

Electronic Supplementary Information

for

Evaluation and comparison of *N*-cycloalkylformylated chitosan bis(arylcarbamate)s as chiral selectors for enantioseparation

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1. ¹H NMR spectra of CSs2-4

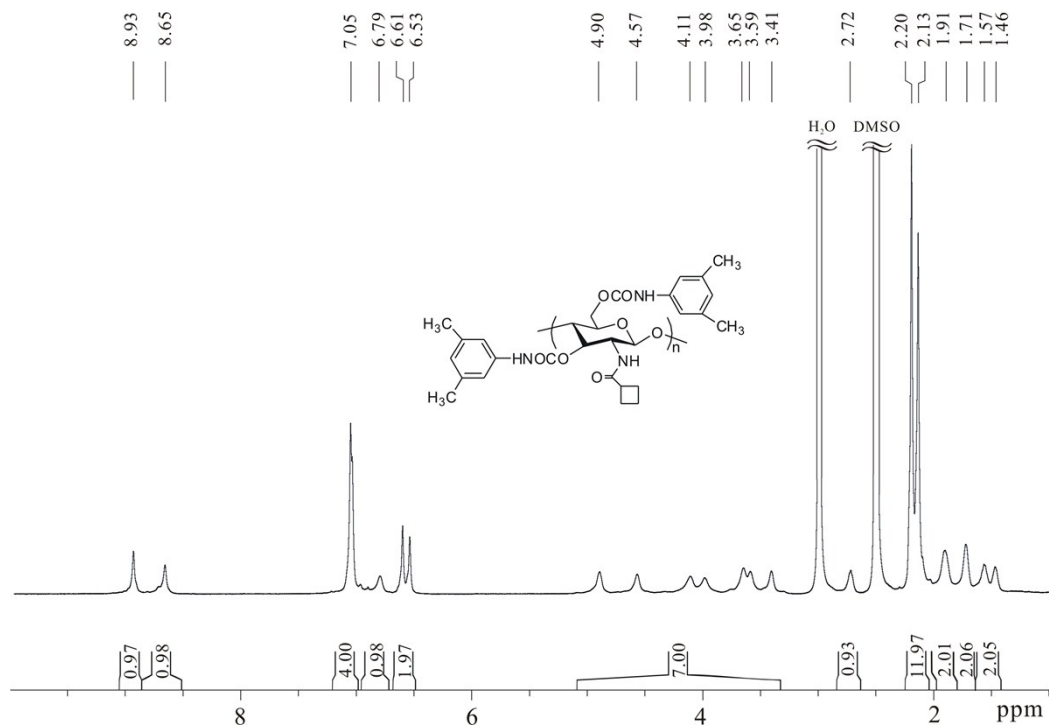


Fig. S1 ¹H NMR spectrum of chitosan bis(3,5-dimethylphenylcarbamate)-(N-cyclobutylformamide) (CS2) (600 MHz, DMSO-*d*₆, 90 °C)

