Supporting information

Chiral differentiation of novel isoxazoline derivatives on "clicked" thioether and triazole bridged cyclodextrin chiral stationary phases

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1. Preparation of **CSP1** and **CSP2**

   The click syntheses of **CSP1** and **CSP2** were depicted in Figure S1.

   *Synthesis of **CSP1***

   Alkynyl functionalized silica (3 g) was suspended in a solution of β-CD derivatives in DMF (30 mL) and then CuI(PPh_3) (10 mmol %) was added. The reaction mixture was heated to 80 °C and kept for two days. The crude products were washed with DMF and thereafter extracted with acetone/methanol for 24 h before being vacuum dried to afford the final **CSP1**. Characterization: FTIR (cm^{-1}, KBr): 2940, 3400. Anal. found: C 13.63%, H 2.51%, N 1.42%.

   *Synthesis of **CSP2***

   Cationic CD (1.5 g) was added to a 20 mL of MeOH and DI water mixture (1:1, v/v) under stirring. After dissolving, thiol silica (3 g) and AIBN (50 mg) was added into the clear solution. The reaction mixture was stirred for 24 h with the protection of N_2. After that, the crude product was obtained by filtration and washed with DI water (2 × 20 mL), MeOH (2 × 20 mL) and acetone (2 × 20 mL) subsequently and vacuum dried at 60 °C (0.1 mbar) to afford the desired **CSP2**. Characterization: FTIR (cm^{-1}, KBr): 2900. Anal. found: C 9.59%, H 1.70%, N 0.48%.

2. Figures

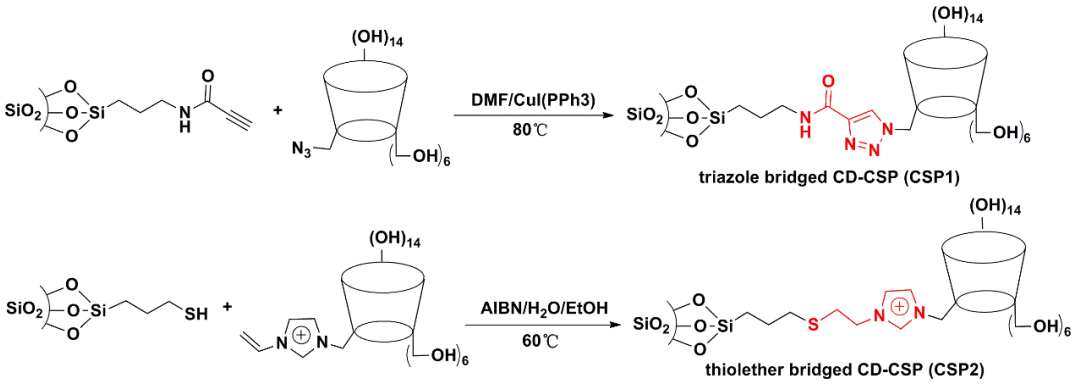


Figure S1 Click syntheses of **CSP1** and **CSP2**

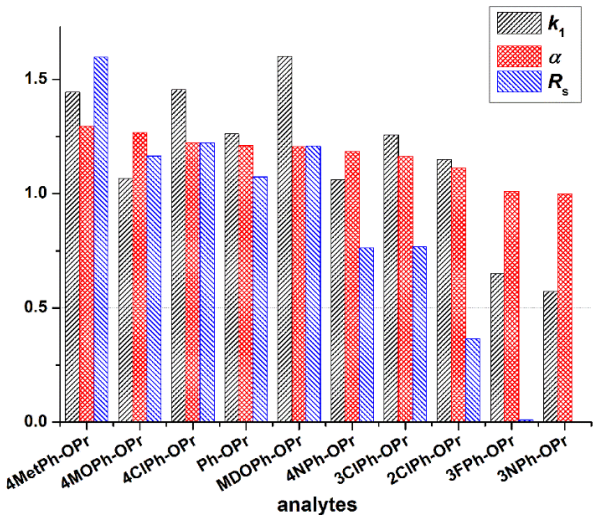
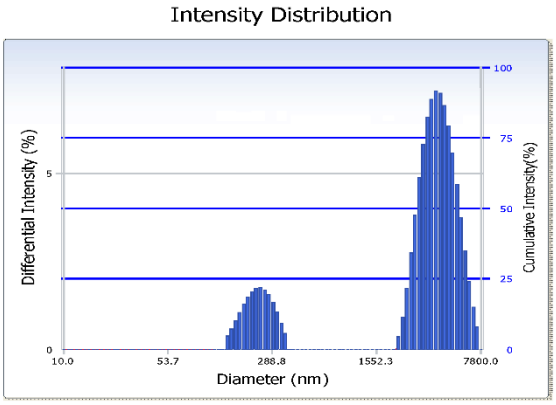


