Supporting information

Developing chiral aggregates exhibiting anti-S-shaped CD-*ee* dependence: Using *meso*-isomer to tune dynamic aggregates induced by enantiomers

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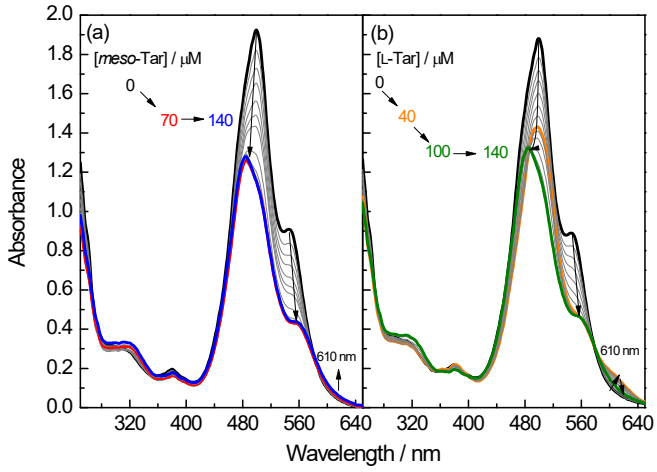

Figure S1. Absorption spectra of **1** in the presence of increasing concentration of (a) *meso*-Tar and (b) L-Tar in pH 5.0 acetate buffer containing 2.5% by volume DMSO. [**1**] = 50 μM.

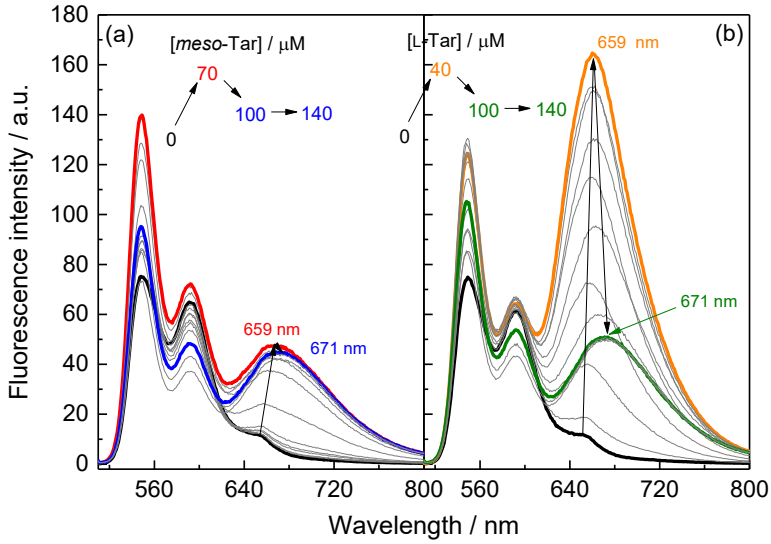

Figure S2. Fluorescence spectra of **1** in the presence of (a) *meso*-Tar and (b) L-Tar in pH 5.0 acetate buffer containing 2.5% by volume DMSO. The long-wavelength emission is due to the excimer of **1**. [**1**] = 50 μM; λ_{ex} = 499 nm, $slit_{ex}$ = $slit_{em}$ = 5 nm.

