

Electronic Supplementary Information

**Design and high-throughput synthesis of cyclodextrin-based
polyurethanes with enhanced molecular recognition
properties**

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Table 1s Compositions for the high-throughput synthesized CDPs; values are given in μmol

CDPs	α -CD	β -CD	γ -CD	DMPA	DHBA	DHTA	DHNA	PDI	TDI	IPDI	HDI
CDP51	8.2	—	—	—	—	—	—	24.6	—	—	—
CDP52	8.2	—	—	—	—	—	—	—	24.6	—	—
CDP53	8.2	—	—	—	—	—	—	—	—	24.6	—
CDP54	8.2	—	—	—	—	—	—	—	—	—	24.6
CDP55	8.2	—	—	4.1	—	—	—	28.7	—	—	—
CDP56	8.2	—	—	—	4.1	—	—	28.7	—	—	—
CDP57	8.2	—	—	—	—	4.1	—	28.7	—	—	—
CDP58	8.2	—	—	—	—	—	4.1	28.7	—	—	—
CDP59*	8.2	—	—	4.1	—	—	—	—	28.7	—	—
CDP60	8.2	—	—	—	4.1	—	—	—	28.7	—	—
CDP61	8.2	—	—	—	—	4.1	—	—	28.7	—	—
CDP62	8.2	—	—	—	—	—	4.1	—	28.7	—	—
CDP63*	8.2	—	—	4.1	—	—	—	—	—	28.7	—
CDP64*	8.2	—	—	—	4.1	—	—	—	—	28.7	—
CDP65*	8.2	—	—	—	—	4.1	—	—	—	28.7	—
CDP66*	8.2	—	—	—	—	—	4.1	—	—	28.7	—
CDP67	8.2	—	—	4.1	—	—	—	—	—	—	28.7
CDP68	8.2	—	—	—	4.1	—	—	—	—	—	28.7
CDP69	8.2	—	—	—	—	4.1	—	—	—	—	28.7
CDP70	8.2	—	—	—	—	—	4.1	—	—	—	28.7
CDP71	—	7.0	—	—	—	—	—	24.5	—	—	—
CDP72	—	7.0	—	—	—	—	—	—	24.5	—	—
CDP73	—	7.0	—	—	—	—	—	—	—	24.5	—
CDP74	—	7.0	—	—	—	—	—	—	—	—	24.5
CDP75	—	7.0	—	3.5	—	—	—	28.0	—	—	—
CDP76	—	7.0	—	—	3.5	—	—	28.0	—	—	—
CDP77	—	7.0	—	—	—	3.5	—	28.0	—	—	—
CDP78	—	7.0	—	—	—	—	3.5	28.0	—	—	—
CDP79	—	7.0	—	3.5	—	—	—	—	28.0	—	—
CDP80	—	7.0	—	—	3.5	—	—	—	28.0	—	—
CDP81	—	7.0	—	—	—	3.5	—	—	28.0	—	—
CDP82	—	7.0	—	—	—	—	3.5	—	28.0	—	—
CDP83	—	7.0	—	3.5	—	—	—	—	—	28.0	—
CDP84*	—	7.0	—	—	3.5	—	—	—	—	28.0	—
CDP85*	—	7.0	—	—	—	3.5	—	—	—	28.0	—
CDP86*	—	7.0	—	—	—	—	3.5	—	—	28.0	—
CDP87	—	7.0	—	3.5	—	—	—	—	—	—	28.0
