A new strategy for constructing the β-cyclodextrin-based magnetic nano-carriers: Molecule docking technique

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Supplementary information

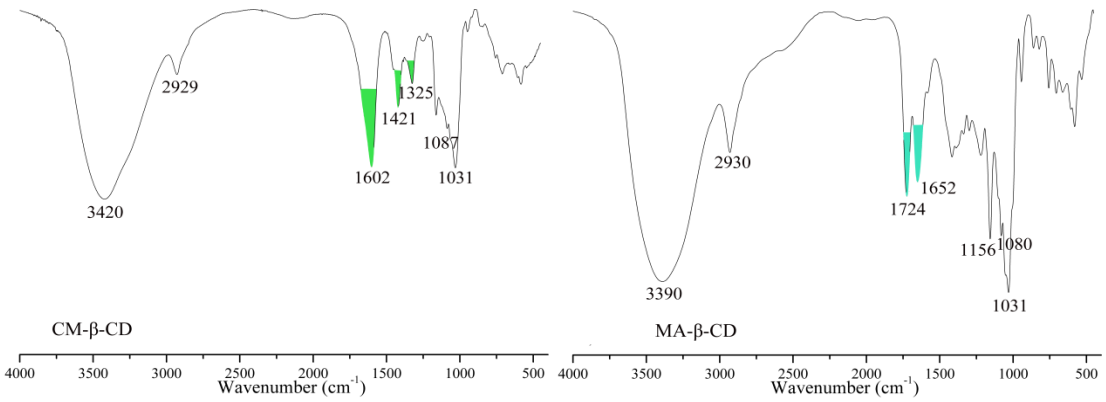

Figure S1 The FT-IR spectra of CM-β-CD and MA-β-CD

As seen in Fig. S1, the characteristic peaks at 1602 cm^{-1}, 1421 cm^{-1} and 1325 cm^{-1} in the FT-IR spectra of CM-β-CD were assigned to CO_2^- stretching vibration of carbonyl groups which indicated the attachment of carboxymethyl group on β-CD. In the spectra of MA-β-CD, the new characteristic peaks at 1724 cm^{-1} and 1652 cm^{-1}, corresponding to the stretching vibration of C=O and C=C, respectively, confirmed the successful synthesis of MA-β-CD.

