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Electronic Supplementary information (ESI)

Single step synthesis of carbon dots embedded chitosan nanoparticles for cell imaging and hydrophobic drug delivery

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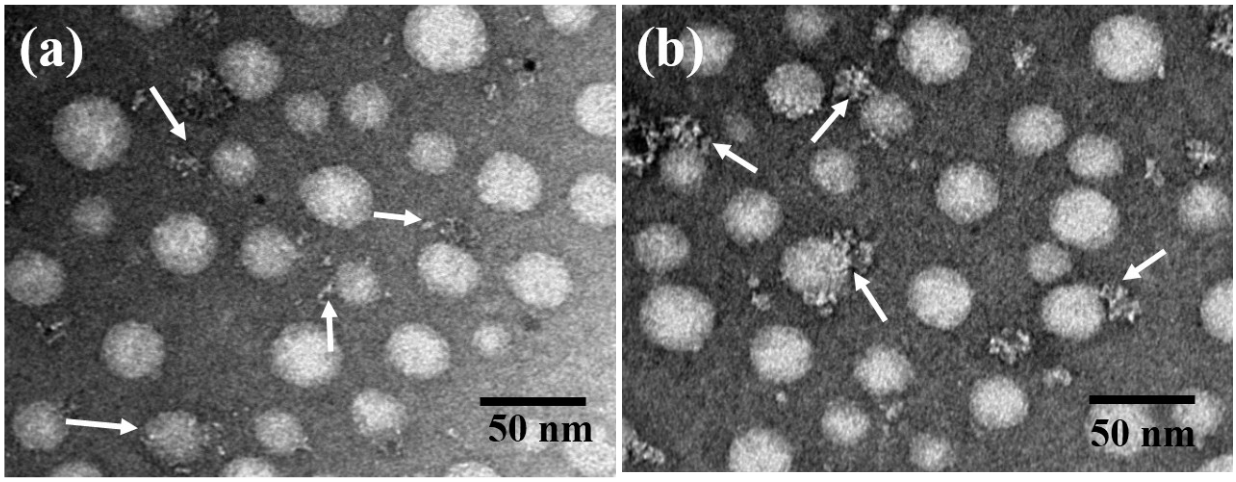


Fig. S1. TEM images of carbon dot conjugated OCMC-MMA nanoparticle synthesized at 135 °C (a) and 150 °C (b).

