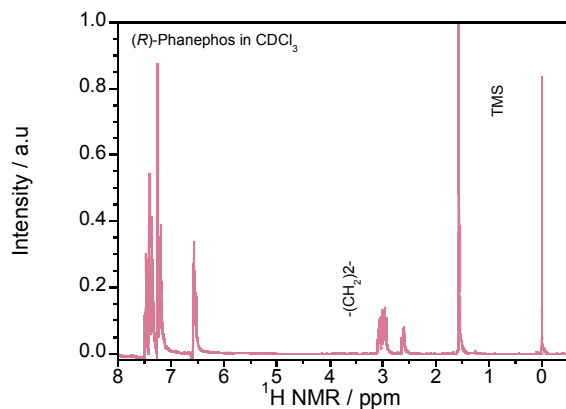
Fig. S9-a. ¹H-NMR spectrum of (*R*)-Phanephos without Tb(hfa)₃ in CDCl₃.

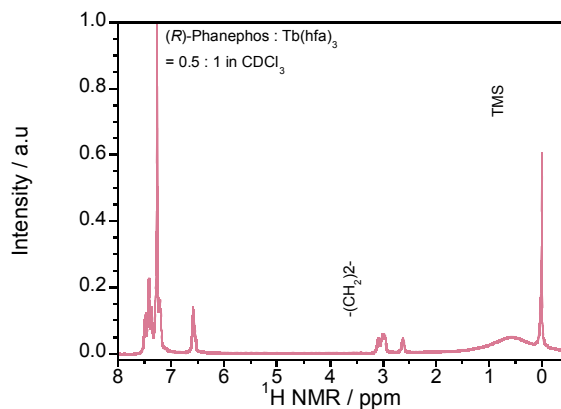**Fig. S9-b.** ¹H-NMR spectrum of (*R*)-Phanephos with Tb(hfa)₃ (0.5:1) in CDCl₃.

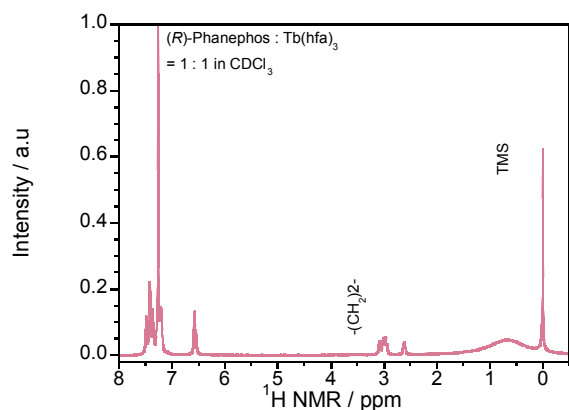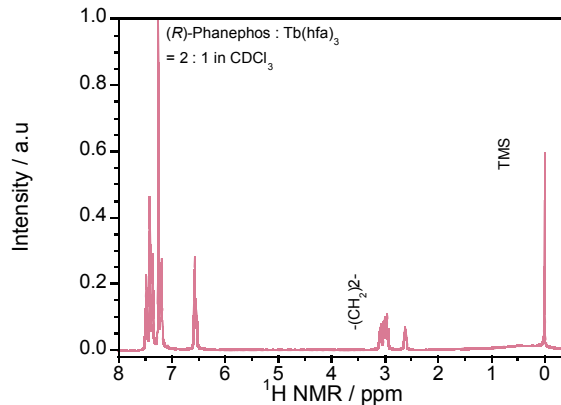**Fig. S9-c.** ¹H-NMR spectrum of (*R*)-Phanephos with Tb(hfa)₃ (1:1) in CDCl₃.

Fig. S9-d. ¹H-NMR spectrum of (*R*)-Phanephos with Tb(hfa)₃ (2:1) in CDCl₃.

Fig. S9-e. ¹H-NMR spectrum of (*R*)-Phanephos with Tb(hfa)₃ (3:1) in CDCl₃.