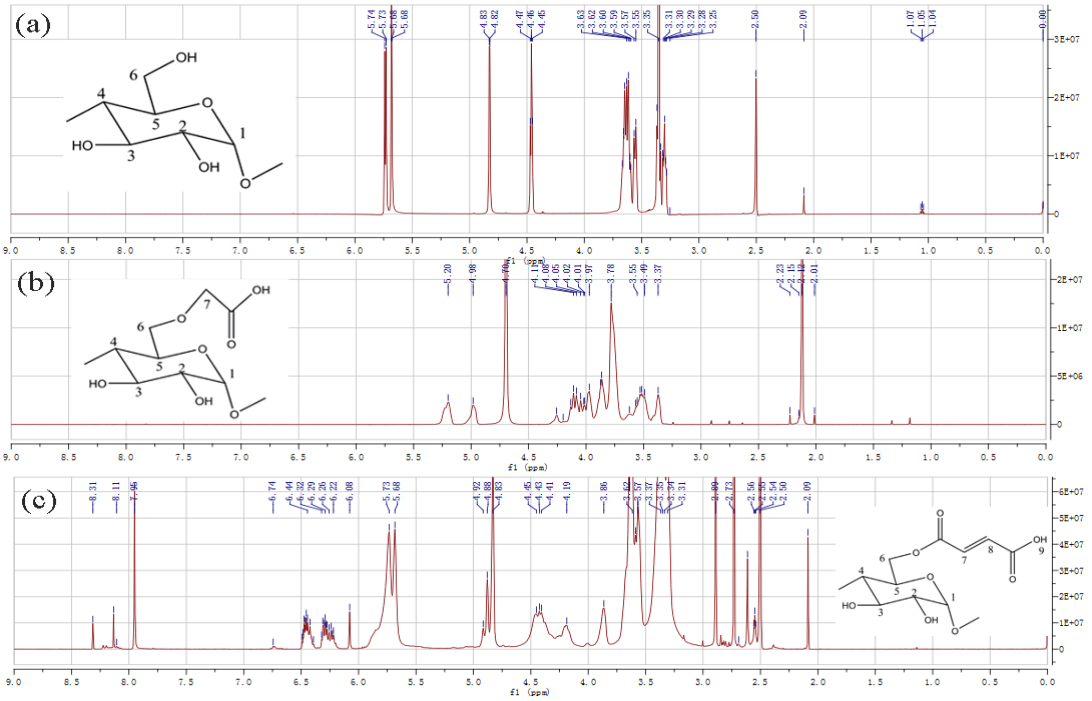

Figure S2 The ^{1}H NMR (600 MHz) spectral for the β-CD, CM-β-CD and MA-β-CD

Table S1 ^{1}H NMR (600 MHz) spectral data for the β-CD, CM-β-CD and MA-β-CD

	β-CD	CM-β-CD	MA-β-CD
H-1	4.46	4.26	4.43
H-2	3.28	3.37	3.31
H-3	3.59	3.97	3.65
H-4	3.35	3.49	3.35
H-5	3.55	3.78	3.57
H-6 a, b	3.62	4.01	4.19
H-7	-	2.12	6.29
H-8	-	-	6.44
OH-2	5.73	5.2	5.73
OH-3	5.68	4.98	5.68
OH-6	4.82	-	4.88
OH-9	-	-	7.96

As illustrated in Table S1 and Fig. S2, the disappeared peak at δ = 4.82 in the spectrum of CM-β-CD indicated the substitution reaction occurred at OH-6. As for MA-β-CD, the similar peak shape and height at δ = 5.68 and δ = 5.73 suggested the

same proportion of proton, which demonstrated there was no involved reaction at OH-2. While the peak area at δ = 4.82 was less than that of δ = 5.73, which was ascribed to the partial substitution occurring at OH-6. Therefore, the substitution reaction of the CM-β-CD and MA-β-CD both occurred at OH-6.

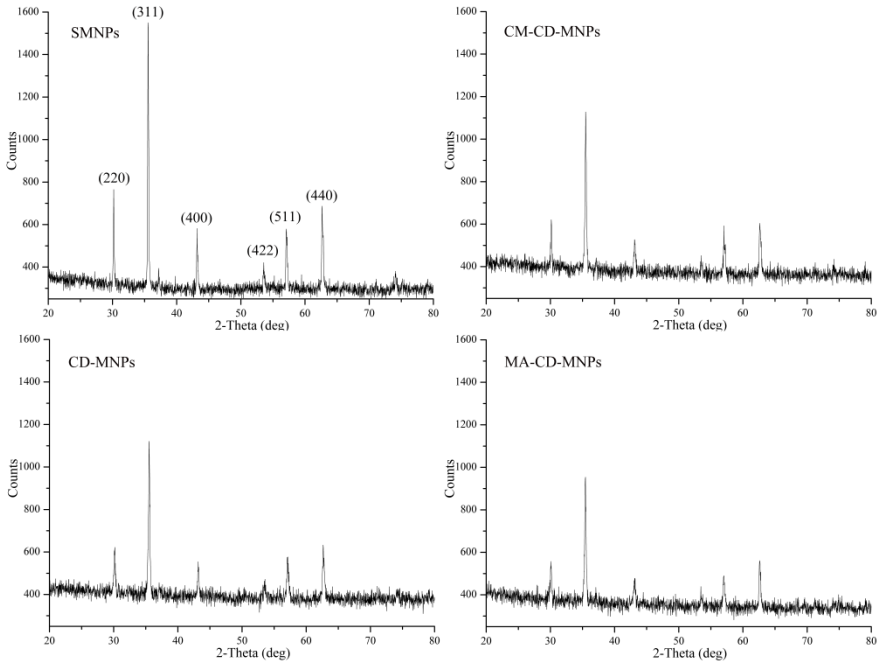

Figure S3 The XRPD spectral for SMNPs, CM-CD-MNPs, CD-MNPs and MA-CD-MNPs

The XRPD patterns for these nanoparticles were shown in Fig. S3. For all the samples, the six characteristic peaks occur at 2θ = 30.1, 35.5, 43.1, 53.4, 57.0 and 62.6 and their indices are: (220), (311), (400), (422), (511), and (440), respectively, because of the presence of Fe_3O_4 according to the standard XRPD data cards of the Fe_3O_4 crystal (JCPDS no. 85-1436). The results suggested that the grafting process did not change the phase of the Fe_3O_4 particles. It was worth noting that the intensity of the XRPD peaks obviously decreased when the SMNPs were coated with the polymers, and this proved that successful surface modification occurred.

Table S2 Elemental analysis of SMNPs and the modified SMNPs

Samples	C (%)	H (%)	N (%)
SMNPs	2.99	1.11	-
SMNPs-KH540	3.87	1.23	0.87
SMNPs-KH560	4.02	1.30	-
SMNPs-KH570	4.16	1.32	-

Table S3 The optimal loading conditions of three types of magnetic nano-carriers

	pH	t (h)	C_o (mg/L)[a]	solid-liquid ratio (mg/mL)[b]	T (^oC)
CD-MNPs	2	4	40	15:40	35
CM-CD-MNPs	2	4	20	15:30	35
MA-CD-MNPs	2	4	50	15:40	35

a: the initial concentration of HCFU

b: the ratio of amount of nano-carriers to volume of solution