Electronic Supplementary Information

for

Performance evaluation of enantioseparation materials based on chitosan isobutylurea derivatives

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1. Structures of chiral analytes

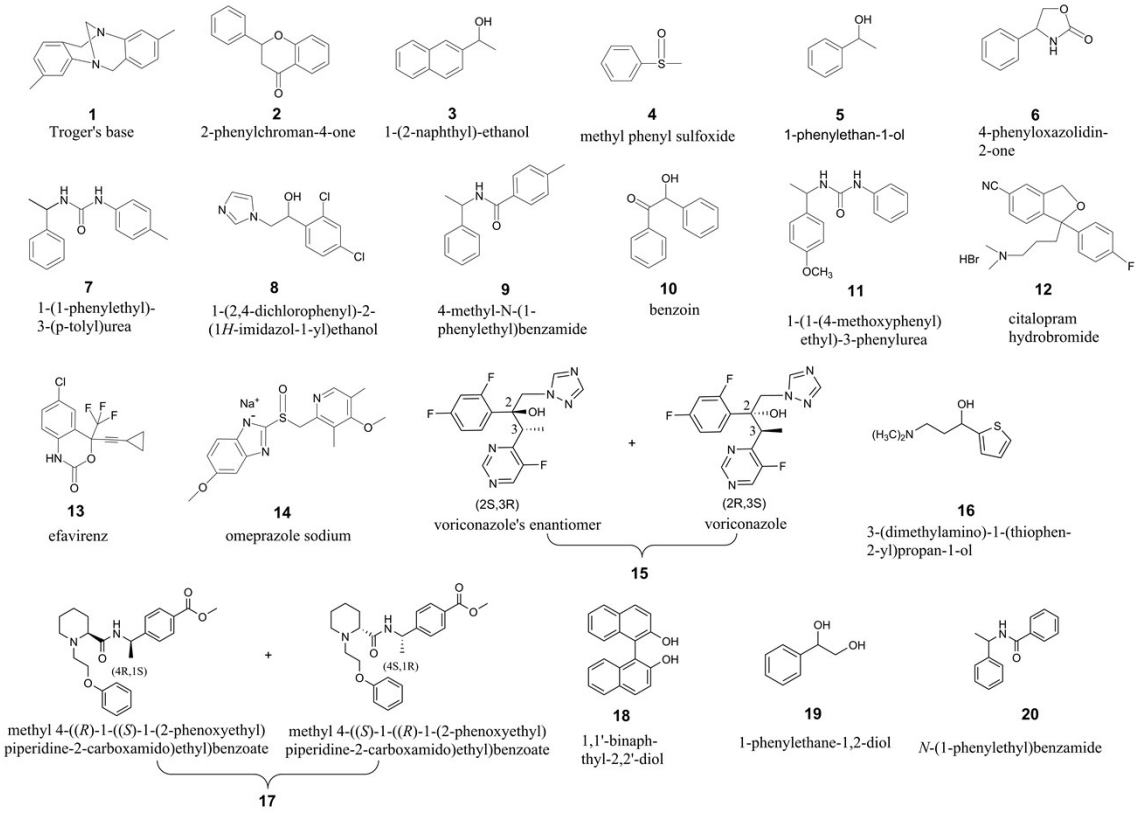

Fig. S1 Structures of chiral analytes[1]

