Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information:

Table S1. Yields of IC1113 as a function of amounts of added CP1113 in 25mL saturated aqueous solutions of β-CD (0.16 mol L^{-1})

Items	***Ex.1***	***Ex.2***	***Ex.3***	***Ex.4***	***Ex.5***	***Ex.6***	***Ex.7***	***Ex.8***
Mass of Added CP1113 *(g)*	0.0000	0.1000	0.2000	0.3000	0.4000	0.5000	0.6000	0.7000
Amount of added CP1113 *(mmol)*	0.0000	0.04153	0.08306	0.1246	0.1661	0.2076	0.2492	0.2907
Concentrtion of added CP1113 *(mmol L^{-1})* [a]	0.0000	1.6612	3.3224	4.9840	6.6440	8.3040	9.9680	11.6280
Theoretical precipitated β-CD *(g)* [b]	4.1250	4.1250	4.1250	4.1250	4.1250	4.1250	4.1250	4.1250
Actually mass of β-CD residue *(g)* [c]	4.1150	4.0510	3.7331	3.4691	2.7885	2.2192	2.2522	2.2275
Theoretically calculated amount of β-CD in ICs *(g)* [d]	0.0200	0.0740	0.3919	0.6559	1.3365	1.9058	1.8728	1.8975
Theoretical calculated amount of β-CD in ICs *(mmol)*	0.01762	0.06520	0.3453	0.5779	1.1178	1.6791	1.6500	1.6718
Theoretical calculated amount of ICs *(g)* [e]	0.0200	0.1740	0.5919	0.9559	1.7365	2.4058	2.4728	2.5975
Actual amount of ICs *(g)*	0.0000	0.1515	0.5619	0.9084	1.7015	2.4683	2.4228	2.5300
Actual yields of ICs *(%)* [f]	0.4848	1.7939	9.5006	15.9006	32.4000	46.2012	45.4012	46.0000
Errors of yields of ICs *(%)* [g]	-0.4848	-0.5455	-0.7273	-1.1515	-0.8485	+1.5152	-1.2121	-1.6364
The molar stoichiometry ratio between β-CD and CP1113 [h]	—	1.5699	4.1572	4.6380	6.7297	8.0882	6.6212	5.7909

a:*Concentrtion of added CP1113 (mmol L^{-1}) was calculated in accordance with a volume-fixed 25 mL β-CD solution;*

b:*Theoretical precipitated β-CD (g) was calculated to be constant value according to the solubility differences between 80°C to 20°C in a volume-fixed 25 mL solution;*

c:*Actually mass of β-CD residue (g) was separated from the mother liquor or in crystal state at the flask bottom without complexation;*

d:*Theoretically calculated amount of β-CD in ICs (g) was calculated from [Theoretical precipitated β-CD] subtracting [Actually mass of β-CD residue];*

e:*Theoretical calculated amount of ICs (g) was calculated from [Theoretically calculated amount of β-CD in ICs] + [Mass of Added CP1113];*

f:*Actual yields of ICs (%) was calculated from [Theoretical calculated amount of β-CD in ICs]/[Theoretical precipitated β-CD];*

g:*Errors of yields of ICs (%) was calculated from [(Theoretical calculated amount of ICs)-(Actual amount of ICs)]/[Theoretical precipitated β-CD];*

h:*The molar stoichiometry ratio between β-CD and CP1113 was calculated from [Theoretical calculated amount of β-CD in ICs]/[Amount of added CP1113].*