Figure S2 Enantioseparation of Ar-OPr on **CSP1**. Separation conditions: ACN/H_2O (v/v)=30/70, flow rate = 0.6 mL·min^{-1}, 25 ^{o}C



Distribution Results (Contin)

Peak	Diameter (nm)	Std. Dev.
1	222.3	1,106.8
2	4,771.8	61.5
3	0.0	0.0
4	0.0	0.0
5	0.0	0.0
Average	4,023.7	195.2

Figure S3 Particle size distribution of **CSP1**

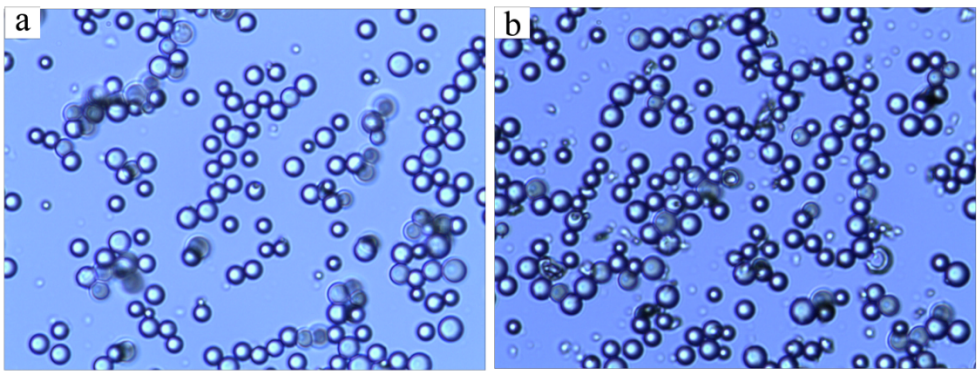


Figure S4 Electron Microscopy images of bare silica (a)and **CSP1** (b)