2. ^{1}H NMR spectrum of chitosan isobutylurea

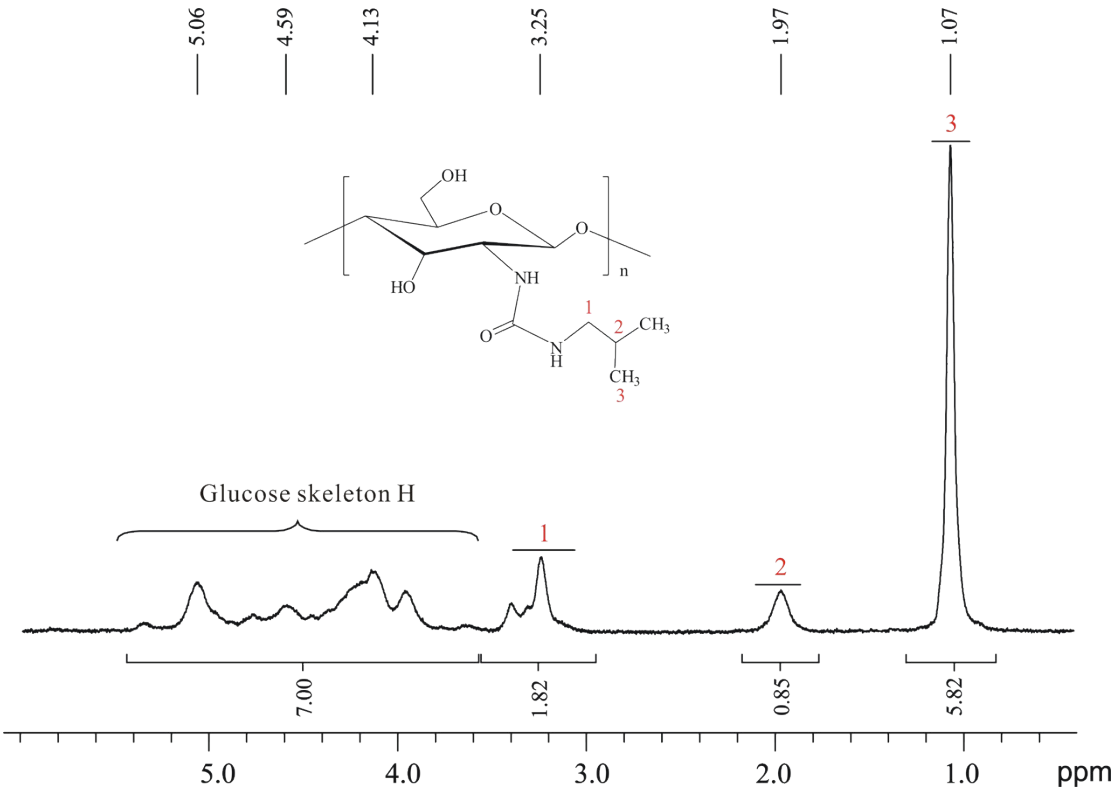

Fig. S2 ^{1}H NMR spectrum of chitosan isobutylurea (400 MHz, CF_3COOD, 25 ^{o}C).