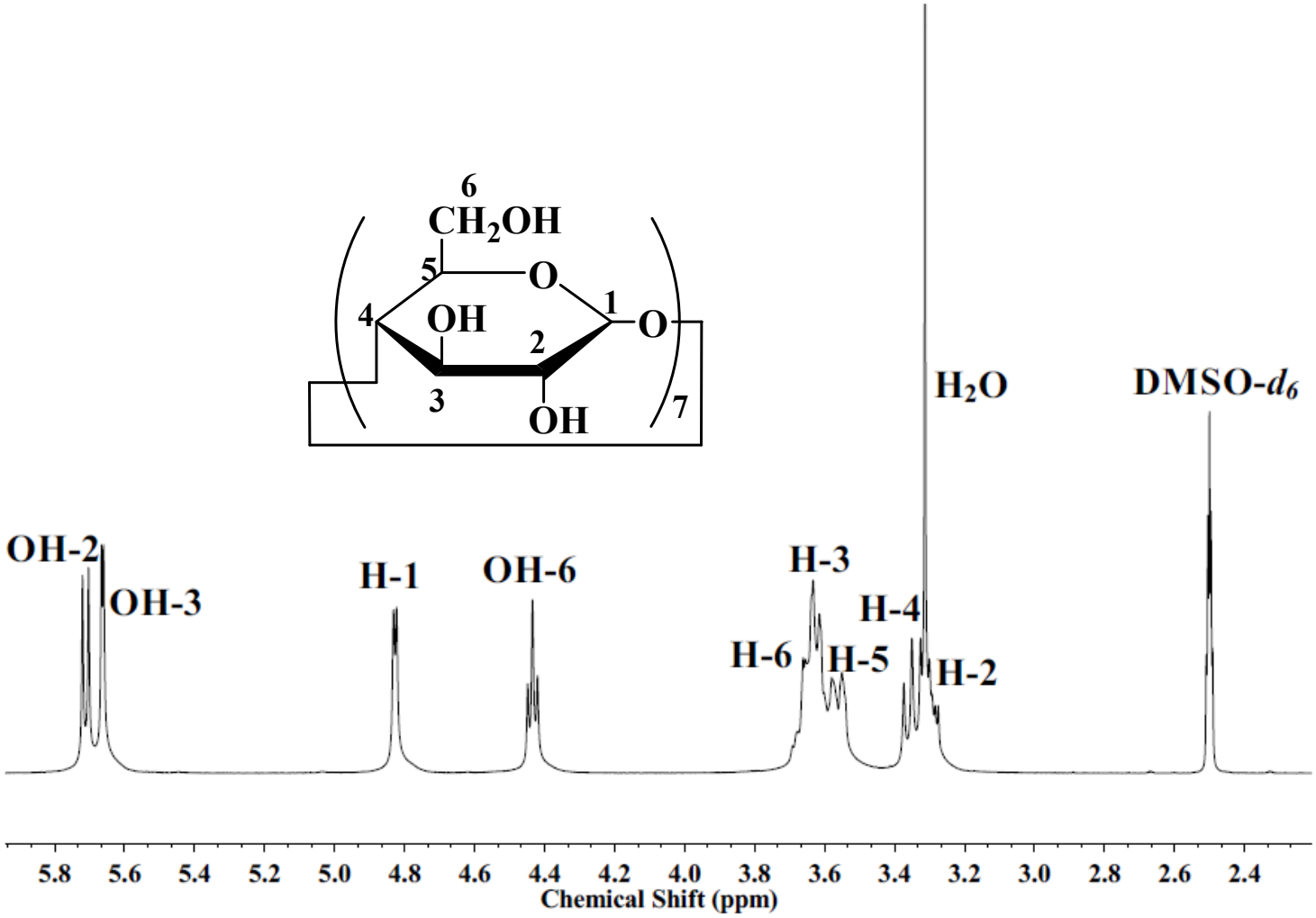

Fig.S1 ^{1}H-NMR spectrum of β-CD in DMSO-d$_6$ at 298.15K.