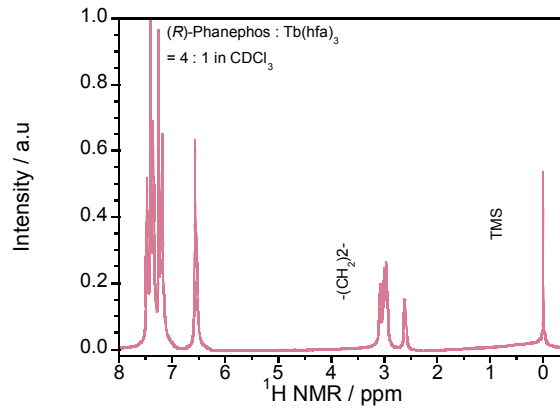**Fig. S9-f.** ¹H-NMR spectrum of (*R*)-Phanephos with Tb(hfa)₃ (4:1) in CDCl₃.

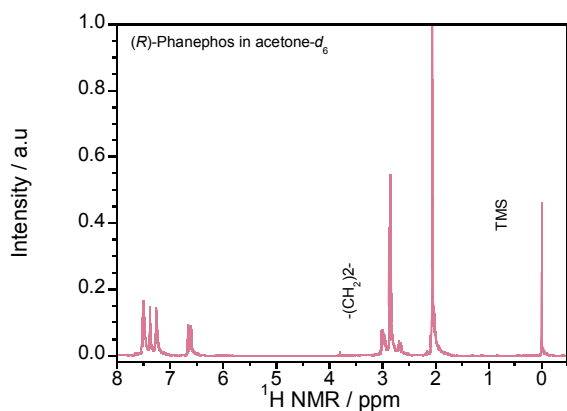**Fig. S9.** ¹H -NMR spectra of (*R*)-Phanephos as a function of (*R*)-Phanephos-to-Tb(hfa)₃ ratio in CDCl₃.

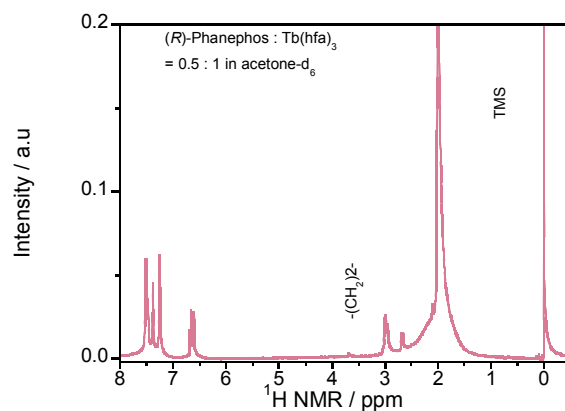**Fig. S10-a.** ^{1}H-NMR spectrum of (*R*)-Phanephos without Tb(hfa)$_3$ in acetone-*d*$_6$

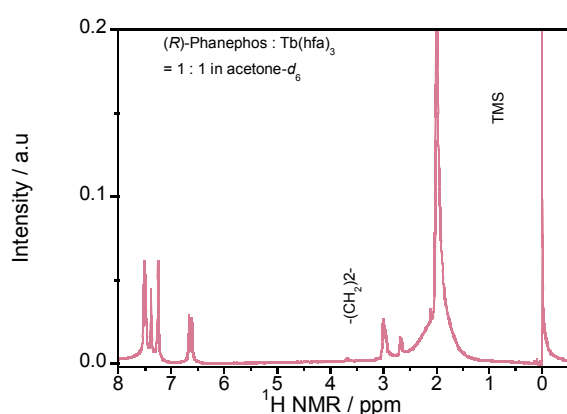**Fig. S10-b.** ^{1}H-NMR spectrum of (*R*)-Phanephos with Tb(hfa)$_3$ (0.5:1) in acetone-*d*$_6$.

Fig. S10-c. ^{1}H-NMR spectrum of (*R*)-Phanephos with Tb(hfa)$_3$ (1:1) in acetone-*d*$_6$.

