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Supporting Information

Circular Dichroism of Multi-Component Assemblies for Chiral Amine Recognition and Rapid *Ee* Determination

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Materials and Methods

All reagents and solvents were used as purchased from commercial sources. The program used to carry out principal component analysis (PCA) and linear discriminant analysis (LDA) studies was XLSTAT 20011. ^{1}H-NMR and ^{13}C-NMR spectra were recorded on a Varian Mercury 400 MHz spectrometer. All CD measurements were performed at 25°C on a Jasco J-815 circular dichroism spectropolarimeter using a 0.1 cm cuvette.

Experimental:

4 mM stock solutions of FPBA, BINOL and derivatives and all α-chiral primary amines (MBA, CHEA, AH, NEA, DMBA, and IPCA) were prepared by stirring the appropriate mass or volume in HPLC grade acetonitrile. All CD spectra were collected after a dilution step to make all samples 0.4 mM, with the 3-component assembly being prepared by mixing 100μL of the FPBA, BINOL-type species and amine stock solutions and adding HPLC grade acetonitrile until achieving volumes of 1mL. The titration experiments were performed by measuring the CD signal for a collection of samples of 0.4 mM in FPBA and BINOL and varying concentrations of the amine. The solutions of known *ee*% were prepared by mixing the appropriate amounts of enantiopure amines and the *ee*% values used for the final error determination calculated accordingly.

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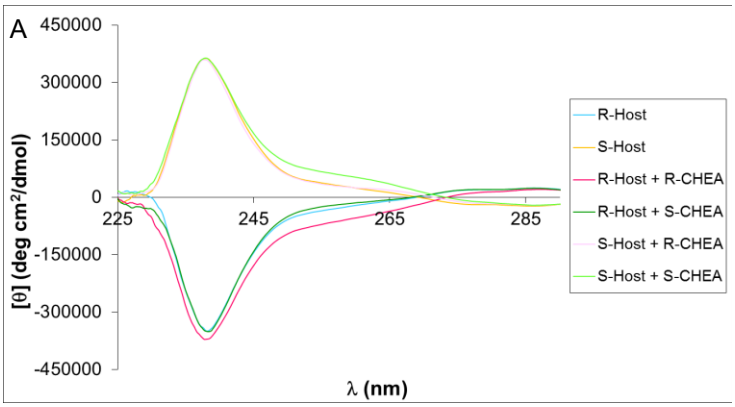
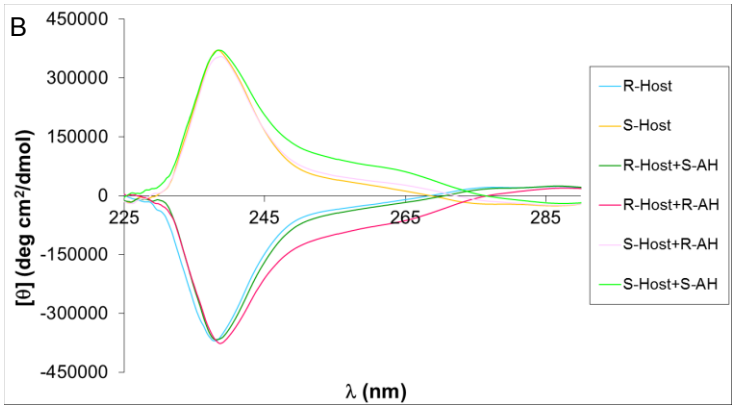
Characterization data

(*S*)-BINOL + FPBA + (*R*)-AH assembly product: ^{1}H-NMR (400MHz, $CDCl_3$) δ 8.8 (s, 1H), 8.5 (d, 2H), 8.1 (d, 2H), 7.9 (m, 3H), 7.6 (m, 7H), 7.1 (d, 2H), 3.4 (m, 1H), 1.7 (m, 2H), 1.4 (m, 5H), 1.3 (m, 4H), 0.9 (t, 3H); *m/z* (ESI-MS) 495.5 $[M]^{+}$.