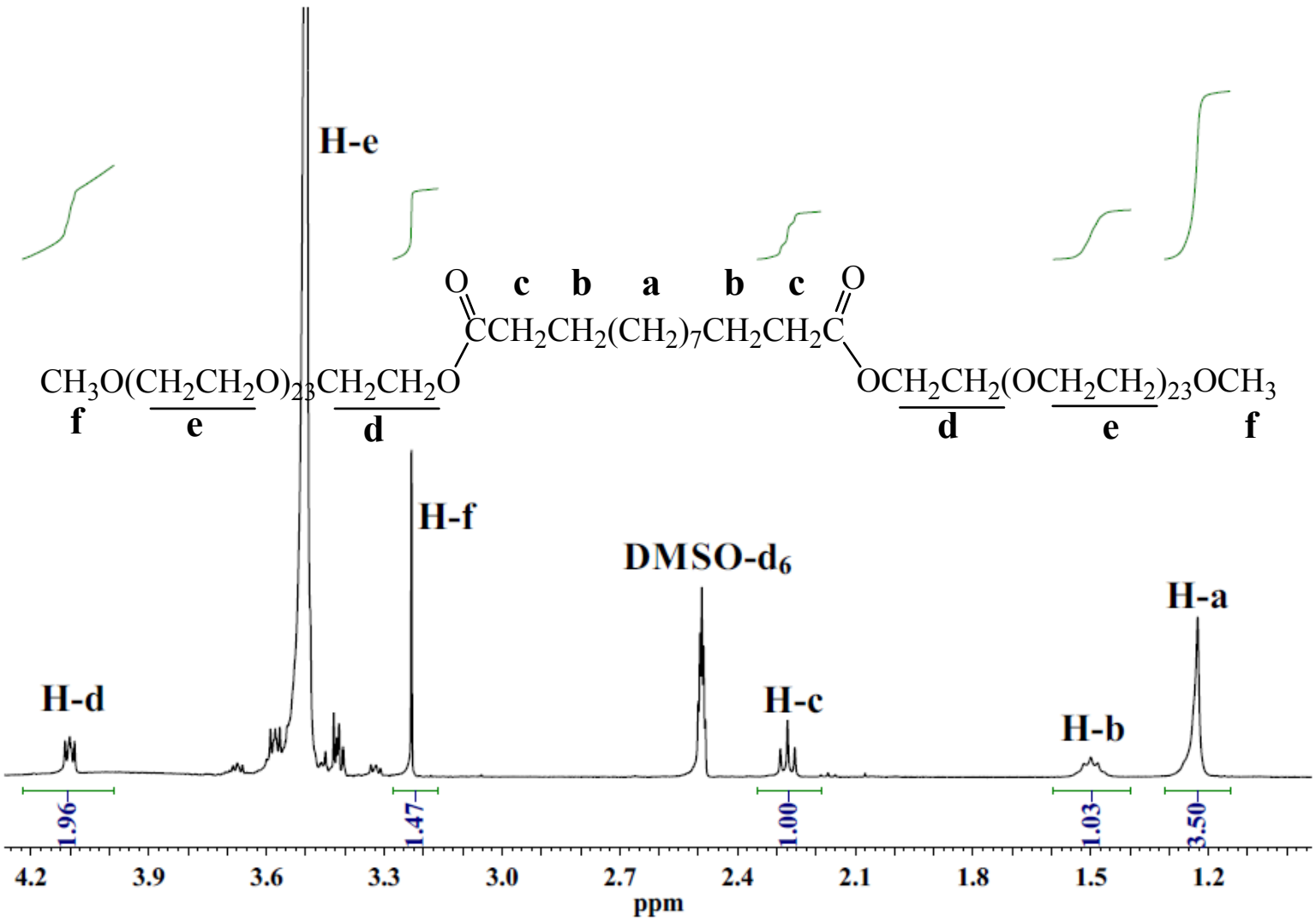

Fig.S2 ^{1}H-NMR spectrum of CP1113 in DMSO-d_6 at 298.15K.

