A simple method of synthesis of ($\pm$)-2,3-diarylpiperazines and a novel method of resolution of ($\pm$)-2,3-diphenylpiperazine

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Supporting Information

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^{13}C Spectra of the compound 1a

^{13}C Spectra of the compound 1b

¹³C Spectra of the compound 1c

¹³C Spectra of the compound 1d

^{13}C Spectra of the compound 1e

Crystal Data: For compound **2a**: Molecular formula: $\text{C}_{20}\text{H}_{16}\text{F}_6\text{N}_2\text{O}_2$, MW = 430.35, monoclinic, space group: $P2(1)/c$, $a = 22.3786(10) \text{ \AA}$, $b = 16.5405(7) \text{ \AA}$, $c = 11.1443(5) \text{ \AA}$, $\beta = 103.3050(10)^\circ$, $V = 4014.4(3) \text{ \AA}^3$, $Z = 8$, $\rho_c = 1.424 \text{ Mg M}^{-3}$, $\mu = 0.130 \text{ mm}^{-1}$, $T = 273(2) \text{ K}$. Of the 45980 reflections collected, 9632 were unique ($R_{\text{int}} = 0.0378$). Refinement on all data converged at $R_1 = 0.0799$, $wR_2 = 0.2291$.

Figure S1. ORTEP diagram of the racemic 2a (one enantiomer is shown; thermal ellipsoids are drawn at 20% probability).

Crystal Data: For compound **3a**: Molecular formula: $\text{C}_{20}\text{H}_{28}\text{N}_2\text{O}_8$, MW = 424.44, Orthorhombic, space group: $P2(1)2(1)2$, $a = 9.2088(10) \text{ \AA}$, $b = 35.387(4) \text{ \AA}$, $c = 6.2519(7) \text{ \AA}$, $V = 2037.3(4) \text{ \AA}^3$, $Z = 4$, $\rho_c = 1.384 \text{ Mg M}^{-3}$, $\mu = 0.107 \text{ mm}^{-1}$, $T = 273(2) \text{ K}$. Of the 23736 reflections collected, 4860 were unique ($R_{\text{int}} = 0.0451$). Refinement on all data converged at $R_1 = 0.0483$, $wR_2 = 0.1071$.

Figure S2. ORTEP diagram of the tartrate salt 3a (thermal ellipsoids are drawn at 20% probability)

Figure S3. H-bonding aggregate of tartrate salt 3a