Supplementary Figures





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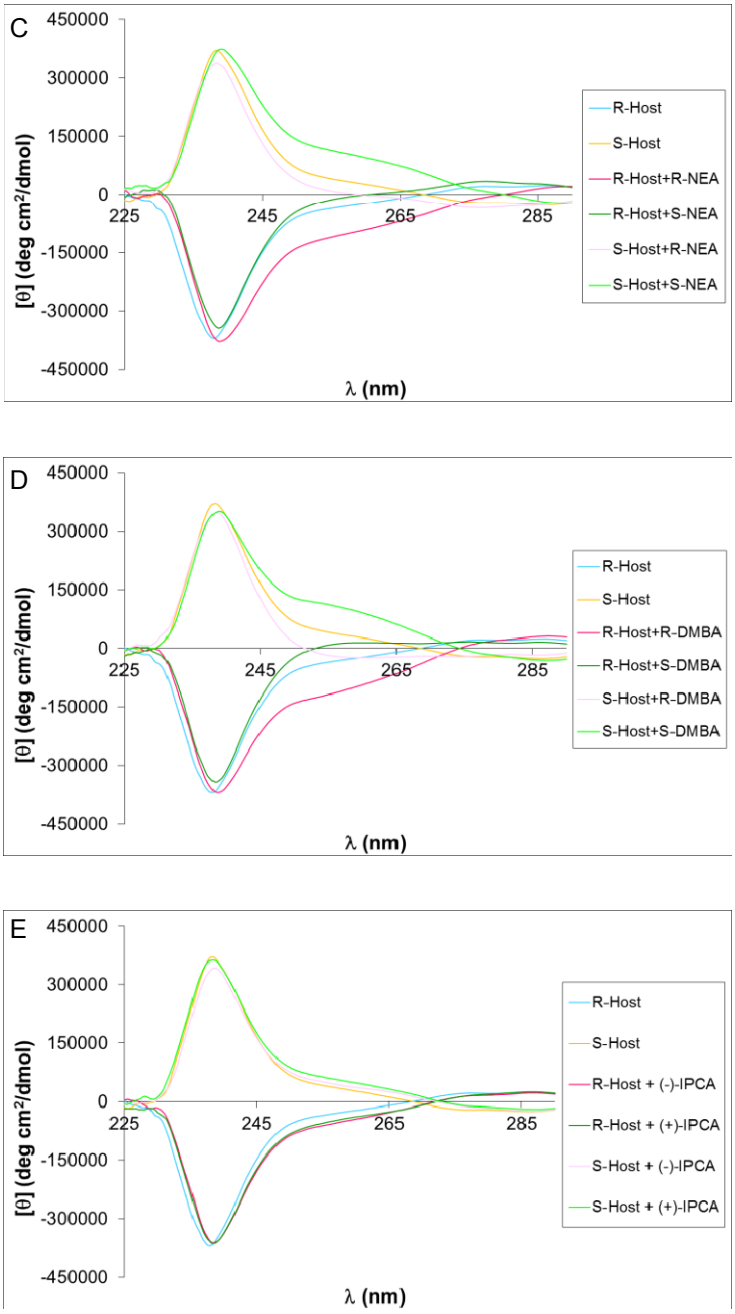

Figure S1. CD spectra for the assembly of BINOL, FPBA and A) CHEA, B) AH, C) NEA, D) DMBA and E) IPCA

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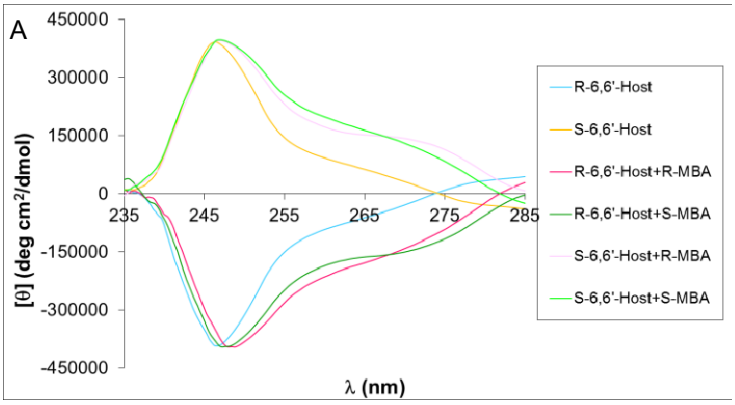