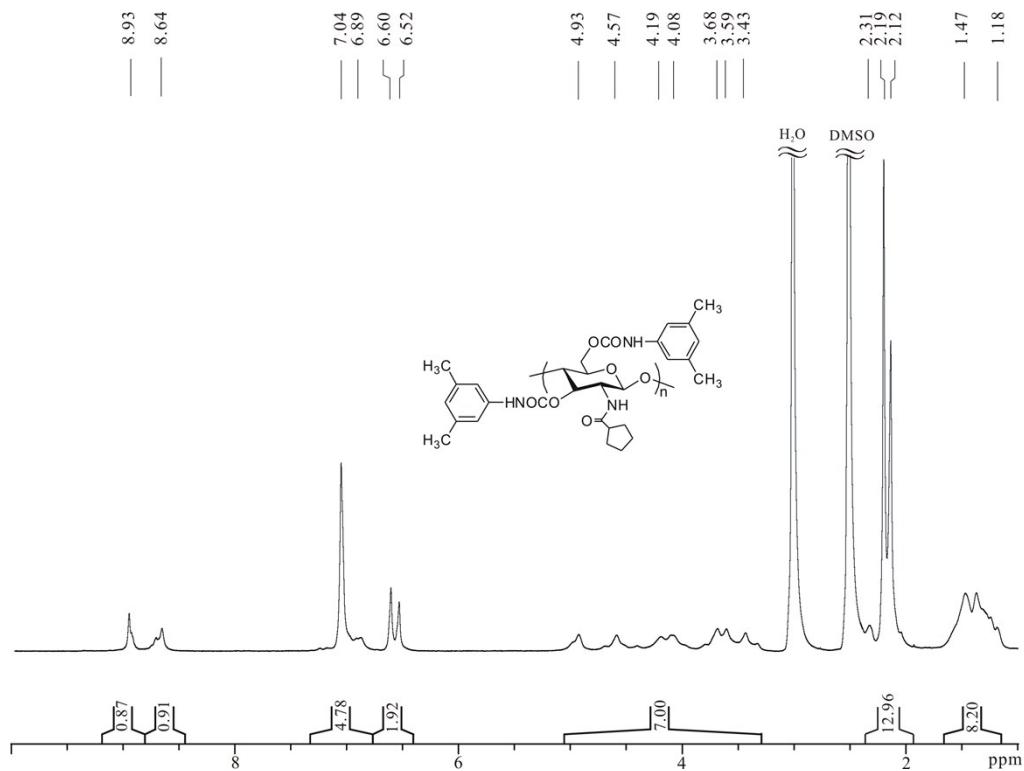


Fig. S2 ^1H NMR spectrum of chitosan bis(3,5-dimethylphenylcarbamate)-(N-cyclopentylformamide) (CS3) (600 MHz, $\text{DMSO-}d_6$, 90 °C)

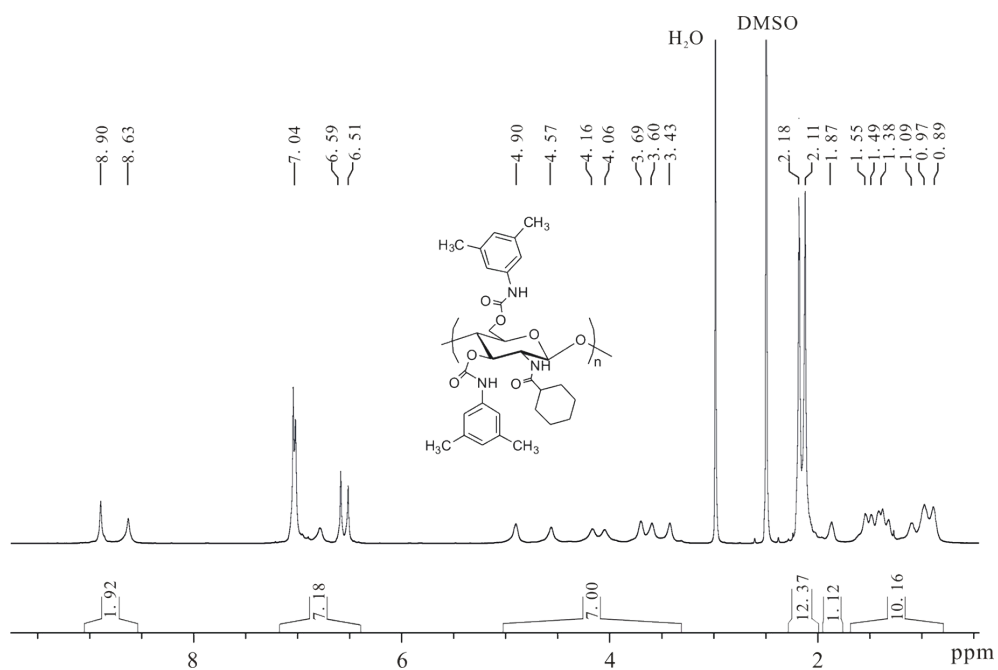


Fig. S3 ^1H NMR spectrum of chitosan bis(3,5-dimethylphenylcarbamate)-(N-cyclohexylformamide) (CS4) (600 MHz, $\text{DMSO-}d_6$, 90 °C)