CDP88	—	7.0	—	—	3.5	—	—	—	—	—	28.0
CDP89	—	7.0	—	—	—	3.5	—	—	—	—	28.0
CDP90	—	7.0	—	—	—	—	3.5	—	—	—	28.0
CDP91	—	—	6.2	—	—	—	—	24.8	—	—	—
CDP92	—	—	6.2	—	—	—	—	—	24.8	—	—
CDP93	—	—	6.2	—	—	—	—	—	—	24.8	—
CDP94	—	—	6.2	—	—	—	—	—	—	—	24.8
CDP95	—	—	6.2	3.1	—	—	—	27.9	—	—	—
CDP96	—	—	6.2	—	3.1	—	—	27.9	—	—	—
CDP97	—	—	6.2	—	—	3.1	—	27.9	—	—	—
CDP98	—	—	6.2	—	—	—	3.1	27.9	—	—	—
CDP99	—	—	6.2	3.1	—	—	—	—	27.9	—	—
CDP100	—	—	6.2	—	3.1	—	—	—	27.9	—	—
CDP101	—	—	6.2	—	—	3.1	—	—	27.9	—	—
CDP102	—	—	6.2	—	—	—	3.1	—	27.9	—	—
CDP103	—	—	6.2	3.1	—	—	—	—	—	27.9	—
CDP104	—	—	6.2	—	3.1	—	—	—	—	27.9	—
CDP105*	—	—	6.2	—	—	3.1	—	—	—	27.9	—
CDP106	—	—	6.2	—	—	—	3.1	—	—	27.9	—
CDP107	—	—	6.2	3.1	—	—	—	—	—	—	27.9
CDP108	—	—	6.2	—	3.1	—	—	—	—	—	27.9
CDP109	—	—	6.2	—	—	3.1	—	—	—	—	27.9
CDP110	—	—	6.2	—	—	—	3.1	—	—	—	27.9

* Marked CDPs: no polymer was obtained after washing steps.

Table 2s Normalized binding percentage (%) of the studied compounds onto the high-throughput synthesized CDPs in the mixed aqueous solution (compound solution: 0.1 mmol L⁻¹, 1 mL; contact time: 2h).

CDPs	APAP	ATE	CAF	OFX	CFX	TC	SMX	CHPH	PRO	DF
CDP51	6.8 ± 1.0	2.0 ± 0.3	16.8 ± 2.1	12.3 ± 0.6	15.2 ± 0.8	3.7 ± 1.4	12.3 ± 1.1	9.4 ± 0.4	6.4 ± 0.6	22.7 ± 0.3
CDP52	5.6 ± 1.0	6.0 ± 1.1	8.8 ± 0.9	13.4 ± 0.7	14.5 ± 0.6	9.3 ± 0.4	8.5 ± 0.6	7.2 ± 0.1	12.7 ± 0.8	20.8 ± 0.2
CDP53	16.4 ± 0.1	1.8 ± 0.4	4.6 ± 1.2	2.3 ± 1.3	1.9 ± 1.5	0	23.6 ± 1.4	13.1 ± 0.3	15.9 ± 1.4	24.1 ± 2.1
CDP54	7.4 ± 1.1	0.5 ± 0.7	2.8 ± 0.9	3.3 ± 1.4	6.3 ± 1.6	0	23.6 ± 1.0	16.3 ± 1.2	17.4 ± 1.3	29.2 ± 2.5
CDP55	5.0 ± 0.8	7.7 ± 0.5	8.0 ± 1.0	14.2 ± 1.8	15.2 ± 2.1	7.8 ± 0.4	7.3 ± 0.6	6.3 ± 0.8	16.6 ± 0.3	15.6 ± 1.5