3. ^{1}H NMR spectra of *CSs1–3*

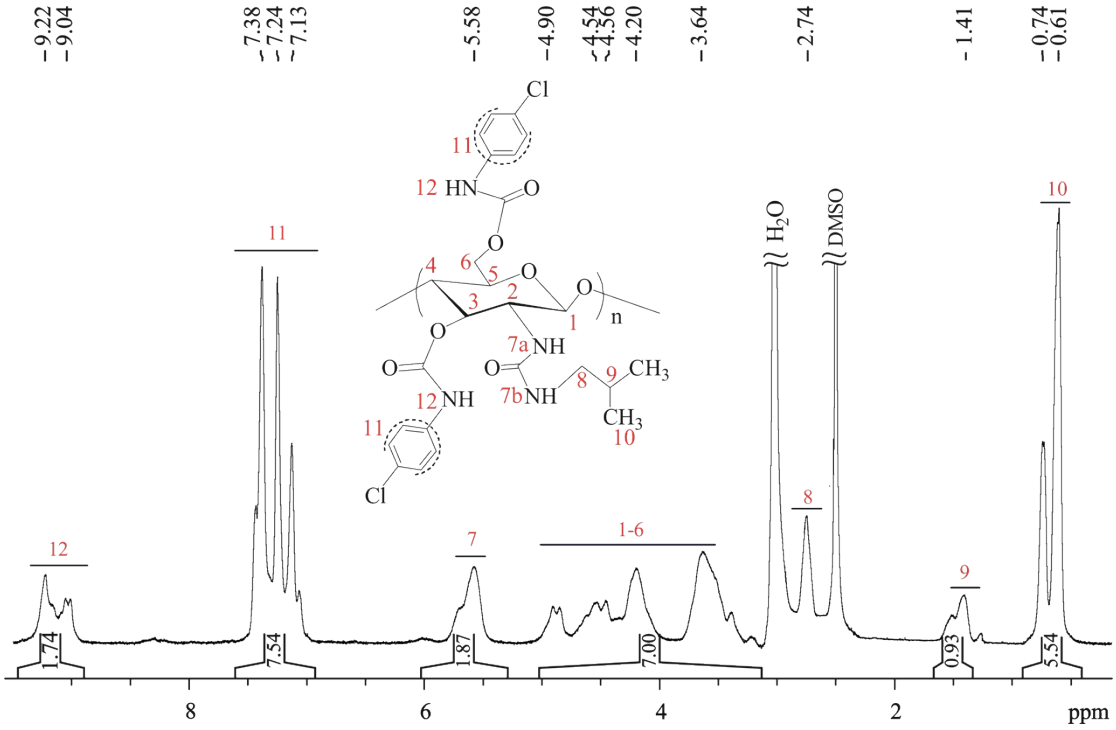

Fig. S3 ^{1}H NMR spectrum of *CS1* (600 MHz, DMSO-d_6, 90 °C)

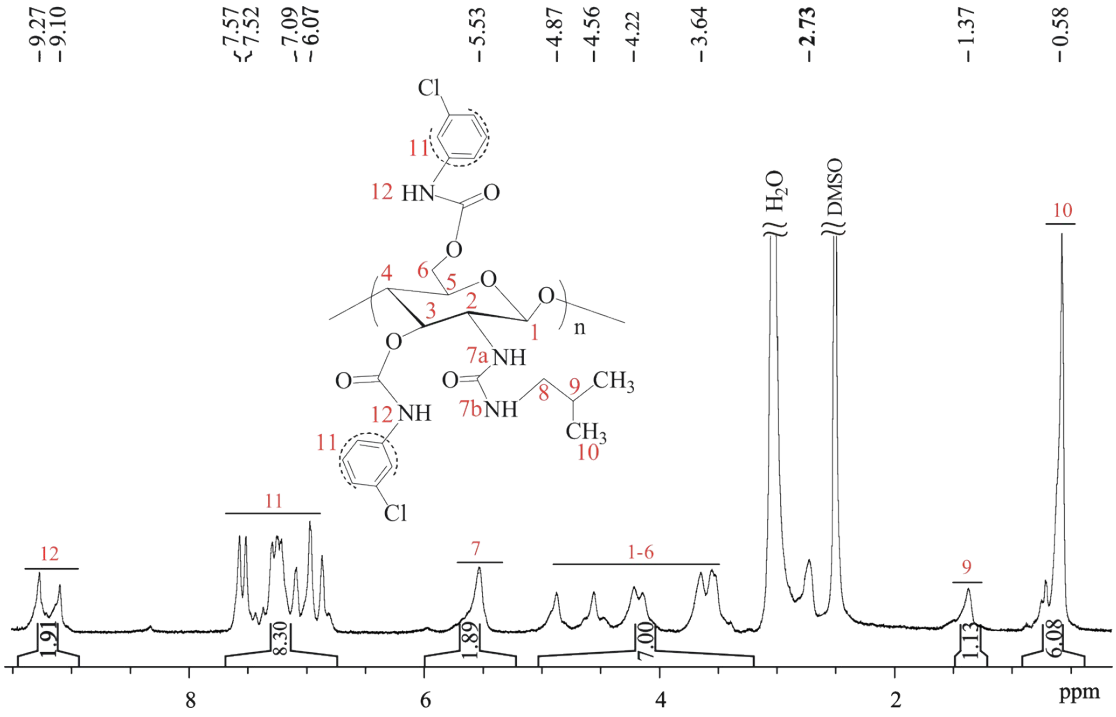

Fig. S4 ^{1}H NMR spectrum of *CS2* (600 MHz, DMSO-d_6, 90 °C)