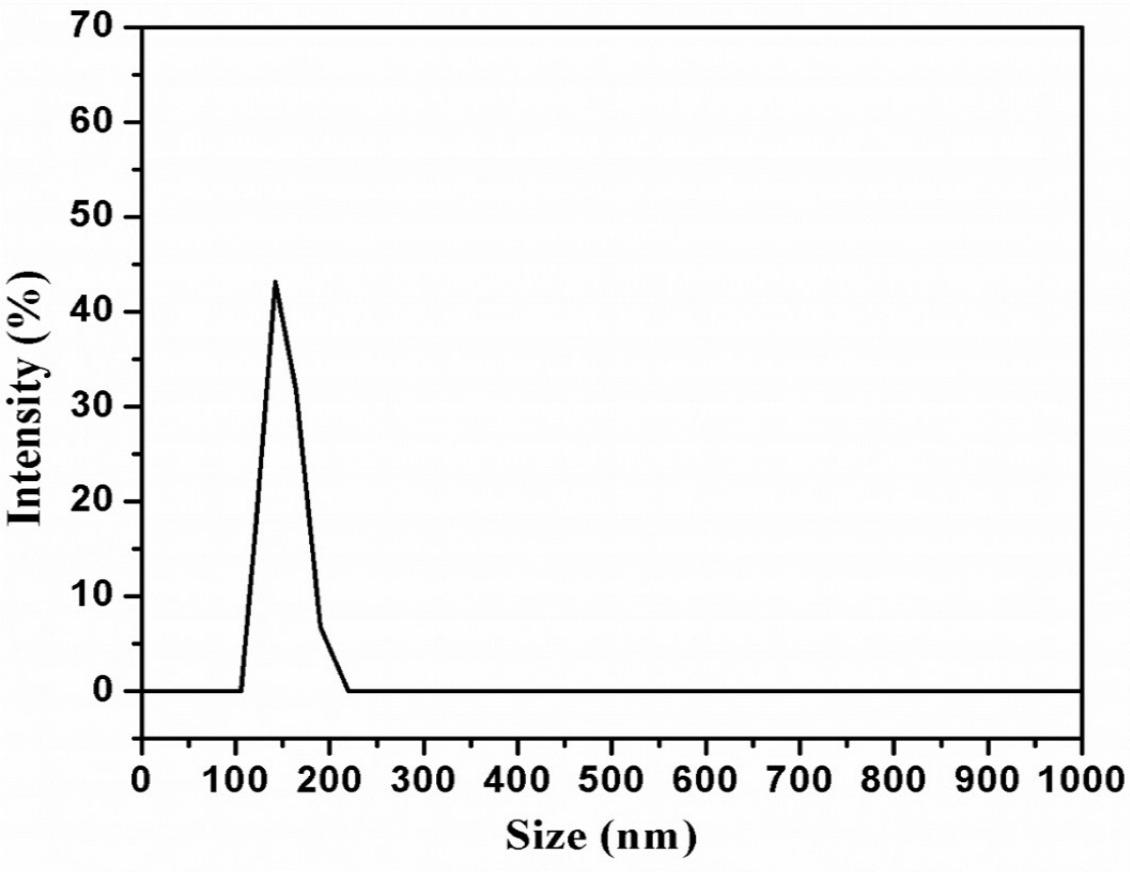


Fig. S2: DLS spectrum of OCMC-MMA nanoparticles

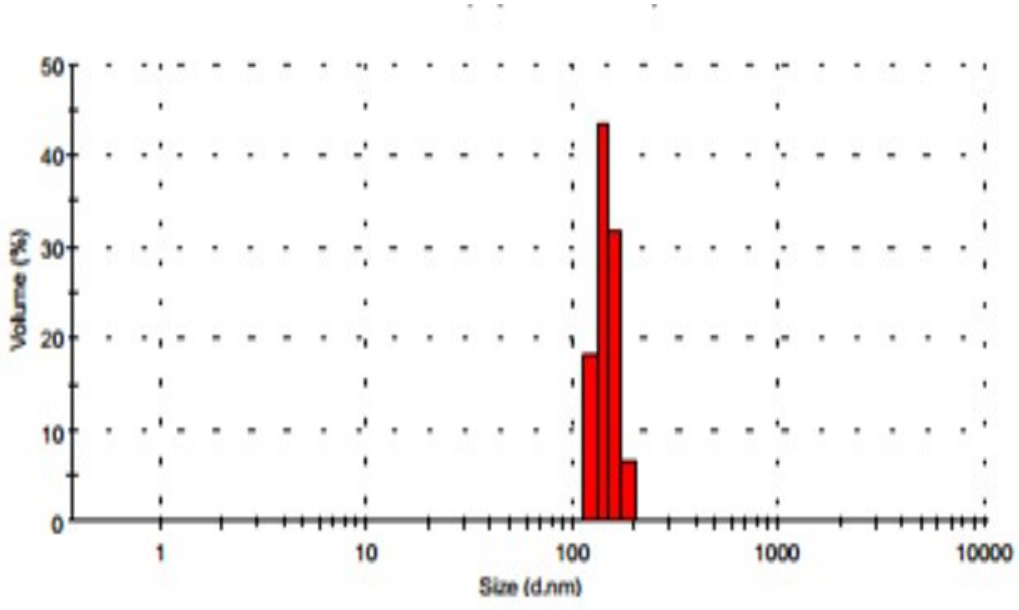


Fig. S3. Size distribution of OCMC@MMA NPs@CDs aggregates as determimed by DLS

Table S1: Intermolecular interaction and second order perturbation energy (E (2), Kcal/mol) between donor and acceptor orbitals of Drug and copolymer molecules.