2. Structures of the tested nineteen racemates

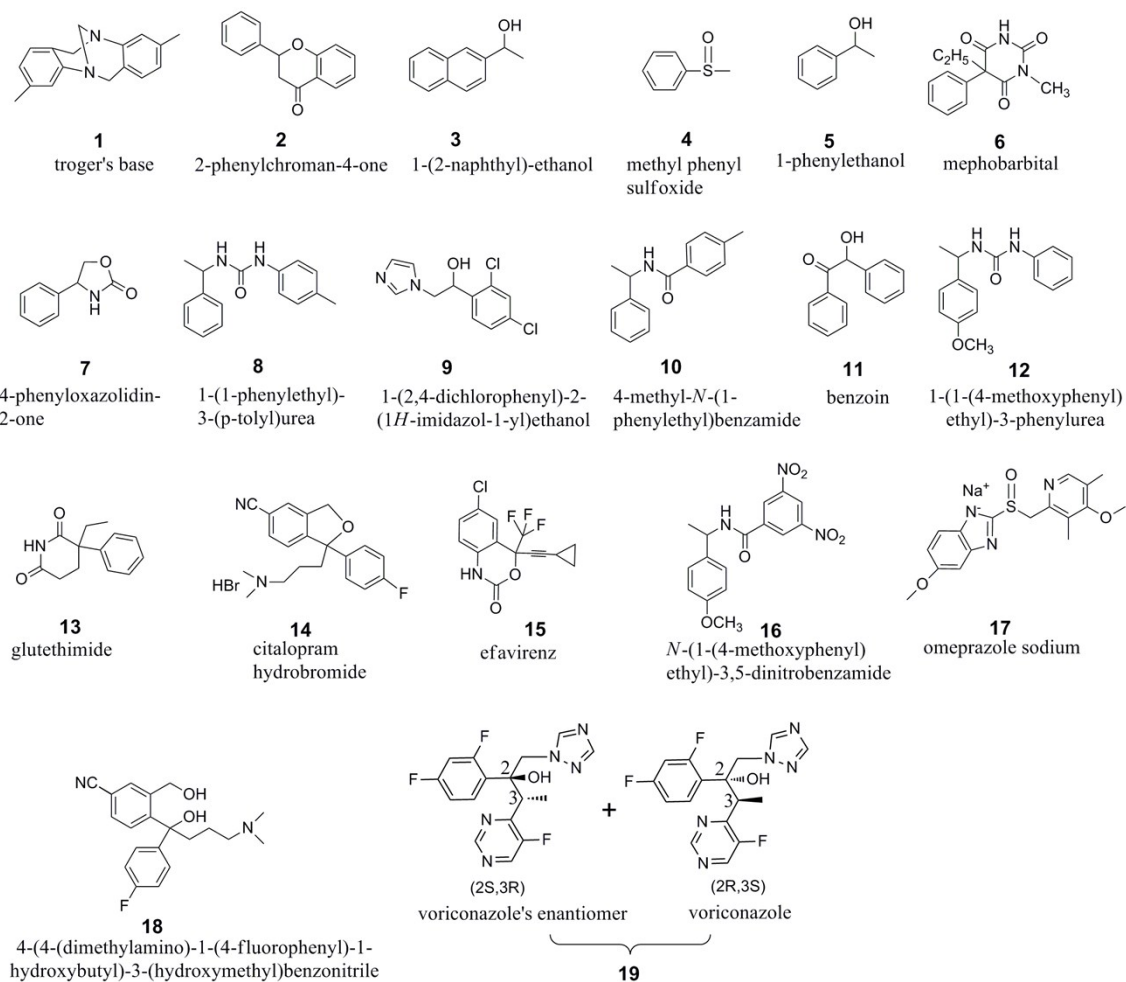


Fig. S4 Structures of the tested nineteen racemates.