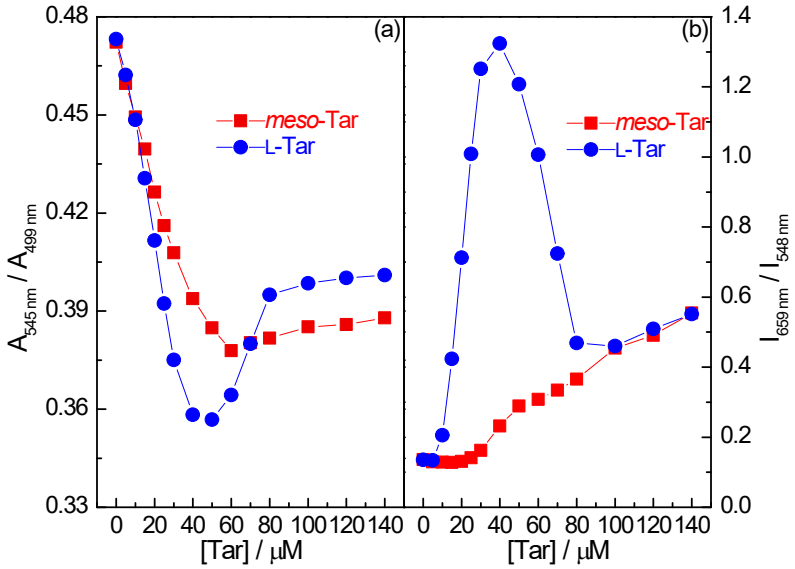

Figure S3. Ratio of (a) absorbance $A_{545\ nm}/A_{499\ nm}$ and (b) fluorescence intensity $I_{659\ nm}/I_{548\ nm}$ of **1** as a function of concentration of *meso*-Tar and L-Tar in pH 5.0 acetate buffer containing 2.5% by volume DMSO. λ_{ex} = 499 nm, $slit_{ex}$ = $slit_{em}$ = 5 nm.

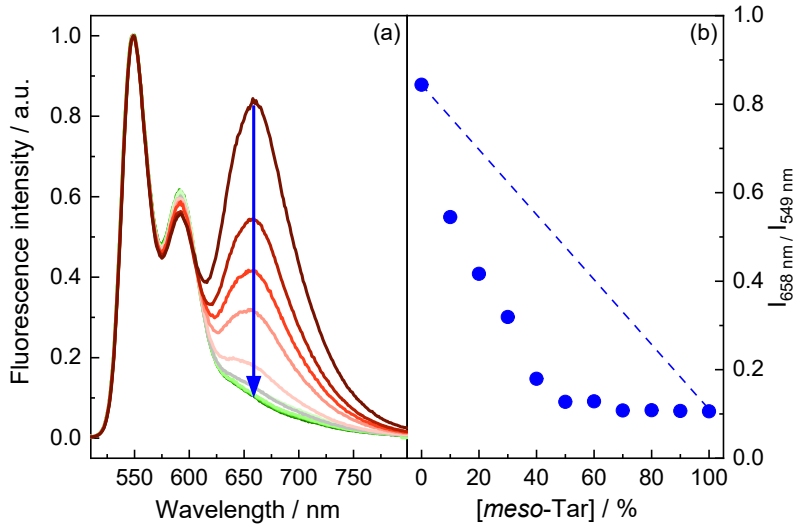

Figure S4. (a) Fluorescence spectra of **1** in the presence of *meso*- and L-Tar mixture of increasing molar fraction of *meso*-Tar and (b) plots of the ratio of fluorescence intensity at 658 nm to that at 549 nm versus molar fraction of *meso*-Tar in pH 5.0 acetate buffer containing 2.5% by volume DMSO. Emission at long-wavelength of 659 nm is due to the excimer of **1**. [**1**] = 50 μM, [L-Tar] + [*meso*-Tar] = 30 μM.

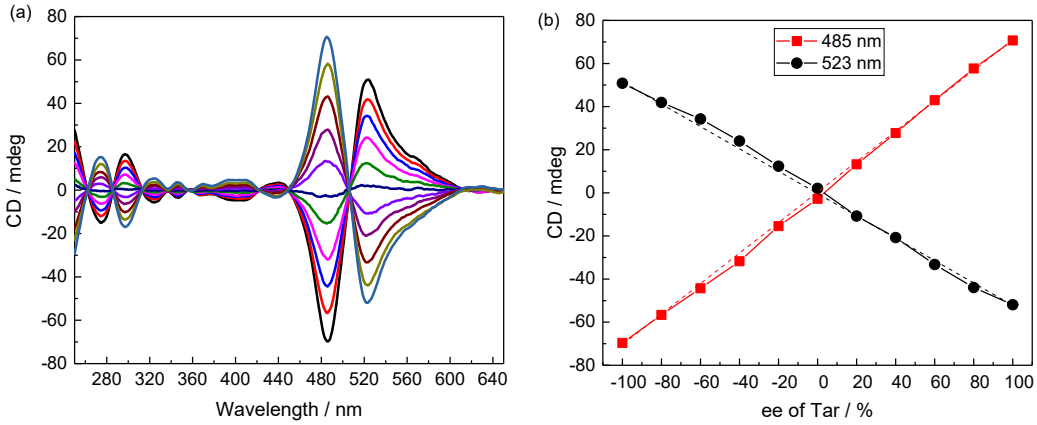

Figure S5. (a) CD spectra of **1** in the presence of Tar of different *ee* and (b) CD-*ee* dependence of the **1**-Tar assembly in pH 5.0 acetate buffer containing 2.5% by volume DMSO. [**1**] = 50 μM, [*meso*-Tar] = 3 μM, [L-Tar] + [D-Tar] = 27 μM.