Where LP =lone pair, BD*= Anti bonding orbital.

Sl No.	Inter molecular interaction	Distance (Å)	Donor	Acceptor	E(2), Kcal/mol
1	1O…1H-N	2.17862	LP (1) 1O	BD*(1)N-1H	3.61
			LP (2) 1O	BD*(1)N-1H	2.12
2	2O…2H-C	2.22249	LP (1) 2O	BD*(1)C-2H	3.22
			LP (2) 2O	BD*(1)C-2H	0.46
3	2O….3H-C	2.59327	LP (2) 2O	BD*(1)C-3H	0.68
4	1N…4H-C	2.68756	LP (1) 1N	BD*(1)C- 4H	1.25
5	1N…5H-C	2.90453	LP (1) 1N	BD*(1)C- 5H	0.31

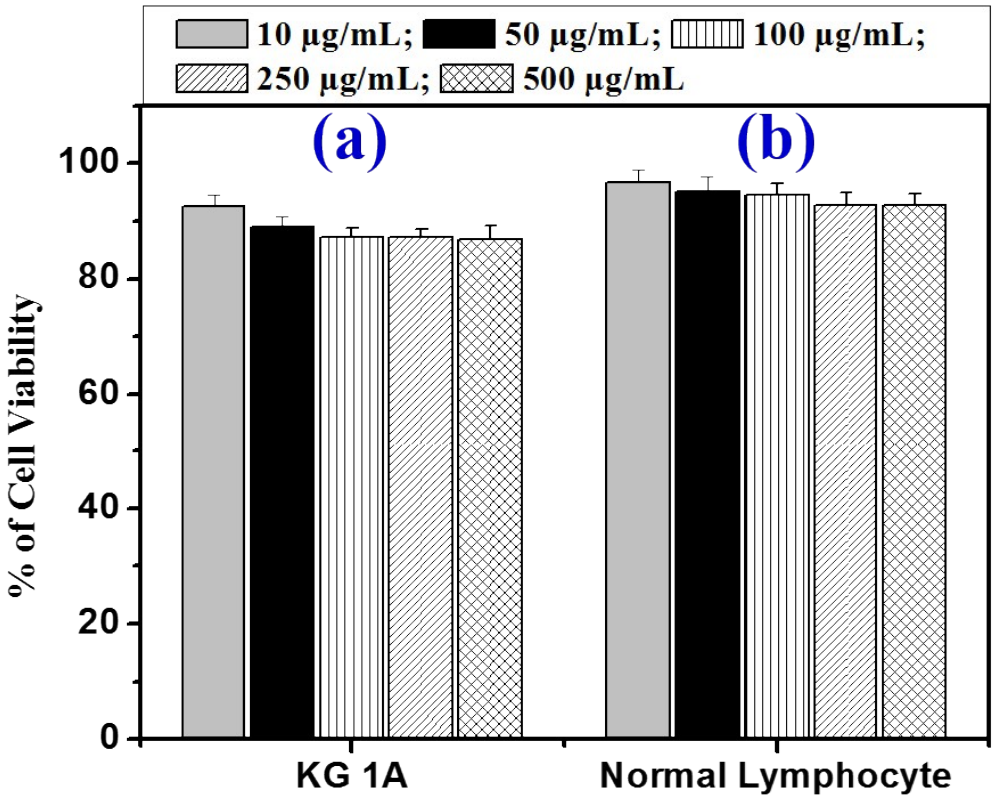


Fig. S4: Graphical presentation represents the cell viability of normal lymphocytes (a) and Cancer cell (b) after exposure with OCMC-MMA@CDs up to 500 µg/ml.