3. Numbers of the racemates recognized and baseline separated by CSPs1–4

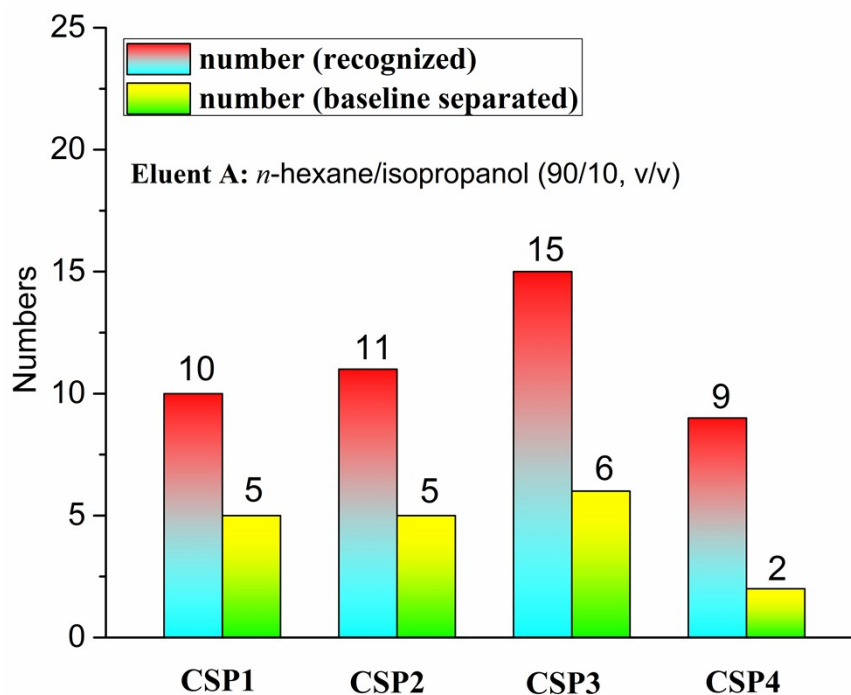


Fig. S5 Numbers of the racemates recognized and baseline separated by CSPs1–4 in eluent A

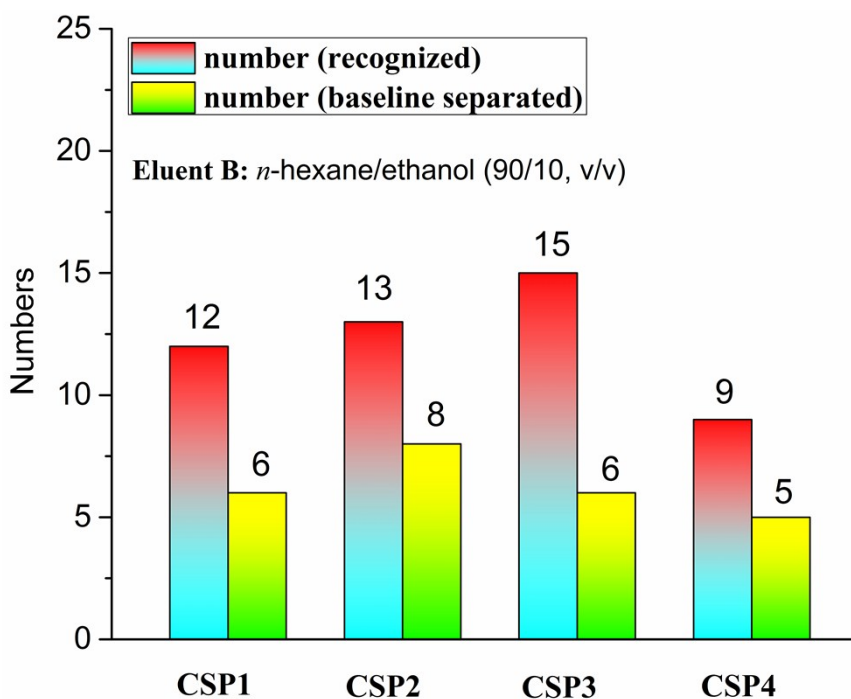


Fig. S6 Numbers of the racemates recognized and baseline separated by CSPs1–4 in eluent B.