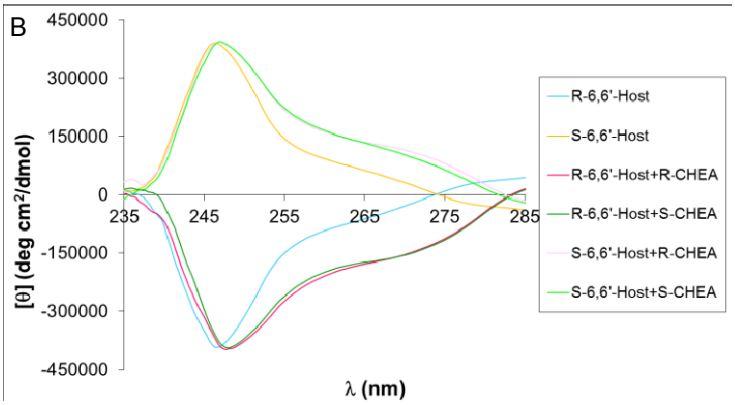

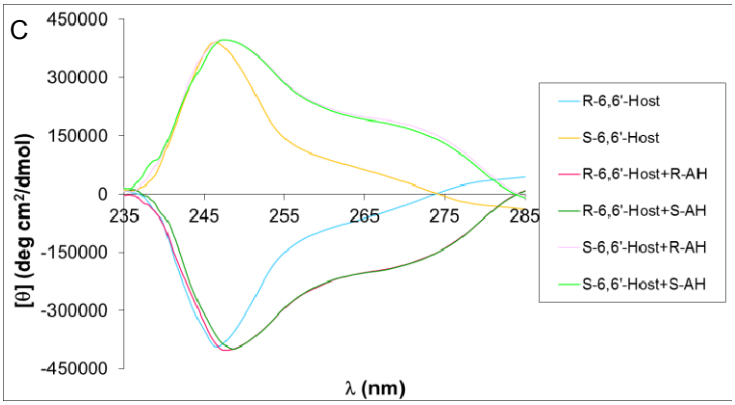

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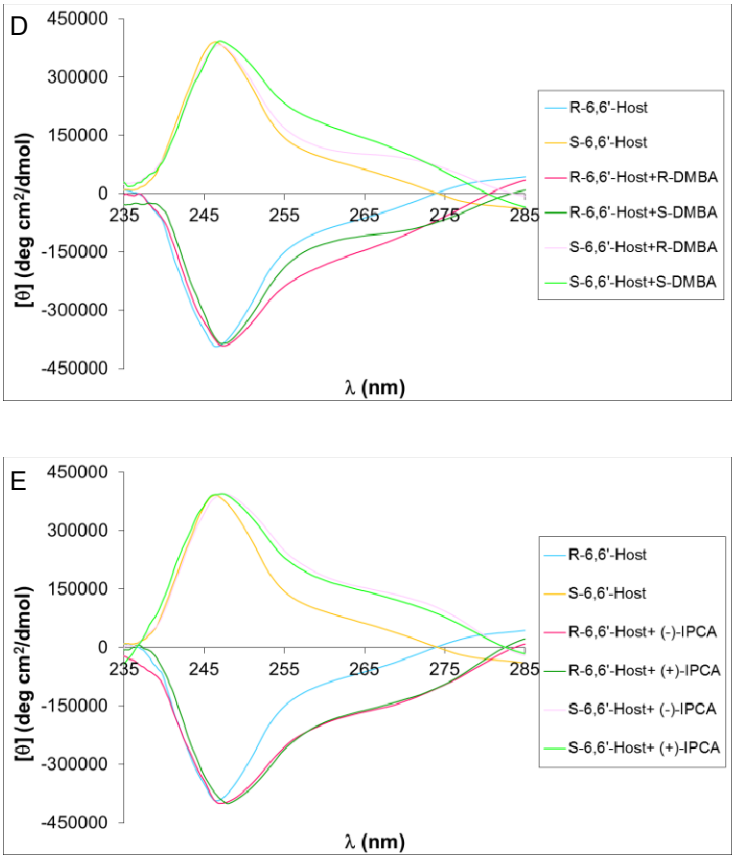