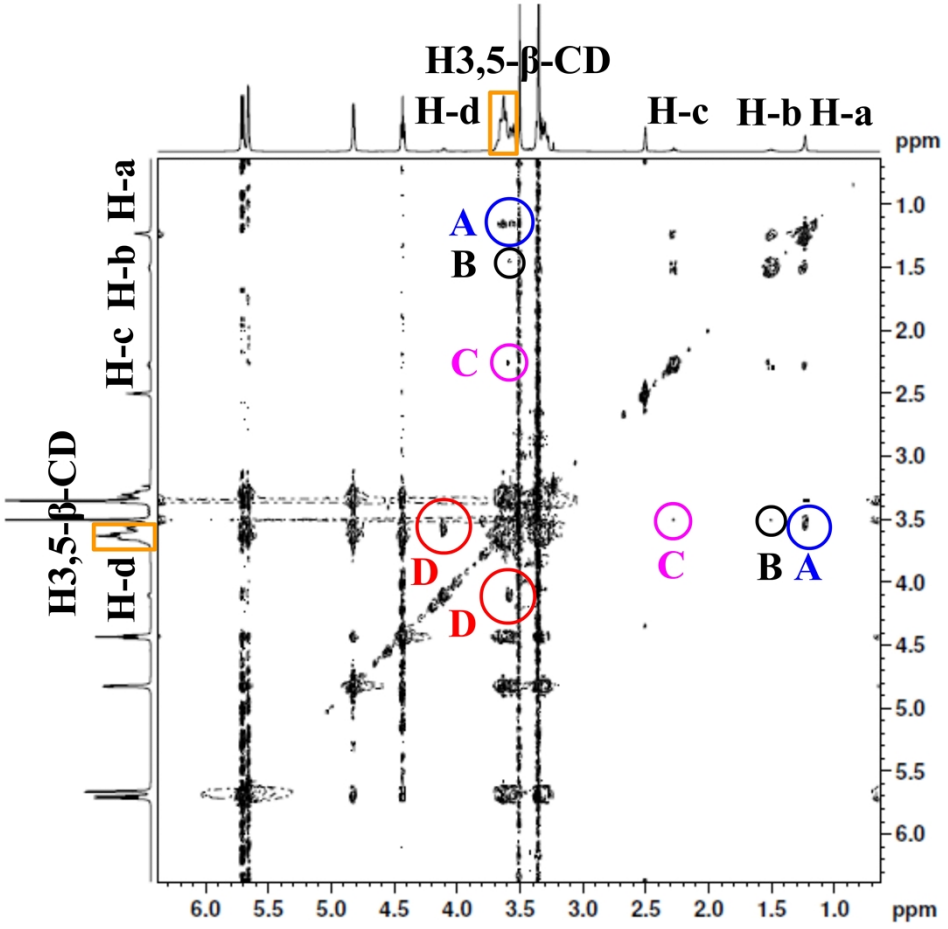

Fig.S3 2D ROSEY spectrum of IC1113 partially dissolved in DMSO-d_6 at 298.15K with 5 min of ultrasonication (four kinds of cross peaks with different strength are assigned to the interactions between H3, H5 of β-CD and : A. H-a, B. H-b, C. H-c, D. H-d of CP1113)