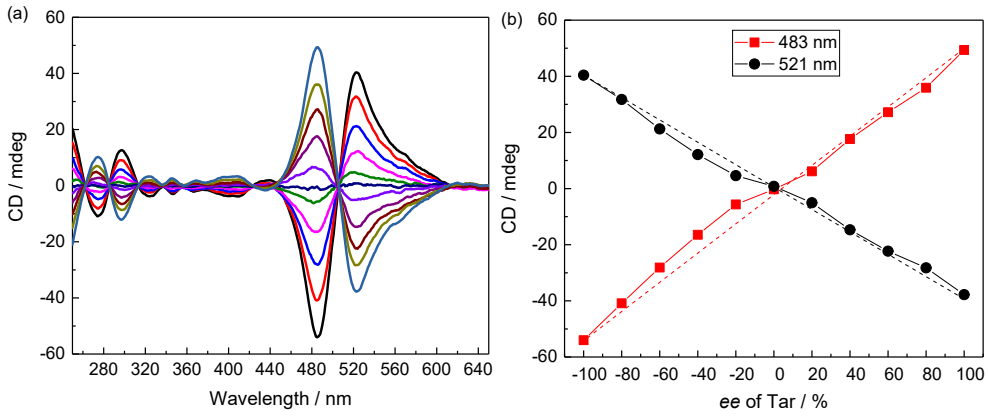

Figure S6. (a) CD spectra of **1** in the presence of Tar of different *ee* and (b) CD-*ee* dependence of **1**-Tar assembly in pH 5.0 acetate buffer containing 2.5% by volume DMSO. [**1**] = 50 μM, [*meso*-Tar] = 6 μM, [L-Tar] + [D-Tar] = 24 μM.

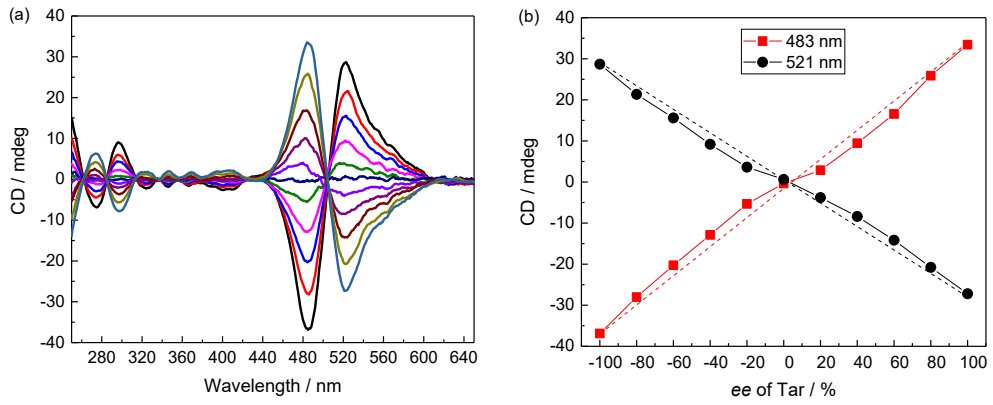

Figure S7. (a) CD spectra of **1** in the presence of Tar of different *ee* and (b) CD-*ee* dependence of **1**-Tar assembly in pH 5.0 acetate buffer containing 2.5% by volume DMSO. [**1**] = 50 μM. [*meso*-Tar] = 9 μM, [L-Tar] + [D-Tar] = 21 μM.

