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Electronic Supplementary Information

Investigation of alkali metal ion binding to the diastereomeric complex between 1 and 2.

a. Representative mass spectra observed with the addition of various alkali acetate salts.

LiOAC



10 µM 1 + 10 µM each (R)-2 and (S)-d₁₀-2 (50/50 MeOH/H₂O + 100 µM LiOAc)

Figure S1 Mass spectrum for competitive binding determination of enantioselectivity in the presence of a 10fold excess (100 μ M) of LiOAc. Besides those peaks labeled, responses for $[1 + (R)-2 + Na]^+$ (m/z = 771), $[1 + (R)-2 + Na]^+$ $(S)-d_{10}-2 + Na]^+ (m/z = 781), [(1)_2 + H]^+ (m/z = 847), and [(1)_2 + Li]^+ (m/z = 853) are also observed.$

KOAc



10 µM 1 + 10 µM each (R)-2 and (S)-d₁₀-2 (50/50 MeOH/H₂O + 100 µM KOAc)

Figure S2 Mass spectrum for competitive binding determination of enantioselectivity in the presence of a 10fold excess (100 μ M) of KOAc. Besides those peaks labeled, responses for $[1 + (R)-2 + Na]^+$ (m/z = 771), $[1 + (R)-2 + Na]^+$ (S)-d₁₀-2 + Na]⁺ (m/z = 781), $[(1)_2 + H]^+$ (m/z = 847), and $[(1)_2 + K]^+$ (m/z = 885) are also observed.

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CsOAc



Figure S3 Mass spectrum for competitive binding determination of enantioselectivity in the presence of a 10-fold excess (100 μ M) of CsOAc. Besides those peaks labeled, responses for $[1 + (R)-2 + Na]^+$ (m/z = 771), $[1 + (S)-d_{10}-2 + Na]^+$ (m/z = 781), $[(1)_2 + H]^+$ (m/z = 847), and $[(1)_2 + Cs]^+$ (m/z = 979) are also observed.

b. Variation in individual ion abundance responses with molar excess alkali acetate present.



Figure S4 Assessment of the increase in α_{MS} (enantioselectivity) for 1 binding isotopomeric quasienantiomers of 2 as a function of LiOAc molar excess (N = 3). Analyte components are present at 10 μ M each.

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Figure S5 Assessment of the increase in α_{MS} (enantioselectivity) for 1 binding isotopomeric quasienantiomers of 2 as a function of KOAc molar excess (N = 3). Analyte components are present at 10 μ M each.



Figure S6 Assessment of the increase in α_{MS} (enantioselectivity) for 1 binding isotopomeric quasienantiomers of 2 as a function of CsOAc molar excess (N = 3). Analyte components are present at 10 μ M each.