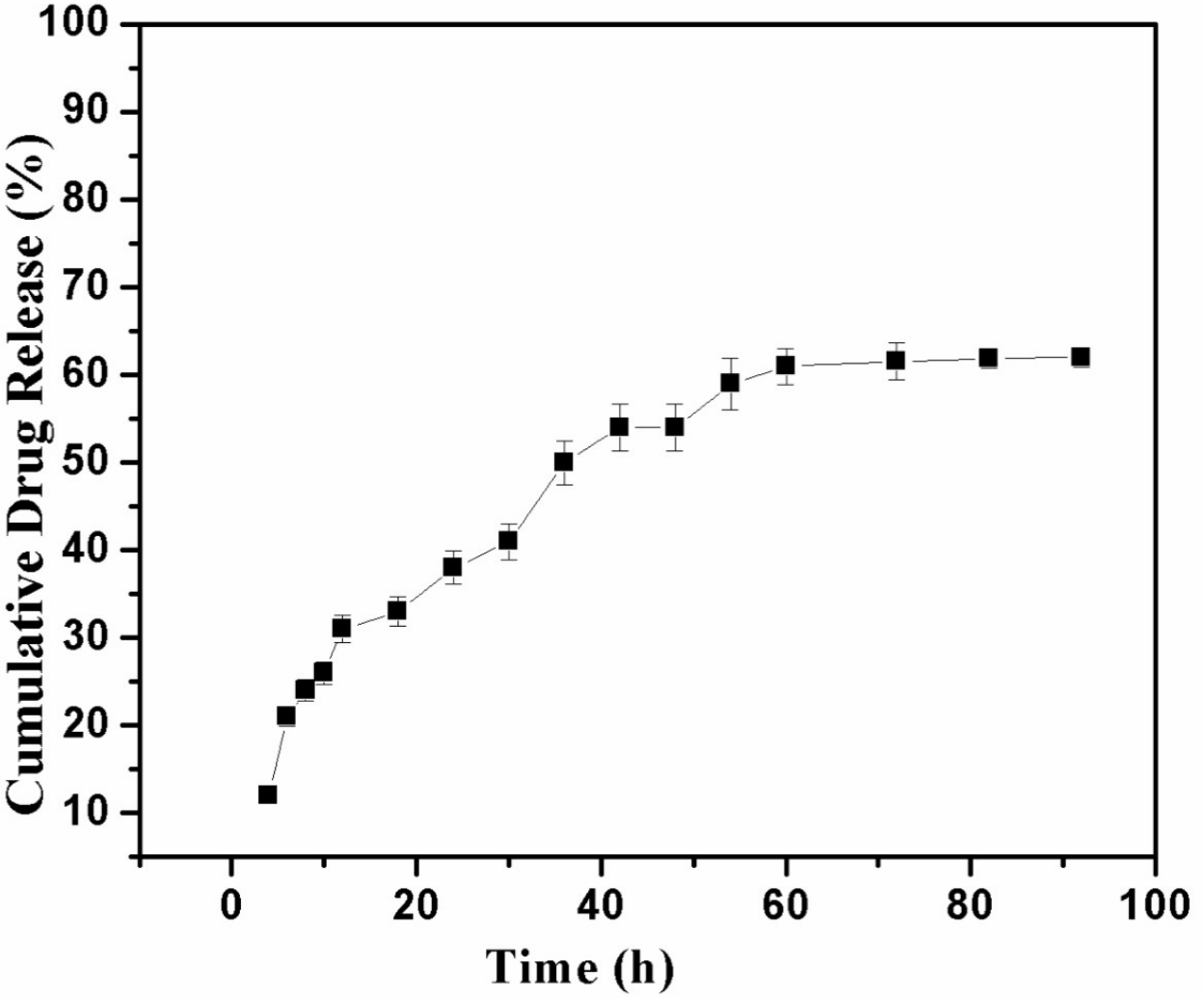