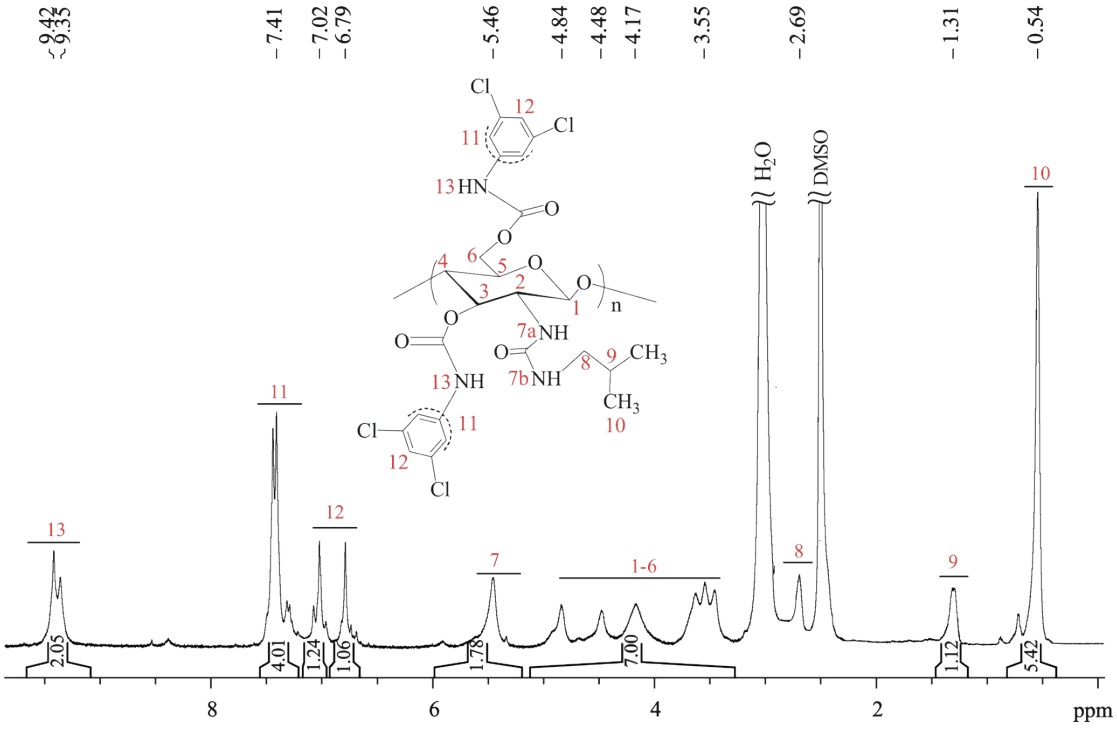

Fig. S5 ^{1}H NMR spectrum of *CS3* (600 MHz, DMSO-d_6, 90 ^{o}C)

4. Enantioseparation results of ADMPC- and CDMPC-based CSPs

Table S1 Enantioseparation results of ADMPC- and CDMPC-based CSPs

S.N.	ADMPC-based CSP			CDMPC-based CSP			M.P.
	k_1	α	R_s	k_1	α	R_s	
1	$^{+}$0.57	1.52	2.04	$^{+}$1.08	1.42	3.17	A
	$^{+}$0.52	1.88	3.73	$^{+}$0.97	1.49	3.90	B
	$^{+}$0.53	1.86	3.84	$^{+}$1.01	1.31	2.71	C
2	$^{+}$1.09	1.22	1.55	$^{-}$1.68	1.30	3.49	A
	$^{+}$1.18	1.49	3.22	$^{-}$1.48	1.23	2.68	B
	$^{+}$1.23	1.72	4.70	$^{-}$1.53	1.28	2.84	C
3	1.09	1.00	0.00	$^{-}$2.15	1.12	1.23	A
	$^{+}$0.75	1.08	0.54	$^{-}$1.78	1.07	0.87	B
	$^{+}$0.70	1.06	0.46	$^{-}$1.83	1.06	0.74	C
4	2.34	1.00	0.00	$^{+}$3.33	1.14	1.78	A
	1.96	1.00	0.00	$^{+}$2.21	1.08	1.02	B
	1.73	1.00	0.00	$^{+}$2.06	1.06	2.77	C
5	0.47	1.00	0.00	$^{+}$0.94	1.16	0.48	A
	0.45	1.00	0.00	$^{+}$0.87	1.17	0.73	B
	0.45	1.00	0.00	$^{+}$0.90	1.23	1.50	C
6	^{R}3.54	1.21	0.91	^{S}7.44	1.12	0.81	A
	^{R}3.59	1.09	0.56	6.06	1.00	0.00	B
	3.13	1.00	0.00	^{R}6.09	1.08	0.70	C
7	^{R}4.99	1.95	3.16	^{R}6.02	1.23	1.56	A
	^{R}1.73	1.38	1.52	^{R}2.03	1.31	2.10	B
	^{R}1.22	1.25	1.31	^{R}1.84	1.22	1.72	C
8	$^{+}$2.67	1.52	2.00	4.46	1.00	0.00	A
	$^{+}$1.41	3.02	5.70	2.43	1.00	0.00	B
	$^{+}$1.29	3.11	6.60	2.25	1.00	0.00	C
9	^{R}3.53	1.69	3.13	^{R}3.49	1.25	2.36	A
	^{R}1.61	1.46	2.14	^{R}1.54	1.21	2.02	B
	^{R}1.16	1.35	2.04	^{R}1.45	1.18	1.83	C
10	3.49	1.00	0.00	$^{+}$2.82	1.45	4.55	A
	$^{+}$2.75	1.08	0.63	$^{+}$2.37	1.40	4.12	B
	$^{+}$2.34	1.09	0.84	$^{+}$2.46	1.39	4.47	C
11	^{R}7.52	1.40	1.94	^{S}8.88	1.13	1.01	A
	^{R}2.69	1.27	1.57	^{S}3.08	1.10	0.90	B
	^{R}1.83	1.24	1.55	^{S}2.78	1.10	0.89	C
12	^{R}1.53	1.46	0.72	^{R}2.12	1.15	0.75	A
	1.66	1.00	0.00	1.67	1.00	0.00	B
	1.56	1.00	0.00	1.74	1.00	0.00	C