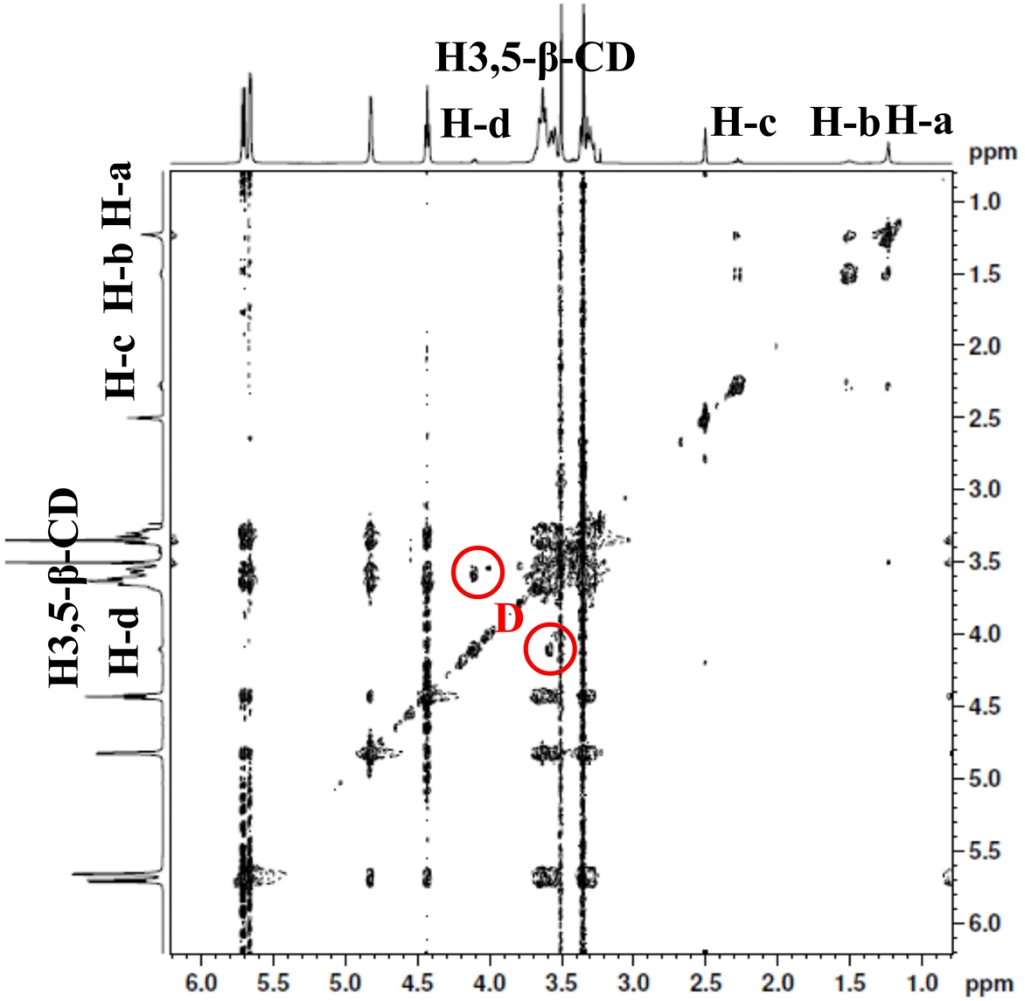

Fig.S4 2D ROSEY spectrum of IC1113 fully dissolved in DMSO-d_6 at 298.15K with 30 min of ultrasonication (two weak cross peaks in red circles are assigned to interaction of H3, H5 of β-CD and H-d of CP1113, the underlined part in $CH_3(OCH_2CH_2)_{23}O$ $\underline{CH_2CH_2}O$-$CO(CH_2)_{11}CO$-$O\underline{CH_2CH_2}O(CH_2CH_2O)_{23}CH_3$)

Table S2. Comparison of experimental results between this work and several previous relevant literatures

Systems	***Molecular structure of guest polymers***	***Molar ratio of β-CDs to the included polymers (or copolymers)***	***Molar ratio of β-CD to non-PEG polymer segments***	***Number of EG segments per β-CD***
IC1113 in this work	$H_3COEG_{\sim 24}(CH_2)_{11}EG_{\sim 24}OCH_3$	~7.8:1	~2:1 (to ME segments) [e]	~8.28 [f]
IC between β-CD and PEG [a]	EG_n, where n was not given	Not given	—	3
IC between β-CD and PPG [b]	$PG_{\sim 17}$	Not given	1:2 (with PG segments) [b]	—
Polypseudorotaxane from β-CD and PPG [c]	H_2N-$PG_{\sim 34}$-NH_2	~13:1	1:2.6 (with PG segments) [c]	—
Polypseudorotaxane prepared from β-CD and PEG-*b*-PPG-*b*-PEG [d]	residue-$EG_{\sim 22}PG_{\sim 39}EG_{\sim 22}$-residue	~17:1 (experimental) ~19:1, (theoretically calculated value according to literature ***b)***	1:2 (with PG segments) [b]	Cannot be determined even if there is [g]
Polyrotaxane prepared from β-CD and PEG-*b*-PPG-*b*-PEG [d]	stopper-$EG_{\sim 22}PG_{\sim 39}EG_{\sim 22}$-stopper	~7:1 (experimental) ~19:1 (theoretically calculated value according to literature ***b)***	1:2 (with PG segments) [b]	Cannot be determined even if there is [g]

a: K. A. Udachin, L.D. Wilson and J.A. Ripmeester, *J. Am. Chem. Soc*, 2000, **122**, 12375-12376.

