

Supramolecular Hydrogels Formed by β -Cyclodextrin Self-Association and Host-Guest Inclusion Complexes

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Supporting information:

Table S1. Composition of the PEG₈-chol_{5,6}/ β CD mixtures discussed in this study.

Gel composition	PEG₈-chol content (% (w/w))	βCD content (% (w/w))	Buffer content (% (w/w))
2 % PEG ₈ 20K-chol _{5,6} + 1 eq. β CD	2	0.6	97.4
5 % PEG ₈ 20K-chol _{5,6} + 1 eq. β CD	5	1.4	93.6
10 % PEG ₈ 20K-chol _{5,6} + 1 eq. β CD	10	2.8	87.2
15 % PEG ₈ 20K-chol _{5,6} + 1 eq. β CD	15	4.1	80.9
20 % PEG ₈ 20K-chol _{5,6} + 1 eq. β CD	20	5.5	74.5
22.5 % PEG ₈ 20K-chol _{5,6} + 1 eq. β CD	22.5	6.2	71.3
25 % PEG ₈ 20K-chol _{5,6} + 1 eq. β CD	25	6.9	68.1
2 % PEG ₈ 20K-chol _{5,6} + 2 eq. β CD	2	1.1	96.9
5 % PEG ₈ 20K-chol _{5,6} + 2 eq. β CD	5	2.8	92.2
10 % PEG ₈ 20K-chol _{5,6} + 2 eq. β CD	10	5.5	84.5
15 % PEG ₈ 20K-chol _{5,6} + 2 eq. β CD	15	8.3	76.7
20 % PEG ₈ 20K-chol _{5,6} + 2 eq. β CD	20	11.0	69.0
22.5 % PEG ₈ 20K-chol _{5,6} + 2 eq. β CD	22.5	12.4	65.1
25 % PEG ₈ 20K-chol _{5,6} + 2 eq. β CD	25	13.8	61.2

22.5 % PEG ₈ 20K-cho _{5,6} + 0.5 eq. β CD	22.5	3.1	74.4
22.5 % PEG ₈ 20K-cho _{5,6} + 4 eq. β CD	22.5	24.8	52.7
15 % PEG ₈ 10K-cho _{5,6} + 2 eq. β CD	15	15.2	69.8
15 % PEG ₈ 40K-cho _{5,7} + 2 eq. β CD	15	4.3	80.7
15 % PEG ₈ 40K-cho _{5,7} + 4 eq. β CD	15	8.5	76.5

Table S2. Composition of the PEG6K-cho_{1,8}/ β CD mixtures discussed in this study.

Gel composition	PEG₈20K-cho_{5,6} content (% (w/w))	βCD content (% (w/w))	Buffer content (% (w/w))
2 % PEG6K-cho _{1,8} + 1 eq. β CD	2	0.5	97.5
5 % PEG6K-cho _{1,8} + 1 eq. β CD	5	1.4	93.6
10 % PEG6K-cho _{1,8} + 1 eq. β CD	10	2.7	87.2
15 % PEG6K-cho _{1,8} + 1 eq. β CD	15	4.1	80.9
20 % PEG6K-cho _{1,8} + 1 eq. β CD	20	5.5	74.5
22.5 % PEG6K-cho _{1,8} + 1 eq. β CD	22.5	6.2	71.3
25 % PEG6K-cho _{1,8} + 1 eq. β CD	25	6.8	68.2
2 % PEG6K-cho _{1,8} + 2 eq. β CD	2	1.1	96.9
5 % PEG6K-cho _{1,8} + 2 eq. β CD	5	2.7	92.3
10 % PEG6K-cho _{1,8} + 2 eq. β CD	10	5.5	84.5
15 % PEG6K-cho _{1,8} + 2 eq. β CD	15	8.2	76.8
20 % PEG6K-cho _{1,8} + 2 eq. β CD	20	11.0	69.0
22.5 % PEG6K-cho _{1,8} + 2 eq. β CD	22.5	12.3	65.2
25 % PEG6K-cho _{1,8} + 2 eq. β CD	25	13.7	61.3

Table S3. T_{gel} (in °C) of PEG₈20K-cho_{5,6}/βCD and PEG6K-cho_{1,8}/βCD hydrogels with increasing PEG-cho_l contents (Average ± STDEV, n=3)

	+ 1 eq. βCD	+ 2 eq. βCD	without βCD
2% (w/w) PEG₈20K-cho_{5,6}	b	b	a
5% (w/w) PEG₈20K-cho_{5,6}	b	b	a
10% (w/w) PEG₈20K-cho_{5,6}	50±4	53±3	42±4
15% (w/w) PEG₈20K-cho_{5,6}	58±2	75±5	a
20% (w/w) PEG₈20K-cho_{5,6}	62±4	>100 ^c	43±1
22.5% (w/w) PEG₈20K-cho_{5,6}	65±5	>100 ^c	a
25% (w/w) PEG₈20K-cho_{5,6}	70±4	>100 ^c	a
	+ 1 eq. βCD	+ 2 eq. βCD	without βCD
2% (w/w) PEG6000-cho_{1,8}	b	b	a
5% (w/w) PEG6000-cho_{1,8}	b	b	a
10% (w/w) PEG6000-cho_{1,8}	38±1	53±1	34±1
15% (w/w) PEG6000-cho_{1,8}	42±1	71±3	a
20% (w/w) PEG6000-cho_{1,8}	55±2	> 90 ^c	a
22.5% (w/w) PEG6000-cho_{1,8}	63±3	> 90 ^c	51±2
25% (w/w) PEG6000-cho_{1,8}	70±4	> 90 ^c	a

^a not determined

^b no T_{gel}

^c Extrapolated values