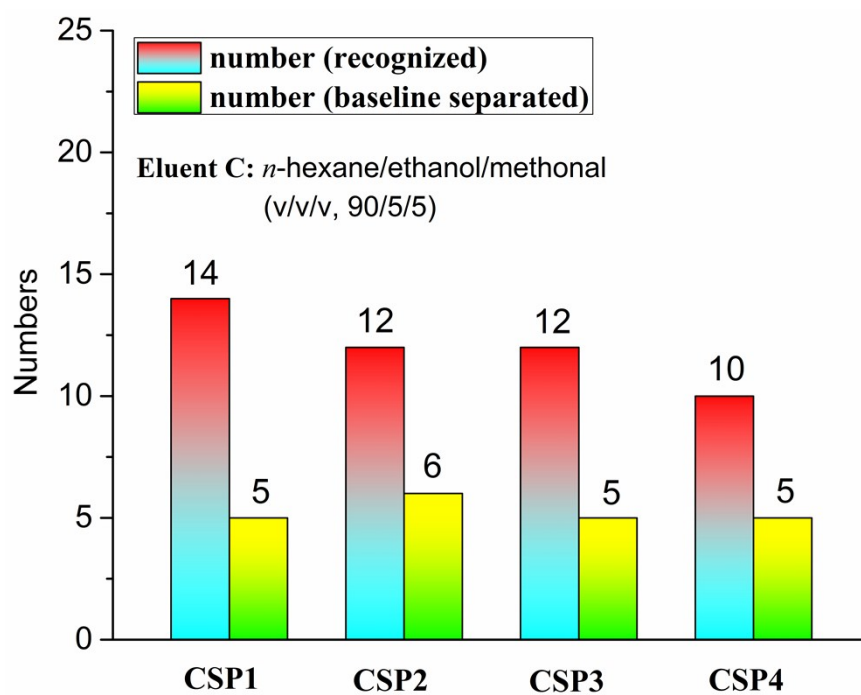


Fig. S7 Numbers of the racemates recognized and baseline separated by **CSPs1–4** in eluent C.

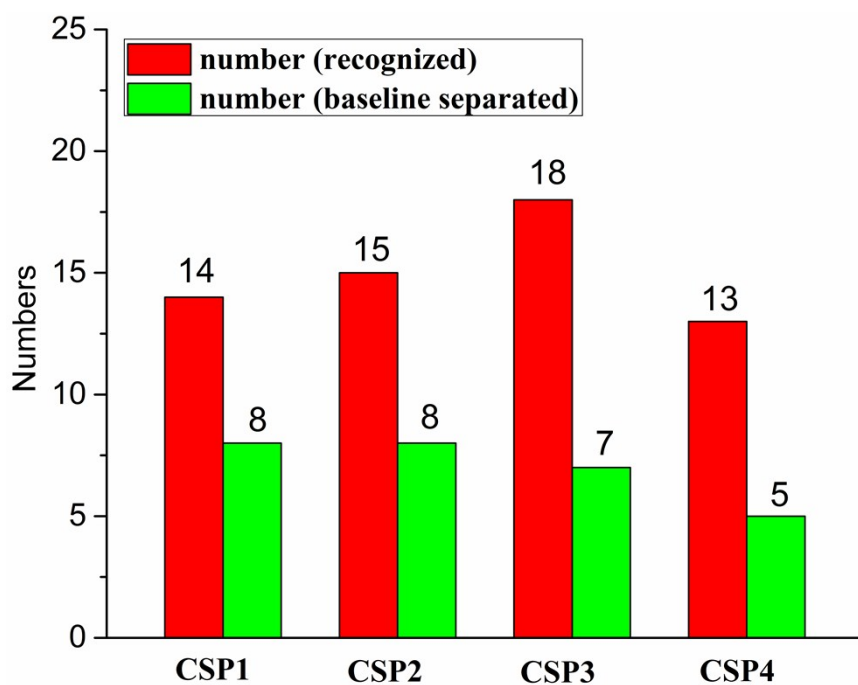


Fig. S8 Total numbers of the racemates recognized and baseline separated by **CSPs1–4** in eluents A, B and C.