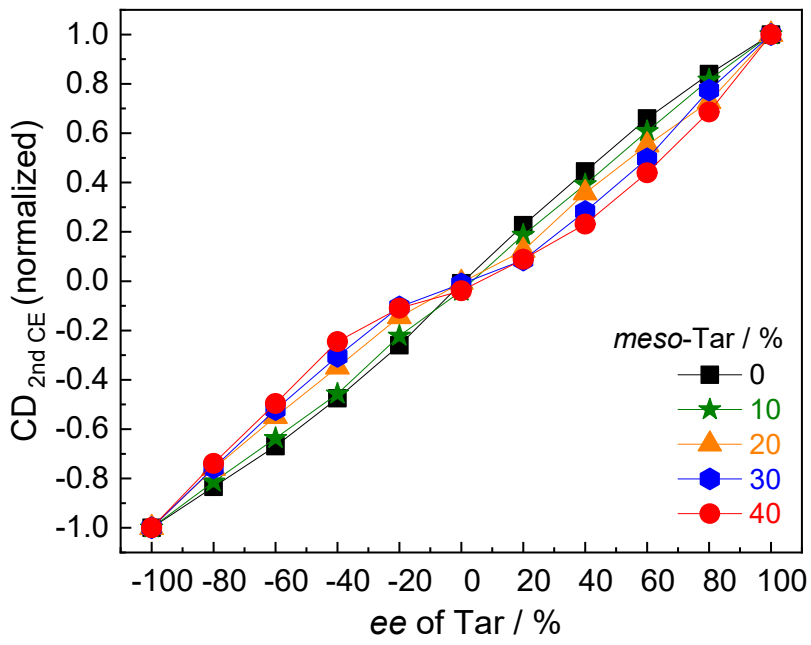

Figure S8. CD-*ee* dependence of **1**-Tar assembly versus *ee* of L- and D-tartaric acid in the mixture of *meso*-, L- and D-tartaric acid of increasing molar fraction of *meso*-Tar in pH 5.0 acetate buffer containing 2.5% by volume DMSO. Note that the curve turns from S- to anti-S-shaped when the molar fraction of *meso*-Tar is over 20%. [**1**] = 50 μM, [*meso*-Tar] + ([L-Tar] + [D-Tar]) = 30 μM.

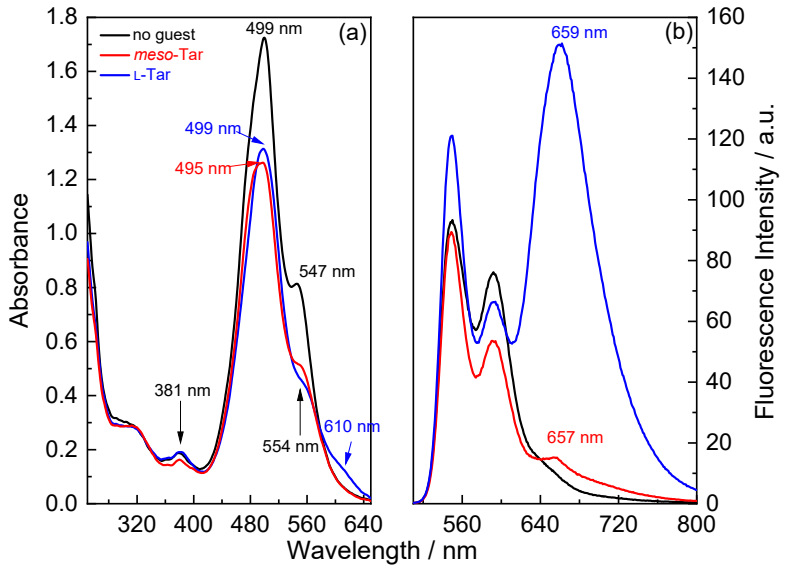

Figure S9. Absorption (a) and fluorescence (b) spectra of **1** in the absence (black lines) and in the presence of *meso*-Tar (red lines) and L-Tar (blue lines) in pH 5.0 acetate buffer containing 2.5% by volume DMSO. [**1**] = 50 μM, [Tar] = 30 μM.

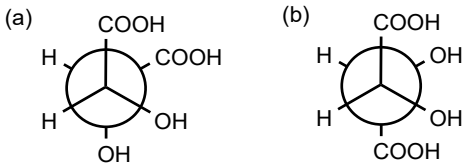

Figure S10. The most stable conformations of (a) *meso*-Tar and (b) L-Tar in aqueous solution.