Figure S2. CD spectra for the assembly of 6,6'-DibromoBINOL, FPBA and A) MBA, B) CHEA, C) AH, D) DMBA and E) IPCA

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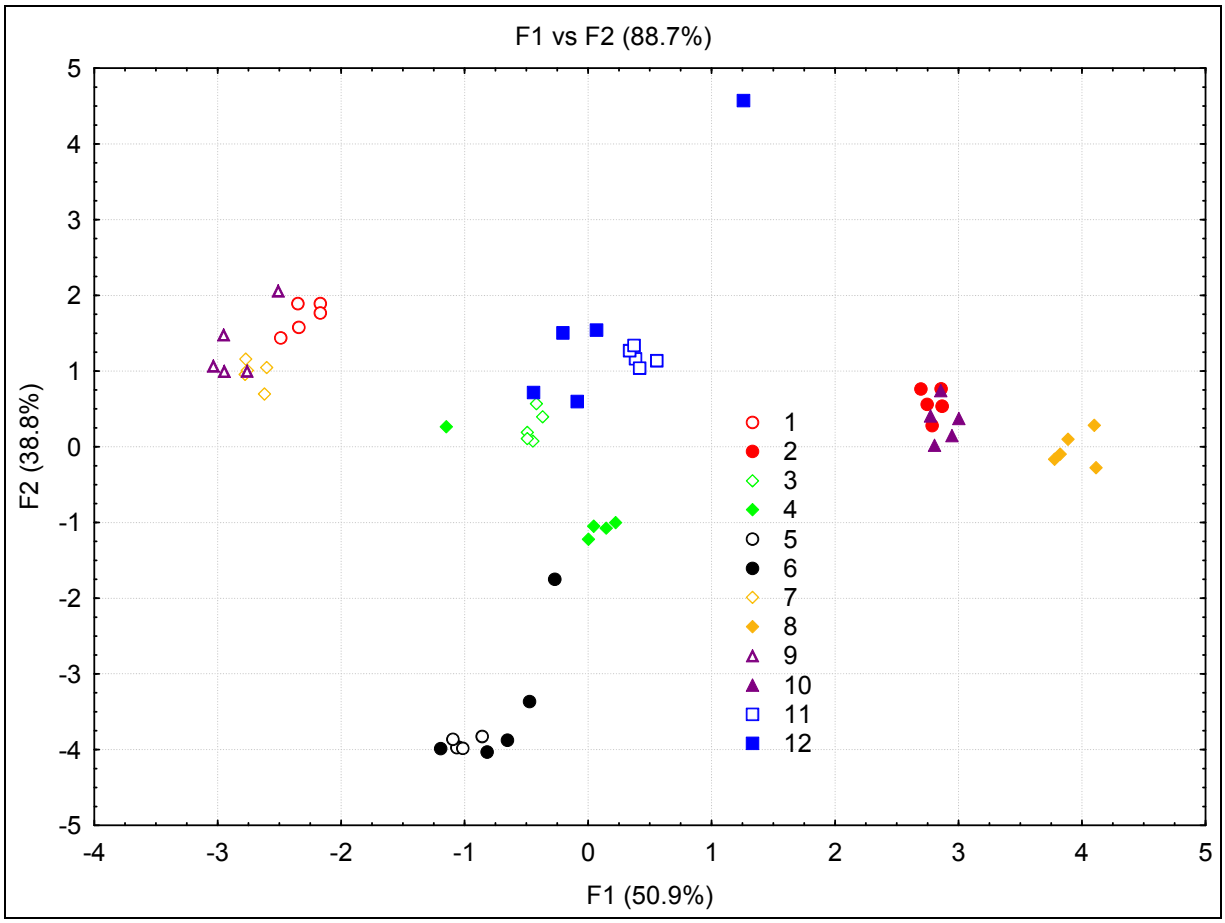