CDP56	5.8 ± 1.0	6.1 ± 0.7	9.2 ± 0.7	13.0 ± 0.8	13.8 ± 0.8	9.1 ± 0.3	8.9 ± 0.3	7.8 ± 0.6	12.5 ± 0.4	17.9 ± 1.3
CDP57	5.6 ± 1.0	6.0 ± 1.1	8.8 ± 0.9	13.4 ± 0.7	14.5 ± 0.6	9.3 ± 0.4	8.5 ± 0.6	7.2 ± 0.1	12.7 ± 0.8	20.8 ± 0.2
CDP58	6.2 ± 0.4	7.0 ± 0.2	9.5 ± 0.1	12.0 ± 0.5	13.4 ± 0.2	9.9 ± 0.2	9.3 ± 0.2	7.8 ± 0.0	12.7 ± 0.3	15.5 ± 1.2
CDP60	8.4 ± 0.8	6.9 ± 0.3	9.3 ± 0.9	10.6 ± 0.4	12.4 ± 0.3	5.7 ± 0.1	9.8 ± 0.4	8.6 ± 0.9	15.2 ± 1.0	16.9 ± 0.9
CDP61	9.6 ± 0.6	3.8 ± 0.8	10.2 ± 0.1	9.0 ± 0.4	10.3 ± 0.8	4.7 ± 0.5	12.1 ± 0.2	8.2 ± 0.2	13.9 ± 0.1	23.6 ± 1.4
CDP62	9.3 ± 1.5	5.9 ± 1.4	8.8 ± 0.4	10.6 ± 0.5	12.9 ± 0.8	6.3 ± 2.0	10.0 ± 0.1	6.6 ± 1.0	14.8 ± 1.5	19.4 ± 2.8
CDP67	2.2 ± 0.8	5.6 ± 0.7	2.7 ± 1.0	11.8 ± 0.3	19.1 ± 0.2	4.7 ± 0.5	8.2 ± 0.6	5.0 ± 0.6	26.3 ± 0.3	18.8 ± 1.6
CDP68	1.8 ± 0.5	0.6 ± 0.6	1.3 ± 0.4	10.0 ± 1.3	19.1 ± 1.6	4.3 ± 0.8	7.5 ± 2.6	4.9 ± 1.2	18.5 ± 2.6	41.4 ± 1.3
CDP69	0.6 ± 0.7	0.3 ± 0.4	0	10.0 ± 0.6	23.1 ± 0.6	3.5 ± 0.7	4.3 ± 0.6	1.6 ± 0.7	22.0 ± 1.4	45.0 ± 0.4
CDP70	2.3 ± 0.5	1.8 ± 0.5	1.4 ± 0.4	9.9 ± 1.5	18.5 ± 1.0	6.6 ± 1.0	8.6 ± 0.4	7.0 ± 0.1	18.1 ± 1.1	33.5 ± 2.0
CDP71	7.1 ± 1.2	0.9 ± 0.8	14.1 ± 0.8	9.9 ± 0.3	11.6 ± 0.3	9.2 ± 0.5	12.4 ± 0.3	9.9 ± 0.2	3.9 ± 0.6	21.0 ± 1.0
CDP72	14.3 ± 2.7	2.6 ± 0.9	14.1 ± 2.2	6.2 ± 1.6	8.0 ± 1.5	4.4 ± 2.4	14.1 ± 1.1	9.8 ± 1.9	6.6 ± 0.4	19.8 ± 1.9
CDP73	10.6 ± 3.3	2.7 ± 3.1	7.3 ± 0.6	4.8 ± 0.8	6.6 ± 0.2	5.5 ± 1.4	14.3 ± 0.6	9.4 ± 1.5	9.7 ± 0.9	29.2 ± 2.3
CDP74	16.5 ± 0.7	2.6 ± 2.1	3.4 ± 0.5	3.2 ± 1.5	2.5 ± 2.8	0.6 ± 1.1	19.4 ± 2.7	10.7 ± 2.1	12.5 ± 0.8	28.6 ± 6.2
CDP75	4.7 ± 0.0	7.1 ± 0.3	7.2 ± 0.1	14.0 ± 0.2	16.3 ± 0.2	8.9 ± 0.7	7.0 ± 0.0	6.6 ± 0.3	14.3 ± 0.2	13.9 ± 0.6