b: A. Harada, M. Okada, J. Li and M. Kamachi, *Macromolecules*, 1995, **28**, 8406-8411.

c: S. Liu, J. Cai, L. Ren, L. Wang and Y.J. Wang, *RSC Adv.*, 2014, **4**, 18608–18611

d: H. Fujita, T. Ooya and N. Yui, *Macromolecules*, 1999, **32**, 2534-2541.

e: J. G. Gao, Y. J. Ding, H. W. Chen, Q. P. Song and Q. J.Zhang, *Chin.J. Chem. Phys*, 2008, **21**, 387-392.

f: Number of EG segments per β-CD was calculated from *[EG segments in one CP1113 mainchain]/[(Molar ratio of β-CDs to the included polymers)- (Molar ratio of β-CD to non-PEG polymer segments)], that is 48/(7.8-2) accordingly.*

g:According to the theoretically molar ratio of β-CD to PG segments of 1:2, the molar ratio of EG segments to β-CD cannot be calculated because the central PG segments (ca. 39) needed more β-CDs (ca. 19) than the experimental numbers (ca. 17 or 7) of the accommodated β-CDs, so it is not sure that β-CDs reside on the PEG segments or not.

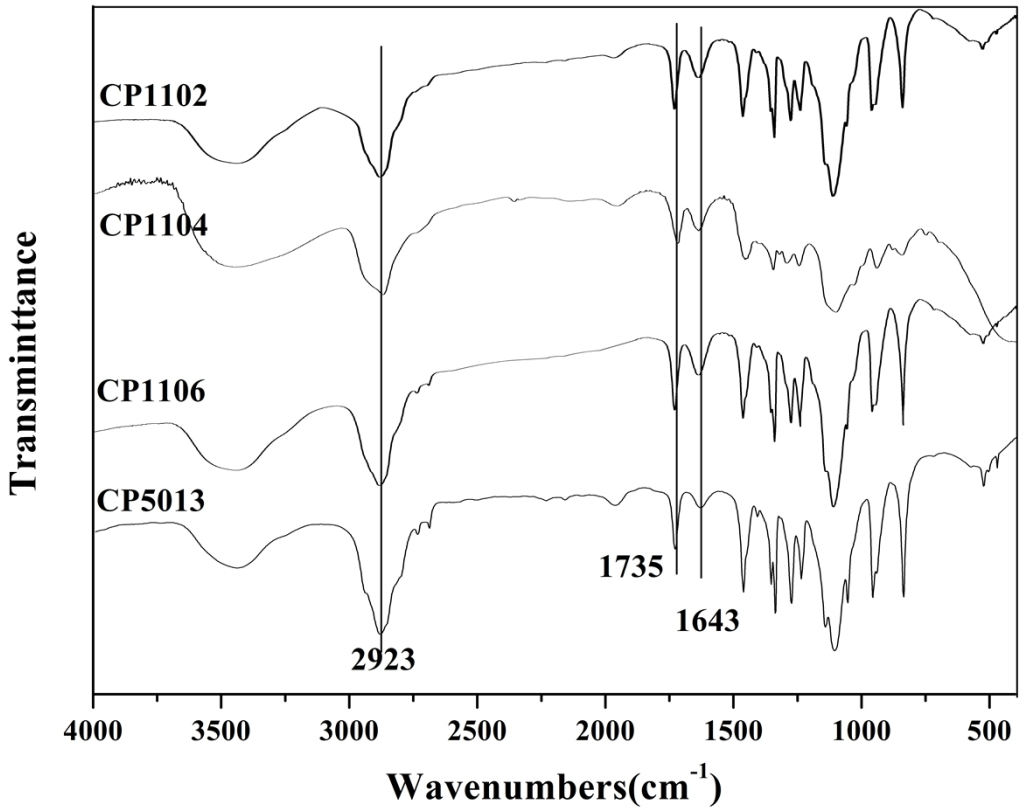

Fig.S5 FTIR spectra of analogous triblock polymers prepared from MePEG and diacids (CP1102: MePEG1100 and oxalic acid; CP1104: MePEG1100 and succinic acid; CP1106: MePEG1100 and adipic acid; CP5013: MePEG5000 and DA13)

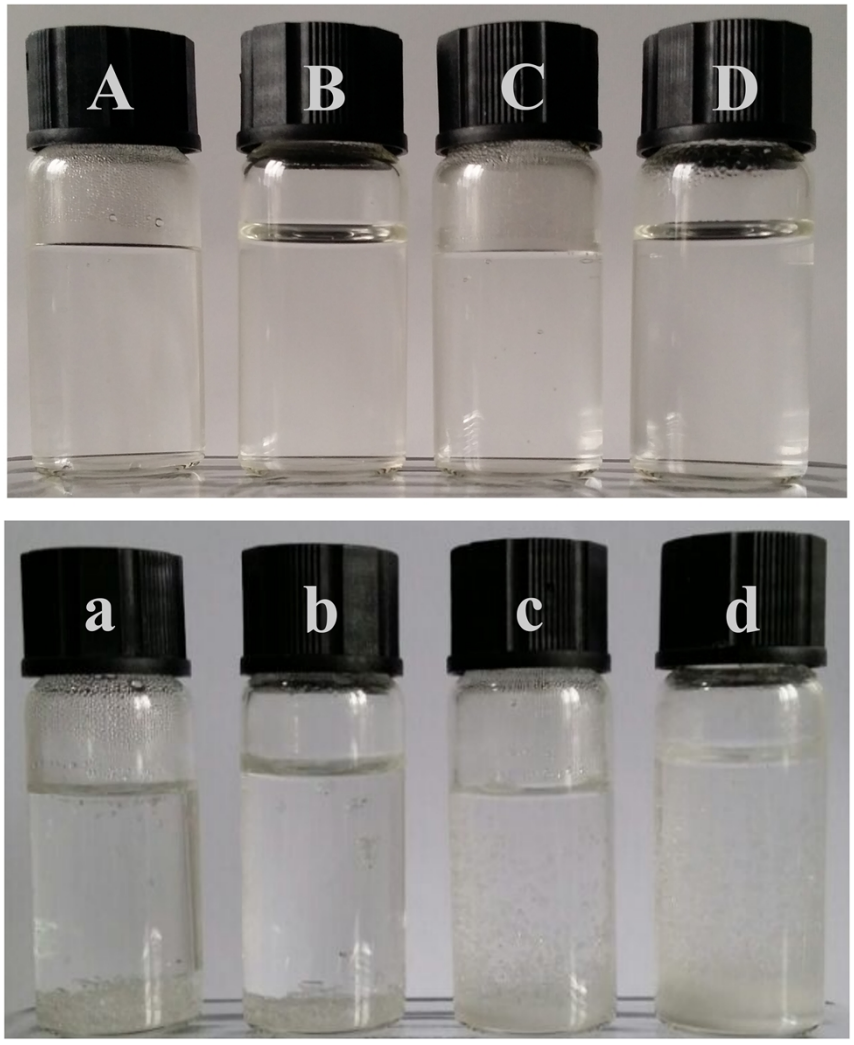

Fig.S6 Optical graphs of the beginning (80 °C, upper) and ending (20 °C, lower) states for four triblock polymers with β-CD (A and a: CP1102; B and b: CP1104; C and c: CP1106; D and d: CP5013).