4. Enantioseparation results of CSPs1–4

Table S1 Enantioseparation results of CSPs1–4

S.N.	CSP1			CSP2			CSP3			CSP4			Eluent
	k_1	α	R_s	k_1	α	R_s	k_1	α	R_s	k_1	α	R_s	
1	0.32	1.00	0.00	0.27	1.00	0.00	0.33 ⁻	1.21	1.00	0.30	1.00	0.00	A
	0.27 ⁻	1.14	0.43	0.22	1.00	0.00	0.26 ⁻	1.25	1.09	0.23	1.00	0.00	B
	0.31 ⁻	1.15	0.55	0.22	1.00	0.00	0.29 ⁻	1.25	1.20	0.23	1.00	0.00	C
2	1.23 ⁻	1.74	6.56	1.21 ⁻	1.57	4.02	1.40 ⁻	1.47	4.53	0.97 ⁻	1.43	2.88	A
	1.03 ⁻	1.78	6.17	0.90 ⁻	1.55	3.99	1.02 ⁻	1.43	4.28	0.70 ⁻	1.34	2.37	B
	1.14 ⁻	1.75	7.60	0.96 ⁻	1.48	3.70	1.11 ⁻	1.40	4.24	0.70 ⁻	1.37	2.40	C
3	1.34	1.00	0.00	1.20	1.00	0.00	1.49	1.00	0.00	1.30	1.00	0.00	A
	0.77	1.00	0.00	0.71	1.00	0.00	0.87 ⁻	1.07	0.19	0.71	1.00	0.00	B
	0.83	1.00	0.00	0.66	1.00	0.00	0.81 ⁻	1.05	0.11	0.69	1.00	0.00	C
4	2.46 ⁺	1.04	0.23	3.12 ⁺	1.10	0.95	3.09 ⁺	1.25	1.02	2.99	1.00	0.00	A
	1.50 ⁺	1.04	0.19	1.63 ⁺	1.11	1.13	1.80 ⁺	1.05	0.30	1.53	1.00	0.00	B
	1.75 ⁺	1.07	0.83	1.30 ⁺	1.09	0.87	1.68	1.00	0.00	1.32	1.00	0.00	C
5	0.81	1.00	0.00	0.42	1.00	0.00	0.81 ⁻	1.11	0.87	0.65 ⁻	1.11	0.24	A
	0.50	1.00	0.00	0.39	1.00	0.00	0.58 ⁻	1.06	0.10	0.51	1.00	0.00	B
	0.53	1.00	0.00	0.40	1.00	0.00	0.61	1.00	0.00	0.51	1.00	0.00	C
6	2.94	1.73	3.84	5.70	1.38	1.33	2.98	1.77	3.02	6.01	1.20	0.34	A
	2.12	1.45	3.35	3.19	1.40	2.73	2.37	1.48	2.92	2.86	1.17	0.85	B
	2.19	1.44	3.36	2.58	1.42	3.36	2.23	1.44	4.01	2.44	1.11	0.48	C
7	12.75 ^R	1.15	1.27	12.93 ^R	1.37	1.85	12.93 ^S	1.35	2.46	11.51	1.00	0.00	A
	6.43 ^R	1.48	4.14	6.63 ^R	1.41	2.98	6.99 ^R	1.33	3.10	5.16 ^R	1.09	0.42	B
	5.51 ^R	1.44	4.21	4.80 ^R	1.29	3.18	5.51 ^R	1.23	2.86	4.30 ^R	1.09	0.88	C

Table S1 to be continued

Continued from Table S1

S.N.	CSP1			CSP2			CSP3			CSP4			Eluent
	k_1	α	R_s	k_1	α	R_s	k_1	α	R_s	k_1	α	R_s	
8	5.84	1.00	0.00	4.05 ^S	1.21	0.82	4.06 ^S	1.38	0.81	6.39	1.00	0.00	A
	1.34	1.00	0.00	1.16 ^S	1.10	0.50	1.31 ^S	1.15	0.38	1.14	1.00	0.00	B
	1.18	1.00	0.00	0.89	1.00	0.00	1.09	1.00	0.00	0.98	1.00	0.00	C
9	3.59 ⁺	1.83	2.80	3.78 ⁺	1.76	3.27	3.90 ⁺	1.58	3.16	3.59 ⁺	1.51	1.75	A
	1.39 ⁺	1.51	2.92	1.58 ⁺	1.48	2.83	1.80 ⁺	1.39	2.36	1.39 ⁺	1.45	1.90	B
	1.45 ⁺	1.30	1.28	1.30 ⁺	1.32	2.14	1.55 ⁺	1.15	1.16	1.35 ⁺	1.48	2.54	C
10	2.31	1.00	0.00	1.88	1.00	0.00	1.91 ^R	1.12	0.16	1.94	1.00	0.00	A
	0.80	1.00	0.00	0.75	1.00	0.00	0.81 ^S	1.10	0.10	0.70	1.00	0.00	B
	0.77	1.00	0.00	0.66	1.00	0.00	0.78	1.00	0.00	0.67	1.00	0.00	C
11	2.46 ⁻	1.19	2.79	2.50 ⁻	1.19	1.52	2.77 ⁻	1.26	2.71	2.50 ⁻	1.13	1.10	A
	1.63 ⁻	1.29	2.05	1.56 ⁻	1.26	2.15	1.91 ⁻	2.45	3.33	1.48 ⁻	1.36	3.06	B
	1.84 ⁻	1.13	1.08	1.45 ⁻	1.17	1.16	1.77 ⁻	1.27	3.87	1.46 ⁻	1.40	3.57	C
12	6.16 ^S	1.33	1.46	6.49 ^S	1.37	1.65	6.59 ^S	1.44	1.70	8.52 ^S	1.04	0.10	A
	1.75 ^S	1.25	0.77	1.77 ^S	1.25	1.50	1.87 ^S	1.28	1.30	1.52	1.00	0.00	B
	2.18 ^S	1.24	0.78	1.33 ^S	1.09	0.60	1.53 ^S	1.10	1.09	1.36	1.00	0.00	C
13	-	-	-	-	-	-	-	-	-	-	-	-	A
	13.44 ⁺	1.14	1.29	15.51 ⁺	1.21	1.94	17.83 ⁺	1.12	1.23	12.06	1.00	0.00	B
	10.33 ⁺	1.16	1.67	10.29 ⁺	1.16	1.96	13.59 ⁺	1.09	1.09	9.12	1.00	0.00	C
14	1.28 ^S	1.48	2.08	1.18 ^S	1.27	0.93	1.45 ^S	1.27	0.23	0.98 ^S	1.24	0.18	A
	0.84 ^S	1.28	1.36	0.77 ^S	1.20	0.87	1.04 ^S	1.26	0.11	0.68 ^S	1.20	0.26	B
	0.97 ^S	1.28	1.43	0.76 ^S	1.17	0.88	0.98 ^S	1.20	0.39	0.70 ^S	1.22	0.93	C