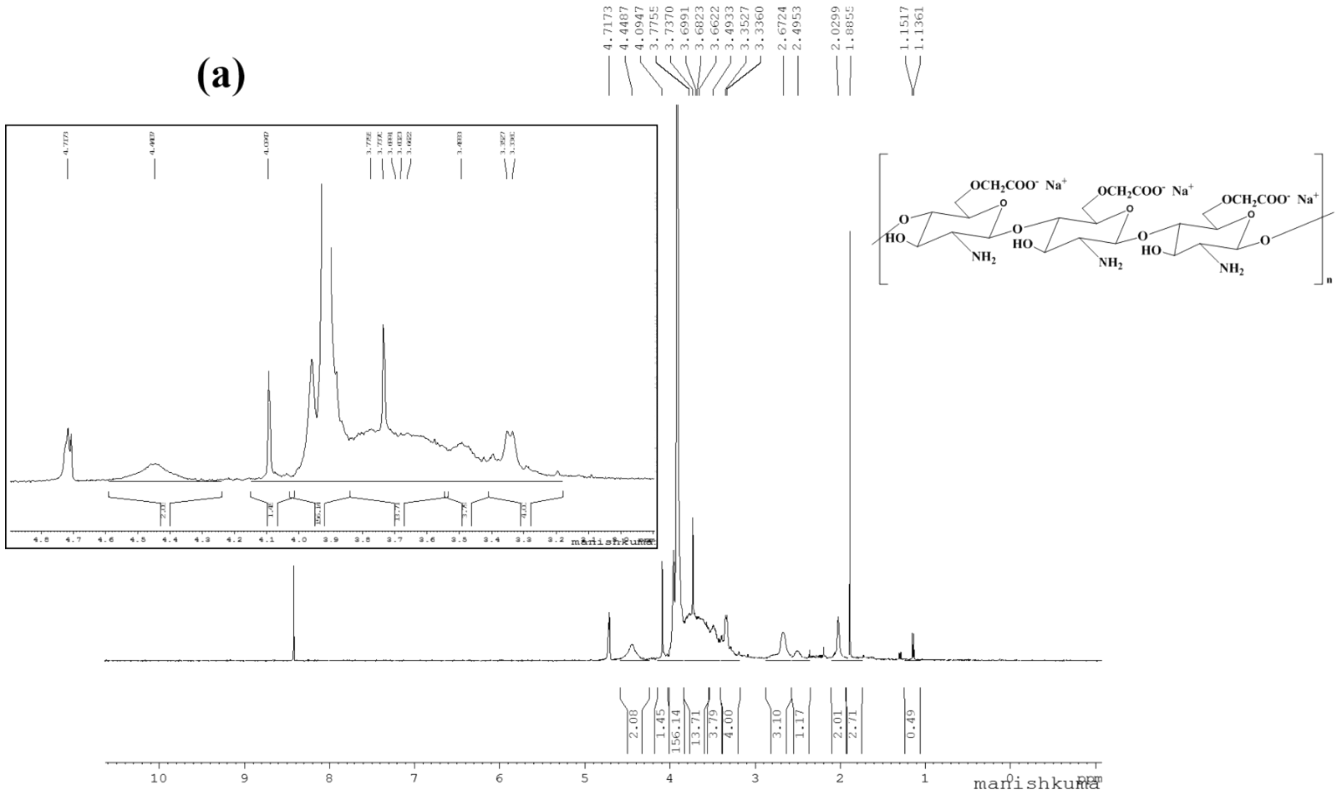