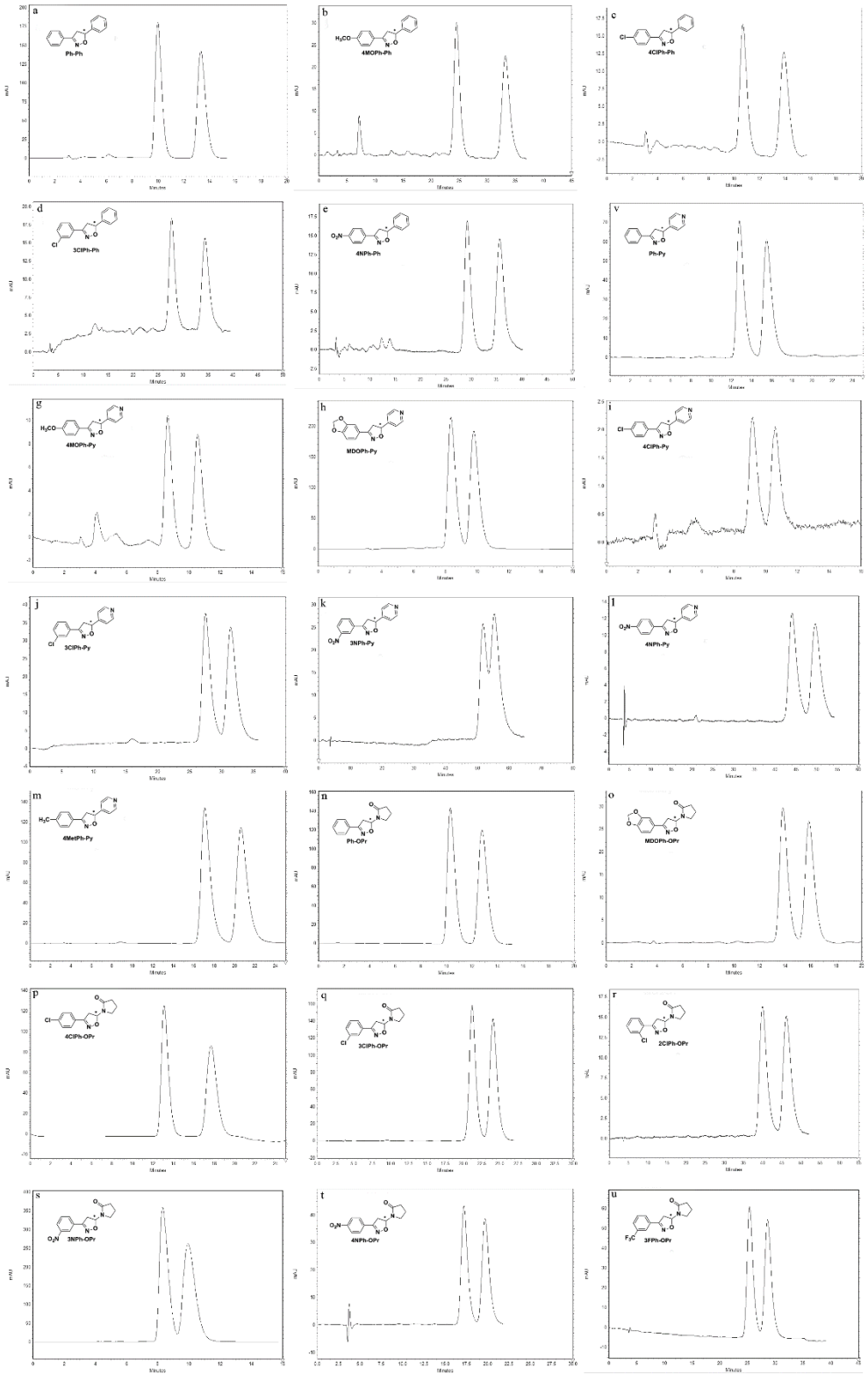


Figure S5 Chromatograms of analytes separated on **CSP1**. Separation conditions: (a, c, g, h, i) ACN/H_2O (v/v)=40/60, flow rate = 0.6 mL·min^{-1}, 25 ^{o}C; (b, d, e, m, v) ACN/H_2O (v/v)=30/70, flow rate = 0.6 mL·min^{-1}, 25 ^{o}C; (o, j) ACN/H_2O (v/v)=25/75, flow rate = 0.6 mL·min^{-1}, 25 ^{o}C; (f, l, q, t) ACN/H_2O (v/v)=20/80, flow rate = 0.6 mL·min^{-1}, 25 ^{o}C; (k, u) ACN/H_2O (v/v)=15/85, flow rate = 0.6 mL·min^{-1}, 25 ^{o}C; (n, p, s) MeOH/H_2O (v/v)=50/50, flow rate = 0.6 mL·min^{-1}, 25 ^{o}C; (r) MeOH/H_2O (v/v)=30/70, flow rate = 0.6 mL·min^{-1}, 25 ^{o}C