CDP76	3.6 ± 0.7	3.3 ± 0.5	8.5 ± 0.7	13.9 ± 0.5	17.4 ± 1.0	6.2 ± 1.0	8.7 ± 0.3	5.8 ± 0.7	13.0 ± 0.4	19.4 ± 1.9
CDP77	4.3 ± 0.8	4.2 ± 0.6	7.4 ± 0.7	13.0 ± 0.2	15.1 ± 0.4	7.2 ± 0.3	10.3 ± 0.4	7.4 ± 0.1	11.7 ± 0.2	19.2 ± 1.6
CDP78	4.0 ± 0.2	3.7 ± 0.5	9.0 ± 0.5	12.7 ± 0.2	14.8 ± 0.5	8.8 ± 0.2	9.5 ± 0.3	7.7 ± 0.2	12.6 ± 0.2	17.1 ± 0.6
CDP79	10.0 ± 1.4	10.0 ± 2.0	8.9 ± 2.6	9.8 ± 3.9	14.5 ± 2.0	0.2 ± 0.4	10.2 ± 0.7	4.2 ± 1.8	19.6 ± 2.1	12.6 ± 1.5
CDP80	8.6 ± 0.3	5.9 ± 0.4	7.0 ± 0.4	10.4 ± 0.1	12.3 ± 0.5	3.8 ± 0.8	12.3 ± 0.3	9.9 ± 1.7	12.9 ± 0.3	16.9 ± 2.5
CDP81	7.7 ± 0.4	3.1 ± 0.2	7.9 ± 0.6	7.5 ± 0.2	9.5 ± 0.7	3.2 ± 0.5	15.6 ± 0.2	9.6 ± 0.9	11.3 ± 0.4	24.3 ± 1.0
CDP82	11.0 ± 2.3	5.2 ± 0.6	8.8 ± 0.7	7.9 ± 1.4	10.4 ± 1.6	2.6 ± 0.6	13.4 ± 0.4	9.0 ± 2.3	12.5 ± 1.2	19.0 ± 1.7
CDP83	2.0 ± 2.2	0.6 ± 1.0	0	8.0 ± 1.0	13.9 ± 9.9	0	10.9 ± 2.7	2.8 ± 2.7	34.2 ± 5.7	27.7 ± 7.5
CDP87	2.6 ± 0.9	6.5 ± 2.0	0.6 ± 0.5	11.2 ± 1.0	20.0 ± 0.5	2.6 ± 2.9	6.6 ± 1.8	2.2 ± 0.5	30.7 ± 3.0	17.0 ± 3.1
CDP88	4.7 ± 1.7	0.3 ± 0.3	1.1 ± 0.2	4.5 ± 0.1	11.3 ± 1.6	0.4 ± 0.4	14.5 ± 1.6	4.5 ± 0.6	18.2 ± 1.1	40.6 ± 2.4
CDP89	0	0	0	5.4 ± 0.6	16.0 ± 0.5	0	6.5 ± 1.4	1.2 ± 2.0	13.1 ± 0.5	57.8 ± 2.8
CDP90	5.1 ± 0.7	1.4 ± 0.1	0	5.3 ± 0.2	13.3 ± 0.7	5.8 ± 0.3	13.6 ± 0.6	8.6 ± 0.5	15.8 ± 0.5	31.1 ± 1.2
CDP91	5.1 ± 0.4	0.8 ± 0.4	16.1 ± 0.5	10.9 ± 0.2	12.4 ± 0.2	5.7 ± 0.5	11.3 ± 0.1	6.4 ± 0.3	4.5 ± 0.2	26.7 ± 0.2
CDP92	8.3 ± 1.6	0.8 ± 0.4	17.0 ± 1.2	7.1 ± 1.0	8.8 ± 1.0	2.5 ± 1.3	14.7 ± 0.8	7.7 ± 0.1	6.4 ± 0.3	26.5 ± 1.0
CDP93	10.1 ± 1.1	0.5 ± 0.4	5.0 ± 1.0	3.1 ± 0.6	4.1 ± 0.7	0.1 ± 0.5	19.2 ± 0.7	9.6 ± 0.5	11.4 ± 0.7	36.8 ± 2.8
CDP94	10.1 ± 1.9	2.9 ± 0.8	3.8 ± 1.0	3.5 ± 0.6	4.6 ± 0.9	0	20.9 ± 0.2	6.8 ± 0.9	16.1 ± 1.4	31.8 ± 2.8