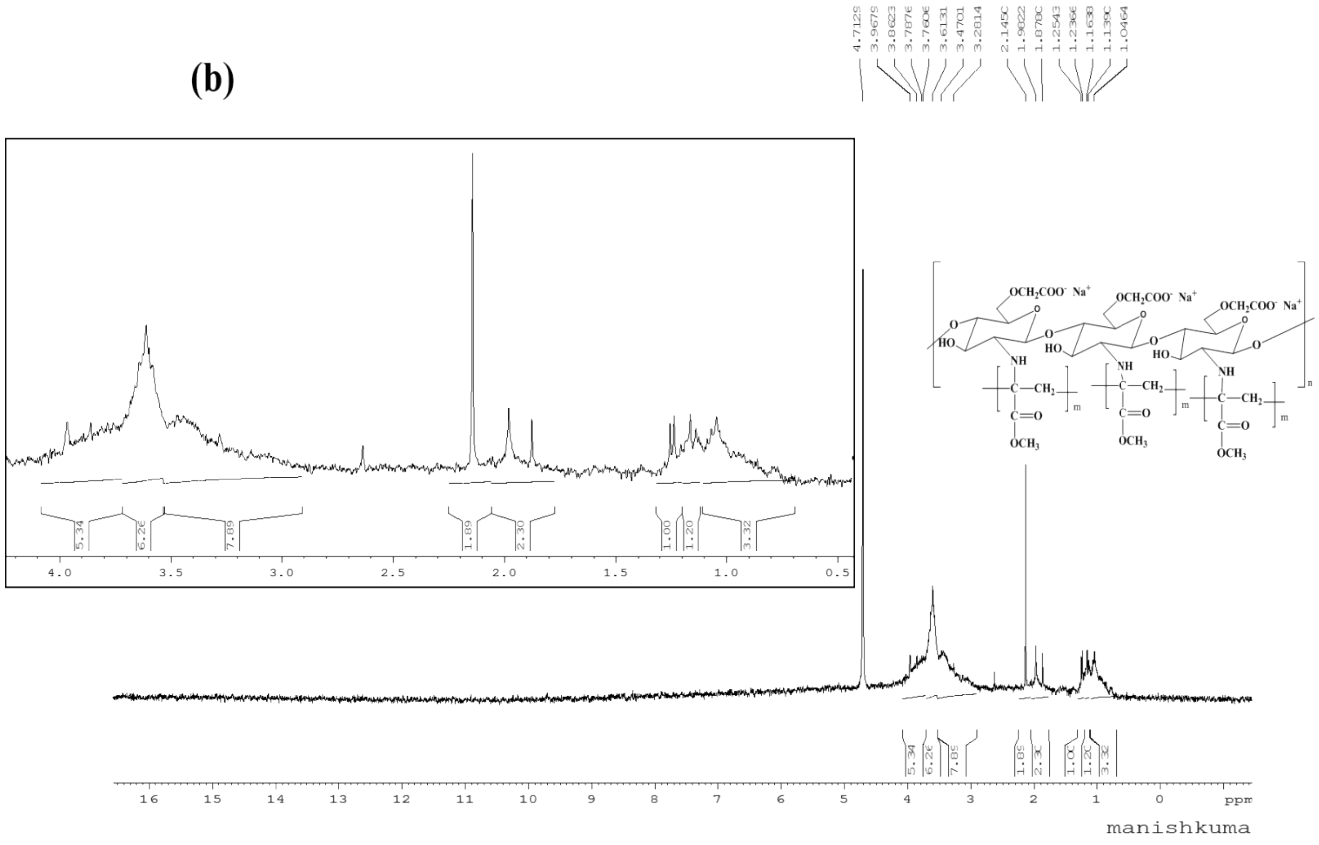