Table S1 to be continued

Continued Table S1

S.N.	ADMPC-based CSP			CDMPC-based CSP			M.P.
	k_1	α	R_s	k_1	α	R_s	
13	0.95	1.00	0.00	^{R}1.38	1.38	2.37	A
	0.69	1.00	0.00	^{R}1.11	1.34	2.62	B
	0.67	1.00	0.00	^{R}1.16	1.22	1.93	C
14	^{R}20.33	1.13	0.53	^{R}11.62	1.19	0.86	A
	^{R}11.54	1.62	2.68	^{R}5.94	1.19	1.47	B
	^{R}9.68	1.81	4.17	^{R}5.54	1.14	1.21	C
15	^{2R,3S}5.49	1.19	0.92	*r.t.* > 120 min			A
	^{2R,3S}4.90	1.18	1.09	^{2R,3S}10.48	1.28	2.48	B
	^{2R,3S}3.77	1.18	1.24	^{2R,3S}7.87	1.26	2.64	C
16	^{S}0.98	1.11	0.44	1.19	1.00	0.00	A
	0.73	1.00	0.00	0.89	1.00	0.00	B
	0.69	1.00	0.00	0.97	1.00	0.00	C
17	^{4R,1S}1.79	1.95	3.87	3.75	1.00	0.00	A
	^{4R,1S}1.65	1.94	3.68	^{4R,1S}2.13	2.32	7.29	B
	^{4R,1S}1.37	1.66	3.05	^{4R,1S}2.15	2.11	7.45	C
18	^{S}4.41	1.10	0.62	^{R}2.12	1.15	0.75	A
	^{S}4.18	1.10	0.58	1.67	1.00	0.00	B
	^{S}2.81	1.09	0.58	1.74	1.00	0.00	C
19	2.41	1.00	0.00	2.31	1.00	0.00	A
	$^{-}$1.75	1.10	0.56	1.91	1.00	0.00	B
	1.55	1.00	0.00	1.89	1.00	0.00	C
20	^{R}3.08	1.44	2.41	^{R}3.50	1.47	3.47	A
	^{R}1.44	1.37	1.92	^{R}1.60	1.25	2.17	B
	^{R}1.02	1.31	1.56	^{R}1.56	1.18	1.77	C

S.N.: series number of analytes; r.t.: retention time. M.P.: mobile phase, A: *n*-hexane/isopropanol (90/10, v/v); B: *n*-hexane/ethanol (90/10, v/v); C: *n*-hexane/ethanol/methanol (90/5/5, v/v/v). +, –, R, S, (2R,3S) and (4R,1S) at the superscript of k_1 refer to the optical rotation or configuration of the first-eluted enantiomer. Flow rate: 1.0 ml min^{-1}; detection temperature: 25 ^{o}C; column size: Φ 250 mm × 4.6 mm; silica gel: 7 μm, 1000 Å. Enantioseparation results of CDMPC-based CSP were cited from Ref. [1].

Reference

1. S. Liang, S. H. Huang, W. Chen and Z. W. Bai, *Anal. Chim. Acta*, 2017, **985**, 183–193.