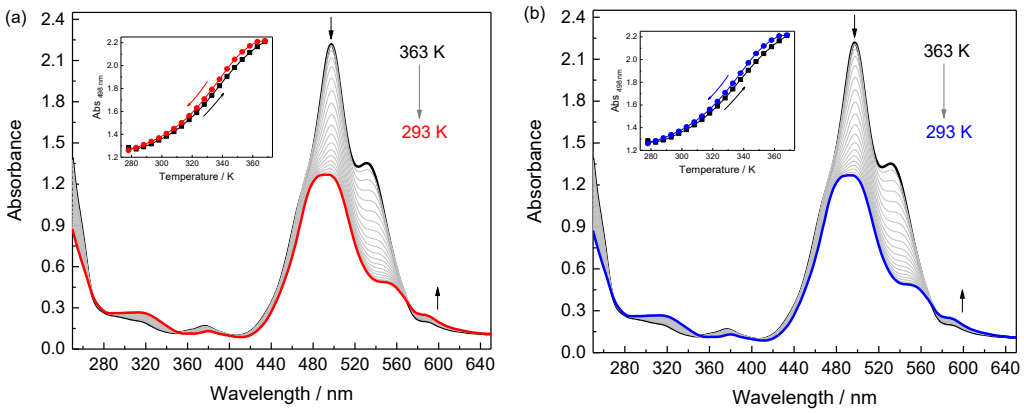

Figure S11. Temperature-dependent absorption spectra of (a) **1**-*meso*-Tar and (b) **1**-L-Tar assemblies during cooling from 363K to 293 K in pH 5.0 acetate buffer containing 2.5% by

volume DMSO. Insets are the corresponding cooling and heating curves of absorbance at 498 nm versus temperature. [**1**] = 50 μM, [Tar] = 30 μM.

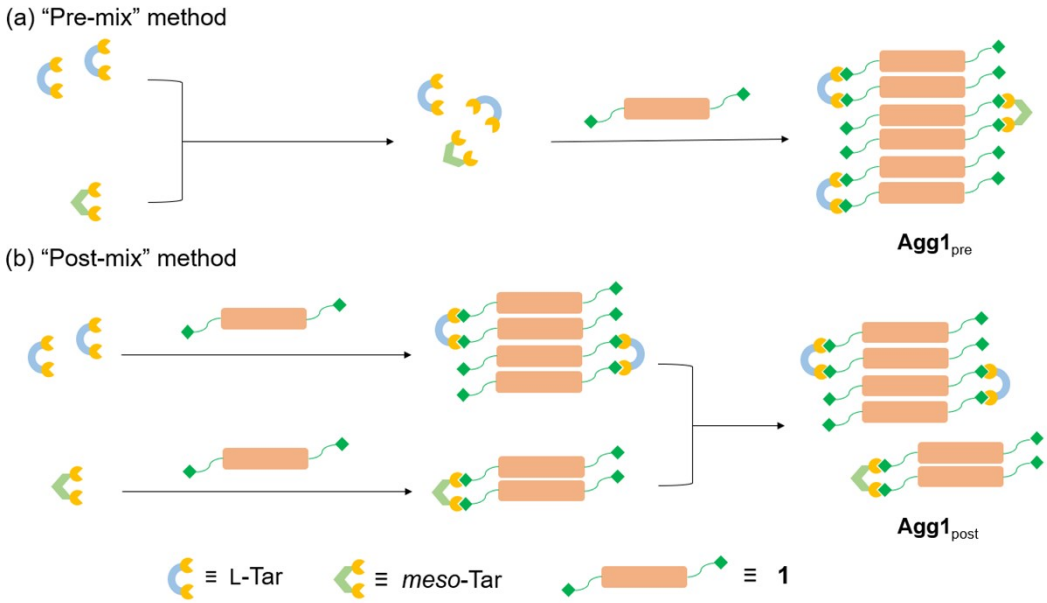

Figure S12. Schematic representation of pre-mix (a) and post-mix (b) methods.