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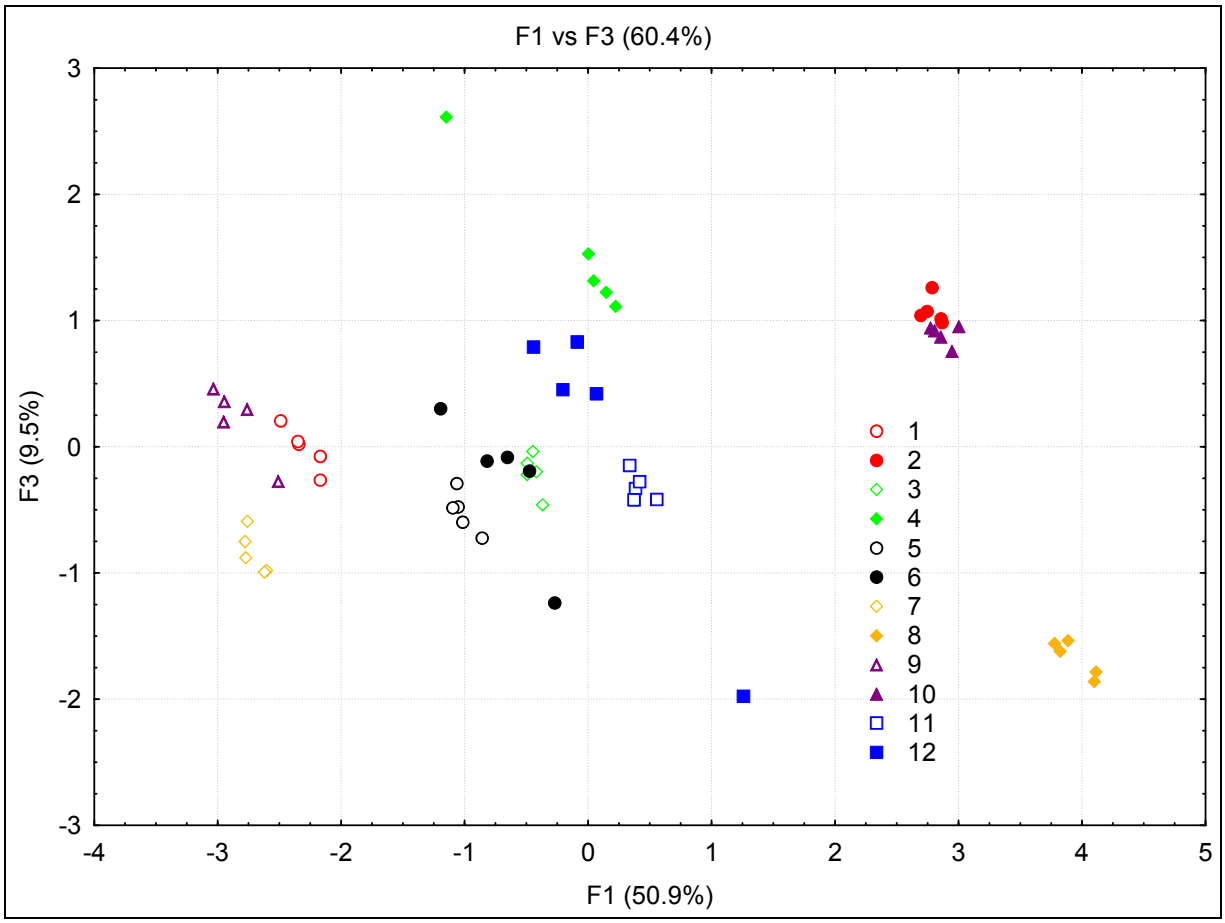