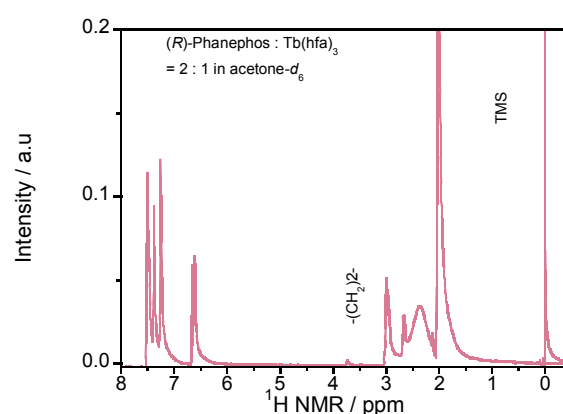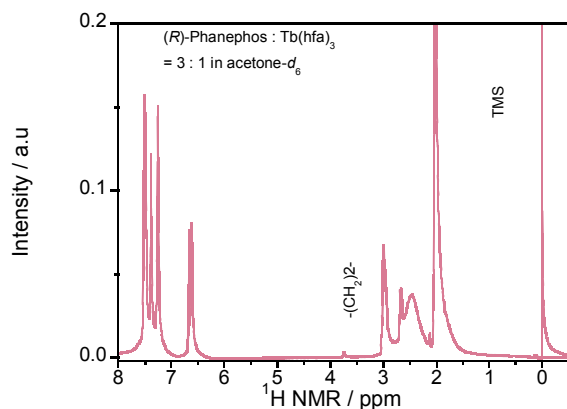**Fig. S10-d.** ^{1}H-NMR spectrum of (*R*)-Phanephos with Tb(hfa)$_3$ (2:1) in acetone-*d*$_6$.

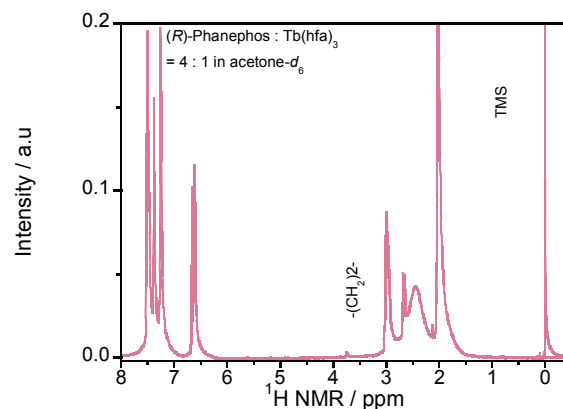**Fig. S10-e.** ^{1}H-NMR spectrum of (*R*)-Phanephos with Tb(hfa)$_3$ (3:1) in acetone-*d*$_6$.

Fig. S10-f ^{1}H-NMR spectrum of (*R*)-Phanephos with Tb(hfa)$_3$ (4:1) in acetone-*d*$_6$.

Fig. S10. ^{1}H -NMR spectra of (*R*)-Phanephos as a function of (*R*)-Phanephos-to-Tb(hfa)$_3$ ratio in acetone-*d*$_6$.
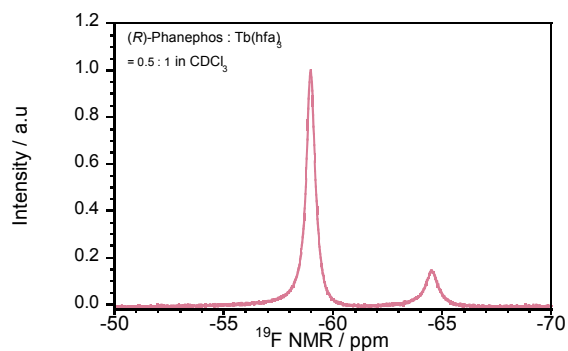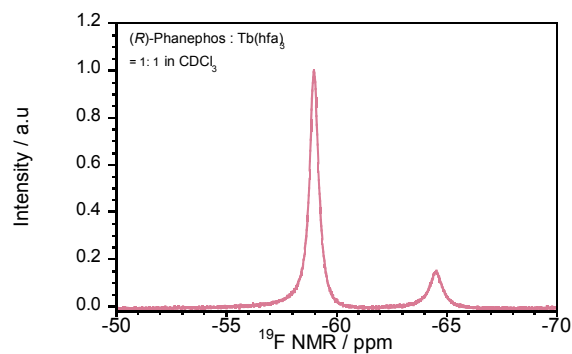
Fig. S11-a. (*R*)-Phanephos and Tb(hfa)$_3$ (0.5:1).