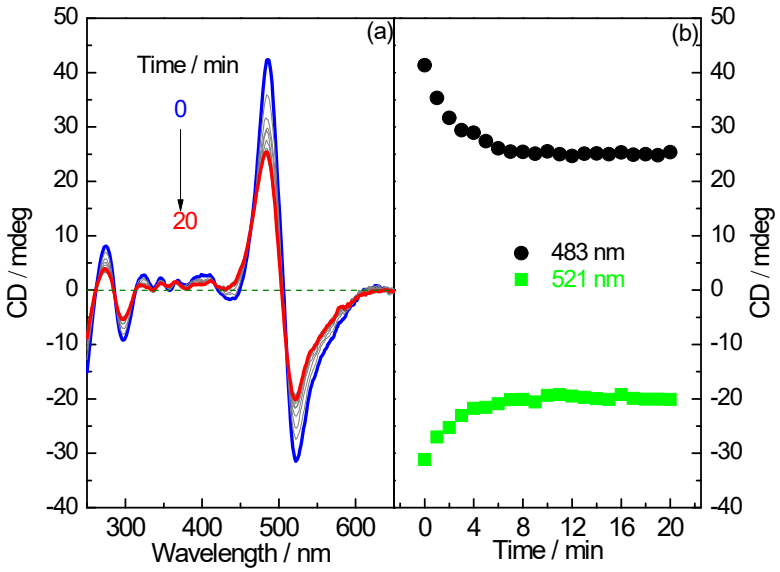

Figure S13 (a) Time-dependent CD spectra of a mixture of **1** (30 μM)/L-Tar (18 μM) assembly and **1** (20 μM)/*meso*-Tar (12 μM) assembly prepared by post-mix method in pH 5.0 acetate buffer containing 2.5% by volume DMSO. (b) Time profiles of CD signals at 483 and 521 nm.

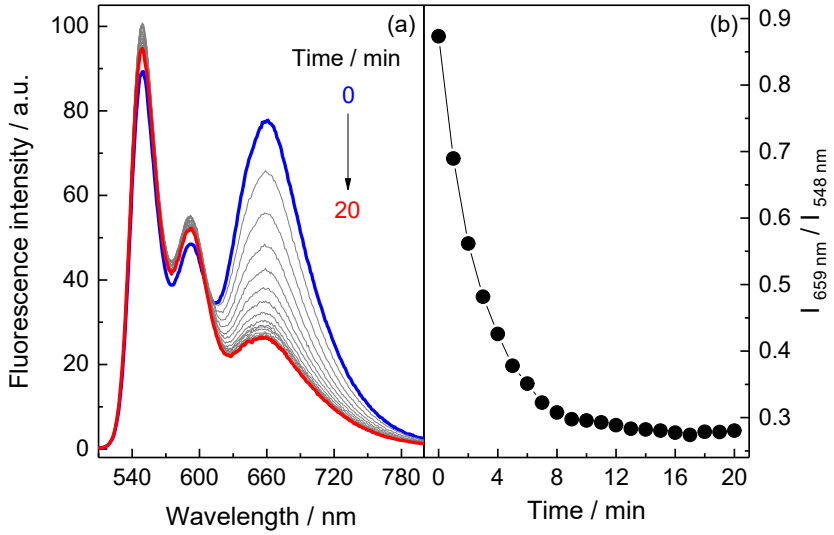

Figure S14. (a) Time-dependent fluorescence spectra of a mixture of **1** (30 μM)/L-Tar (18 μM) assembly and **1** (20 μM)/*meso*-Tar (12 μM) assembly prepared by post-mix method in pH 5.0 acetate buffer containing 2.5% by volume DMSO. (b) Time profile of the intensity ratio of excimer (659 nm) to monomer (548 nm) emission. λ_{ex} = 499 nm, $slit_{ex}$ = $slit_{em}$ = 5 nm.

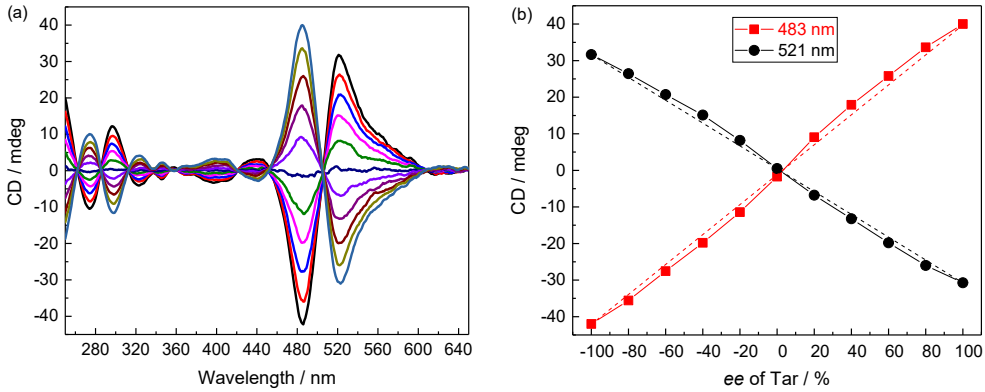

Figure S15. (a) CD spectra of **1** in the presence of Tar of varying *ee* and (b) CD-*ee* dependence of **1**-Tar assembly in pH 5.0 acetate buffer containing 2.5% by volume DMSO. [**1**] = 50 μM, [L-Tar] + [D-Tar] = 18 μM.