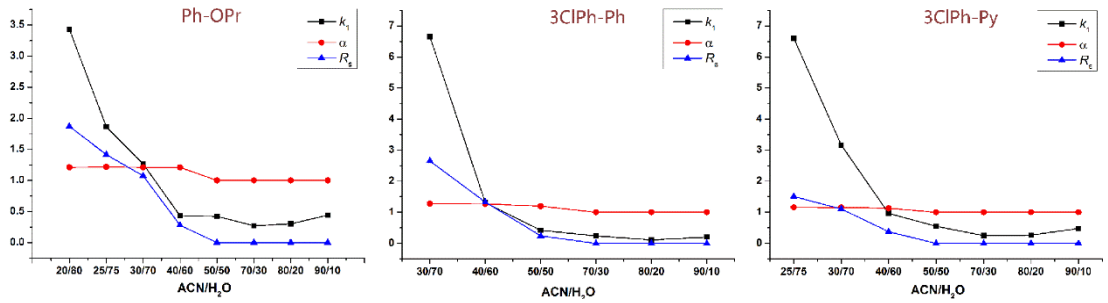


Figure S6 Effect of MP composition. Conditions: 0.6mL·min^{-1}, 25 ^{o}C

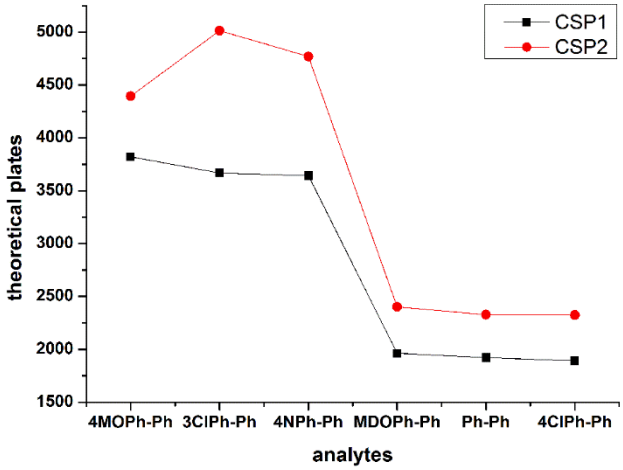


Figure S7 Comparison of column efficiency on **CSP1** and **CSP2**. Conditions: 1. ACN/H_2O=30/70, 0.6mL·min^{-1}, 25 ^{o}C (4MOPh-Ph/3ClPh-Ph/4NPh-Ph) 2. ACN/H_2O=40/60, 0.6mL·min^{-1}, 25 ^{o}C (MDOPh-Ph/4ClPh-Ph/Ph-Ph).

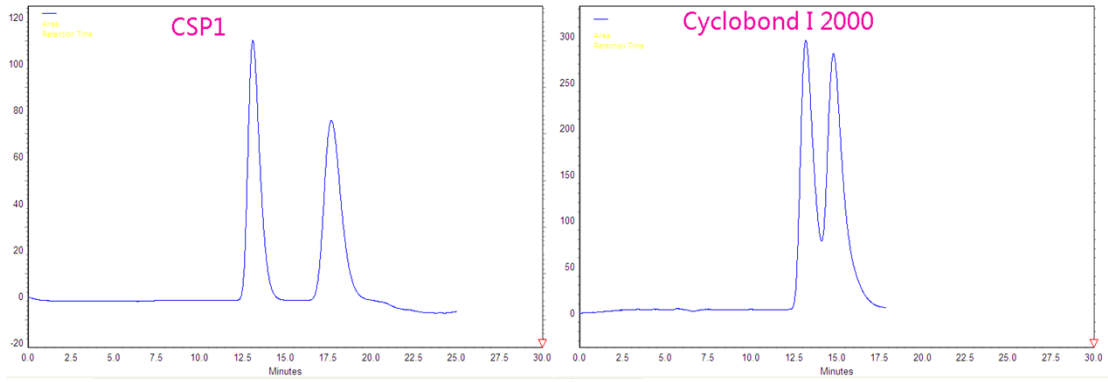


Figure S8. Comparison of enantioseparation of 4ClPh-OPr on **CSP1** and Cyclobond I *2000*. Conditions: flow rate = 0.6 mL·min^{-1}, MeOH/H2O=50/50 (v/v), 25 ^{o}C.