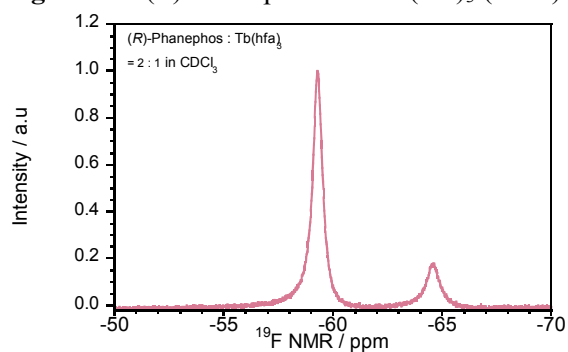**Fig. S11-b.** (*R*)-Phanephos and Tb(hfa)$_3$ (1:1).

Fig. S11-c. (*R*)-Phanephos and Tb(hfa)$_3$ (2:1).

Fig. S11-d. (*R*)-Phanephos and Tb(hfa)$_3$ (3:1).

Fig. S11-e. (*R*)-Phanephos and Tb(hfa)$_3$ (4:1).

Fig. S11. ^{19}F-NMR spectra of Tb(hfa)$_3$ as a function of (*R*)-Phanephos-to-Tb(hfa)$_3$ ratio in CDCl$_3$.

Fig. S13-a. (*R*)-Phanephos and Tb(hfa)$_3$ (0:1).

Fig. S13-b. (*R*)-Phanephos and Tb(hfa)$_3$ (0.5:1).

Fig. S13-c. (*R*)-Phanephos and Tb(hfa)$_3$ (1:1).

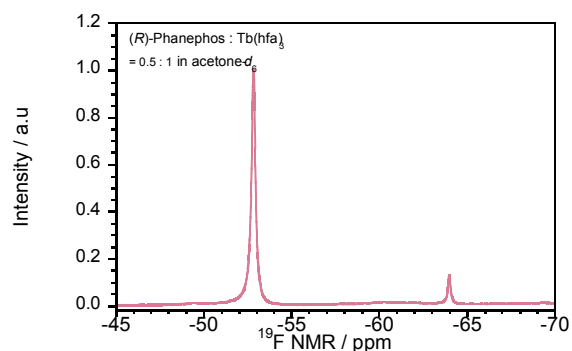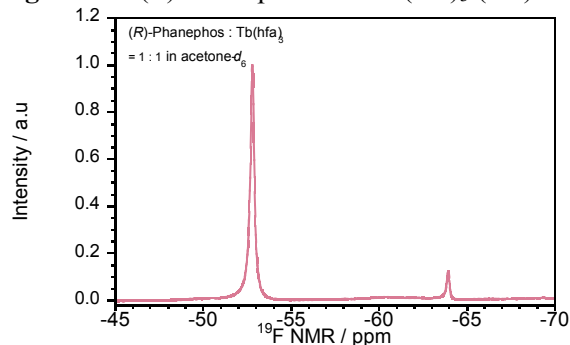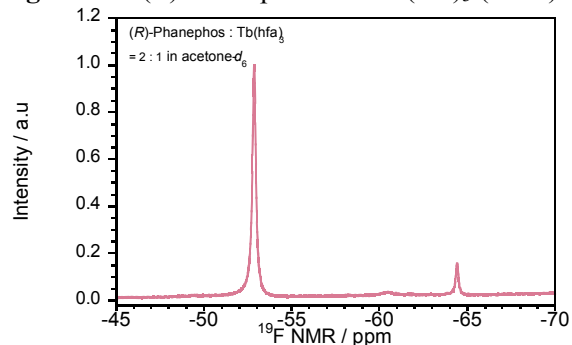**Fig. S13-d.** (*R*)-Phanephos and Tb(hfa)$_3$ (2:1).
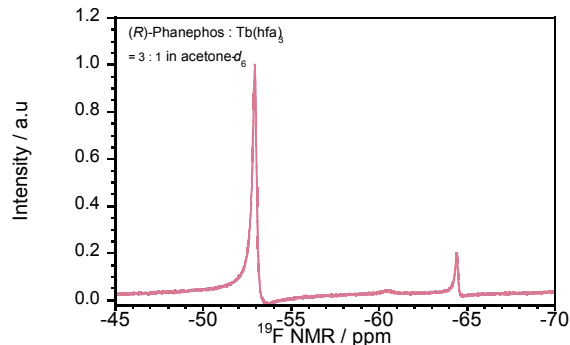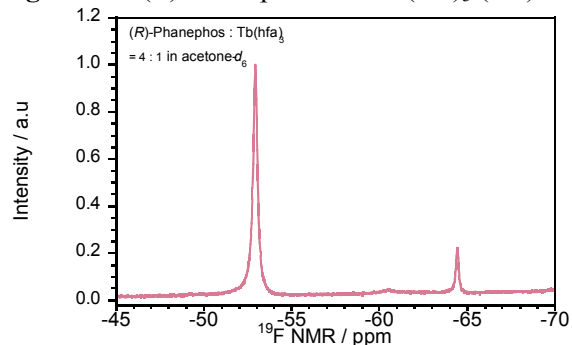
Fig. S13-e. (*R*)-Phanephos and Tb(hfa)$_3$ (3:1).