CDP95	4.2 ± 0.1	5.2 ± 0.4	7.7 ± 0.1	14.3 ± 0.2	15.4 ± 0.1	8.2 ± 0.3	7.9 ± 0.0	6.7 ± 0.1	13.6 ± 0.1	16.8 ± 0.7
CDP96	4.4 ± 0.2	3.9 ± 0.3	8.4 ± 0.3	13.1 ± 0.2	14.6 ± 0.1	7.7 ± 0.1	8.7 ± 0.1	7.1 ± 0.0	12.2 ± 0.2	19.9 ± 0.4
CDP97	4.4 ± 0.2	3.0 ± 0.4	8.0 ± 0.2	13.4 ± 0.1	15.0 ± 0.4	8.7 ± 0.4	8.2 ± 0.1	7.2 ± 0.3	11.2 ± 0.1	20.8 ± 1.2
CDP98	5.1 ± 0.3	4.0 ± 0.3	9.8 ± 0.1	11.9 ± 0.2	13.7 ± 0.1	8.1 ± 0.5	9.3 ± 0.0	8.1 ± 0.1	12.2 ± 0.1	17.6 ± 0.8
CDP99	4.4 ± 0.9	6.1 ± 0.3	4.9 ± 0.4	12.9 ± 1.4	17.8 ± 0.7	2.6 ± 1.8	8.7 ± 0.7	5.0 ± 1.2	23.5 ± 5.8	13.9 ± 2.0
CDP100	8.0 ± 2.2	3.7 ± 0.4	10.4 ± 1.7	5.6 ± 2.9	10.4 ± 1.8	4.4 ± 1.1	12.4 ± 1.0	8.1 ± 0.2	12.8 ± 1.5	24.1 ± 2.1
CDP101	8.6 ± 1.0	0.5 ± 0.8	9.1 ± 0.4	3.3 ± 0.5	6.5 ± 0.5	1.1 ± 0.6	13.9 ± 1.5	5.6 ± 1.0	14.3 ± 1.0	37.0 ± 2.4
CDP102	6.9 ± 0.7	4.1 ± 1.1	7.9 ± 0.5	9.8 ± 0.4	12.1 ± 1.1	5.2 ± 0.8	9.9 ± 0.6	6.8 ± 0.5	14.8 ± 0.5	22.4 ± 0.9
CDP103	11.9 ± 0.5	5.3 ± 1.6	7.1 ± 5.0	4.5 ± 4.2	8.2 ± 3.4	0.2 ± 0.4	14.5 ± 1.7	8.0 ± 2.2	20.0 ± 2.1	20.4 ± 2.1
CDP104	3.9 ± 1.6	0	0	1.1 ± 1.0	6.3 ± 1.8	0.4 ± 0.7	17.1 ± 2.5	5.8 ± 0.9	12.9 ± 0.7	52.4 ± 3.2
CDP106	8.8 ± 2.4	0	1.3 ± 1.0	2.4 ± 2.4	11.9 ± 3.4	15.1 ± 0.7	15.4 ± 3.2	8.0 ± 3.4	6.6 ± 1.7	30.4 ± 3.7
CDP107	4.1 ± 0.2	7.4 ± 0.7	2.3 ± 0.2	10.4 ± 0.7	15.2 ± 0.6	4.9 ± 0.3	10.0 ± 0.3	5.5 ± 0.2	22.4 ± 0.8	17.8 ± 0.8
CDP108	1.4 ± 0.8	0.1 ± 0.2	0.2 ± 0.3	4.5 ± 0.7	11.1 ± 1.0	4.3 ± 0.4	11.0 ± 0.6	5.2 ± 0.5	18.1 ± 0.5	44.1 ± 0.9
CDP109	0.8 ± 0.3	0.1 ± 0.2	0.1 ± 0.2	6.0 ± 0.6	14.4 ± 0.4	4.8 ± 0.4	6.0 ± 0.4	3.8 ± 0.1	14.8 ± 0.1	49.1 ± 1.4
CDP110	2.2 ± 0.7	0.4 ± 0.2	0.9 ± 0.3	6.2 ± 0.3	14.4 ± 0.7	7.6 ± 0.4	10.1 ± 0.1	6.8 ± 0.1	15.7 ± 0.6	35.6 ± 1.4