Electronic supporting Information

Fluorescent chirality recognition by simple boronate ensembles with aggregation-induced emission capability

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General

NMR spectra were taken by a Bruker Avance 500 (¹H: 500 MHz) spectrometer and JEOL JMN-EC S400 (¹¹B: 128 MHz). In ¹H NMR measurements, chemical shifts (δ) are reported downfield from the internal standard Me₄Si. Electrospray ionization (ESI) mass spectrum was recorded on a Mariner System 5231 (Applied Biosystems). Fluorescence spectra were measured using a JASCO FP-6300 spectrophotometers. Powder X-ray diffraction (PXRD) data were collected by a Rigaku RINT-TTR III X-ray diffractometer with Cu K α radiation. Dynamic light scattering (DLS) measurements were performed using an ELSZ-2 (OTSUKA ELECTRONICS) instrument.

Materials

Unless otherwise indicated, reagents used for the synthesis were commercially available and were used as supplied. Synthesis of 4,4'-(2,2-diphenylethane-1,1-diyl)bis(dihydroxyborylbenzene) (**DB-TPE**) was conducted according to the method previously reported (A. Ozawa, A. Shimizu, R. Nishiyabu and Y. Kubo, *Chem. Commun.*, 2015, **51**, 118–121).



Fig. S1 ESI-MS spectrum (negative mode) of a mixture of L-tartaric acid $(7.50 \times 10^{-5} \text{ M})$ and **DB-TPE** $(3.75 \times 10^{-5} \text{ M})$ in THF after aging for 20 h in the presence of molecular sieve 4A. The ESI data were acquired at 100 °C.



Fig. S2 Emission spectra of mixture of L-TPE-TA and (1*S*,2*S*)-1 (blue line) or (1*R*,2*R*)-1 (red line) with an increase in ethanol fraction (*f*) in THF. [L-TPE-TA] = 0.75 mM, [1] = 1.50 mM. λ_{ex} = 365 nm. Data were acquired in 30 min after the addition of each enantiomers of 1.



Fig. S3 Emission spectra of a mixture of **D-TPE-TA** (0.75 mM) upon adding (1*S*,2*S*)-1 (1.50 mM) or (1*R*,2*R*)-1 (1.50 mM) in EtOH/THF (4:1 v/v) at 25 °C. λ_{ex} = 365 nm. Data were acquired in 30 min after the addition of each enantiomer of 1.



Fig. S4 Powder X-ray diffraction patterns of aggregated L-TPE-TA/(1*S*,2*S*)-1 salt (blue line) (a) or L-TPE-TA with (1*R*,2*R*)-1 salt (red line) (b). (c) Salt formation of L-TPE-TA and (1*S*,2*S*)-1. (d) A part of a plausible network structure from the salt formation of L-TPE-TA and (1*R*,2*R*)-1.



Fig. S5 Emission spectra of a mixture of **D-TPE-TA** (0.75 mM) upon adding (1*S*,2*S*)-**2** (1.50 mM) or (1*R*,2*R*)-**2** (1.50 mM) in EtOH/THF (1:5 v/v) at 25 °C. $\lambda_{ex} = 365$ nm. Data were acquired in 30 min after the addition of each enantiomer of **2**.



Fig. S6 Plausible binding modes of L-TPE-TA with (1S,2S)-1 (a) and L-TPE-TA with (1R,2R)-2 (b).



Fig. S7 Emission spectra of a mixture of **D-TPE-TA** (0.50 mM) and cinchonidine (1.00 mM) or cinchonine (1.00 mM) in THF at 25 °C. $\lambda_{ex} = 365$ nm. Data were acquired in 30 min after the addition of cinchonidine or cinchonine.