Table S1 to be continued

Continued from Table S1

S.N.	CSP1			CSP2			CSP3			CSP4			Eluent
	k_1	α	R_s	k_1	α	R_s	k_1	α	R_s	k_1	α	R_s	
15	2.31 ^S	1.09	0.22	2.32 ^S	1.09	0.63	2.23 ^S	1.16	1.20	2.37 ^S	1.14	0.85	A
	1.32	1.00	0.00	1.38	1.00	0.00	1.42	1.00	0.00	1.19	1.00	0.00	B
	1.29 ^R	1.12	1.08	1.19	1.00	0.00	1.29	1.00	0.00	1.14	1.00	0.00	C
16	-	-	-	-	-	-	-	-	-	-	-	-	A
	26.14	1.00	0.00	19.67 ^S	1.18	1.23	21.79	1.00	0.00	15.10 ^R	1.40	2.49	B
	22.05 ^S	1.07	0.40	17.15 ^S	1.07	0.63	22.38	1.00	0.00	15.30 ^R	1.36	2.96	C
17	16.76	1.00	0.00	14.78	1.00	0.00	13.23 ^S	1.11	0.22	-	-	-	A
	5.75	1.00	0.00	6.55	1.00	0.00	5.74	1.00	0.00	4.82 ^S	1.09	0.19	B
	4.47	1.00	0.00	4.33 ^R	1.12	0.83	4.24	1.00	0.00	3.66 ^R	1.16	1.03	C
18	4.13 ^S	1.28	1.05	3.23 ^S	1.17	0.62	4.03 ^S	1.04	0.10	2.68 ^S	1.29	0.21	A
	1.49 ^S	1.20	0.98	1.62 ^S	1.04	0.26	1.81	1.00	0.00	1.44	1.00	0.00	B
	1.71 ^S	1.22	1.17	1.43	1.00	0.00	1.70 ^S	1.03	0.10	1.25 ^R	1.07	0.12	C
19	-	-	-	9.42	1.00	0.00	-	-	-	-	-	-	A
	3.37 ^{2R, 3S}	4.12	10.36	3.24 ^{2R, 3S}	8.64	12.28	3.65 ^{2R, 3S}	5.25	10.92	2.61 ^{2R, 3S}	3.68	7.15	B
	2.51 ^{2R, 3S}	2.80	8.29	2.19 ^{2R, 3S}	5.38	12.95	2.62 ^{2R, 3S}	3.61	10.52	1.93 ^{2R, 3S}	2.14	5.09	C

S.N.: serial number of the racemates. Eluents: A: *n*-hexane/isopropanol (90/10, v/v), B: *n*-hexane/ethanol (90/10, v/v), and C: *n*-hexane/ethanol/methanol (90/5/5, v/v/v); flow rate: 1.0 ml min⁻¹; detection temperature: 25 °C. “-” means that the racemate was retained too long, hence the data were unavailable. “+”, “-”, “R”, “S” and “(2R, 3S)” at the superscript of k_1 refer to the optical rotation or configuration of the first-eluted enantiomer. Enantioseparation results of CSP2 were cited from our previously reported work.¹

References

1. J. Zhang, X. C. Wang, W. Chen and Z. W. Bai, *Analyst*, 2016, **141**, 4470-4480.