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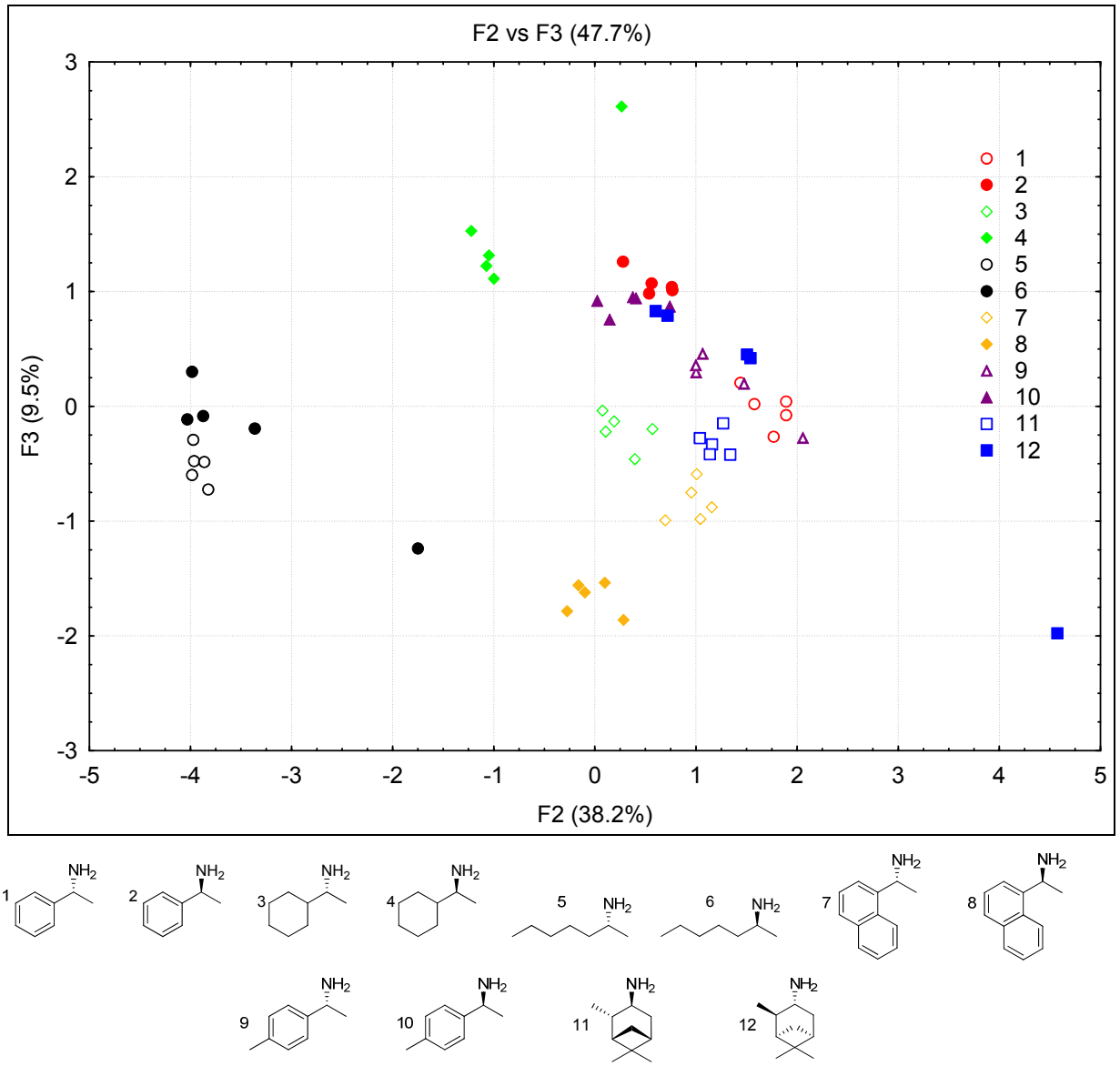

Figure S3. 2D PCA plots