Fig. S13-f. (*R*)-Phanephos and Tb(hfa)$_3$ (4:1).

Fig. S13. ^{19}F-NMR spectra of Tb(hfa)$_3$ as a function of (*R*)-Phanephos-to-Tb(hfa)$_3$ ratio in acetone-d_6.
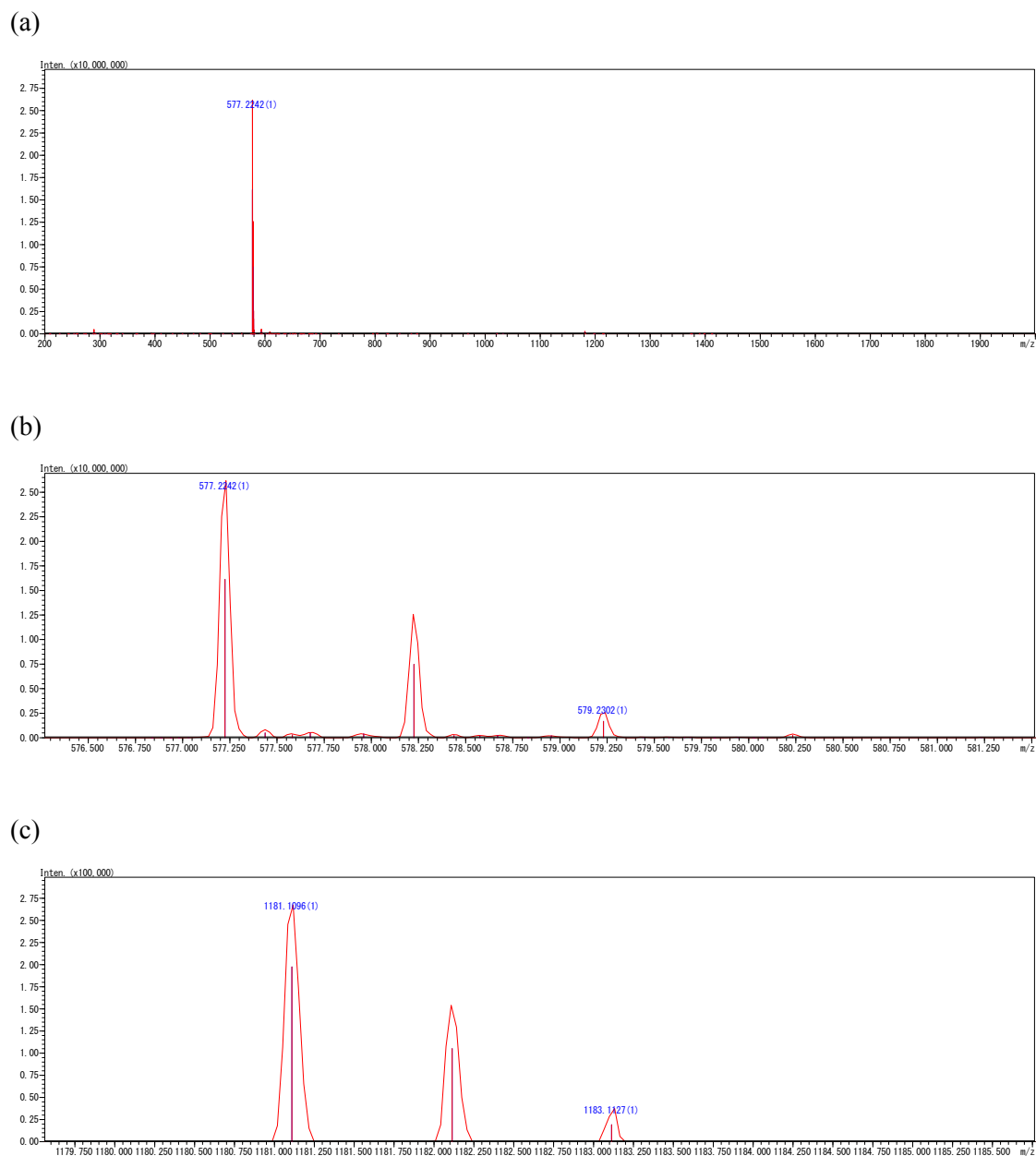
(a)

(b)

(c)

Figure S14. High resolution mass spectra of (*R*)-Phanephos and Tb(hfa)$_3$ (1:1) (a) all range, (b) and (c) expanded range (electrospray ionization, positive mode).
[Phanephos+ H]$^+$ (Phanephos: C$_{40}$H$_{34}$P$_2$) calcd. *m/z* 577.2209
[Tb(Phanephos)(hfac)$_2$]O$_2^+$ (C$_{50}$H$_{36}$O$_6$F$_{12}$P$_2$Tb) calcd *m/z* 1181.1043

Fig. S14a. (*R*)-BINAP: Tb(hfa)$_3$ = 1:1 in acetonitrile
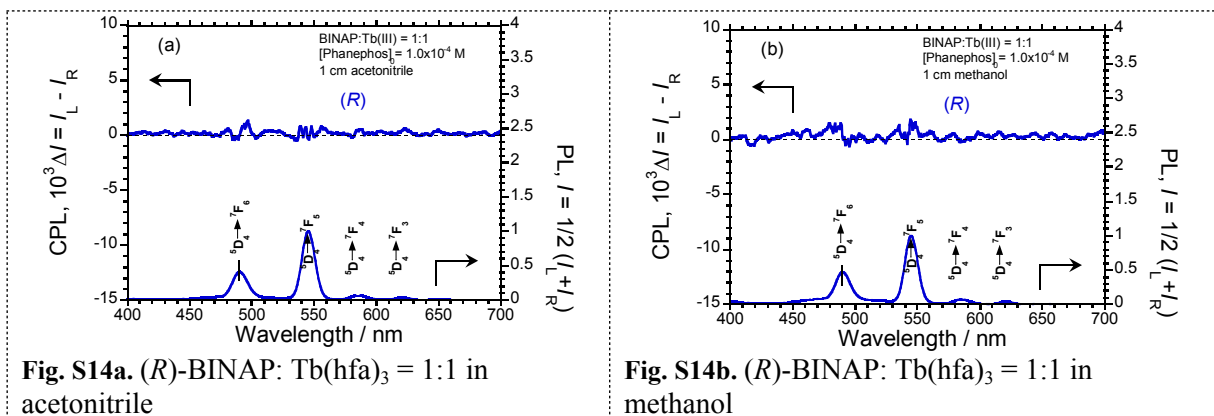
Fig. S14b. (*R*)-BINAP: Tb(hfa)$_3$ = 1:1 in methanol

Fig. S14. CPL and PL spectra as a function of (*R*)-BINAP : Tb(hfa)$_3$ ratio in acetonitrile and methanol. Path length 1.0 cm. λ_{ex} = 300 nm. [Tb(hfa)$_3$]$_0$ = 1.0 × 10^{-4} M. Bandwidth for emission 10 nm, bandwidth for excitation 10 nm, response time of PMT 8 sec, scanning rate 50 nm per min, and two-time scans.