Fig. S5: In vitro *telmisartan* releases from OCMC-MMA@CDs at 7.4 pH solution.


(a)
manishkuma


(b)
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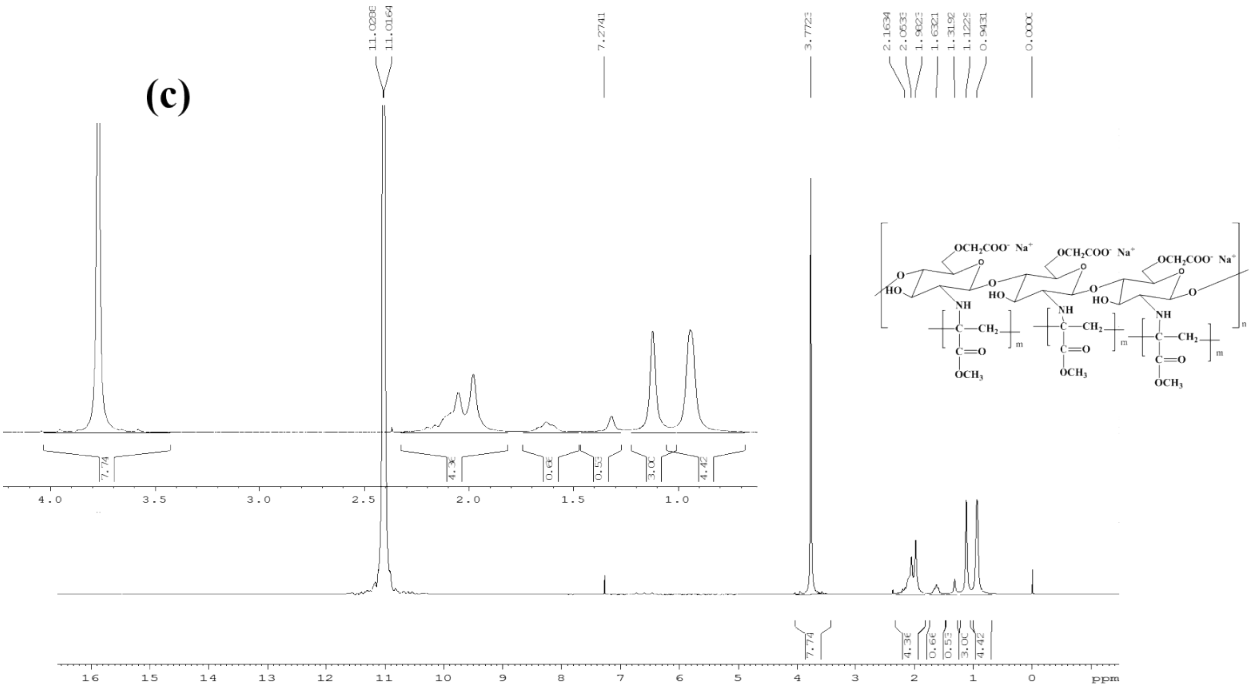

Fig. S6. 1H NMR spectra of OCMC dissolved in D_2O (a), OCMC@MMA NPs dissolved in D_2O (b), and CMC@MMA NPs dissolved in CF3COOD (c).

1HNMR Study

The 1H NMR spectrum of OCMC chitosan dissolved in D_2O is shown in Figure S6 (a). The multiplet proton signals in between 3.0-4.0 ppm confirmed the presence of ring methenyl protons of O-carboxylated chitosan backbones [7-9]. The peaks at 4.71 and 3.73 ppm corresponded to the -CH- group in the sugar ring while 3.92 ppm referred to the -CH_2- group of the carboxymethyl segment [10]. Which indicated the linkage of carboxymethyl groups to the hydroxyl position of chitosan. MMA is grafted at the NH_2 group of the OCMC backbone. Proton signals at 2.01 ppm is due to the methyl hydrogen of N-acetylglucosamine. The 1H NMR spectrum of OCMC-MMA NPs dispersed in D_2O was given in Figure S6 (b). The proton signals only due to the OCMC is prominent. When the OCMC-MMA NPs is dispersed in CF_3COOD, all the characteristic peaks including CH_3 (0.9-1.0 ppm), methylene-methine envelope (1-2.5 ppm) was observed for PMMA and 3.0-4.0 ppm were detected for the OCMC, as shown in fig S6 (c) [10]. The hydrophobic compartment i.e., PMMA is limited when OCMC-MMA is dissolve in D_2O, thus causing shielding of the proton signal in OCMC-MMA. As OCMC-MMA was dissolved, the dissociation of OCMC-MMA led to orientation of the hydrophobic chains to the aqueous phase, and the alkyl groups appeared accordingly. Therefore, the hydrophilic carboxylated chitosan and the hydrophobic acrylate polymer portions spontaneously formed nanoparticles with core-shell structures in aqueous solution

Table S2: Comparison of drug loading efficiency with relevant literature.

	Carrier	Drug	%Loading Efficiency	%Encapsulation Efficiency	Reference
Shi et al	Glycyrrhizin-modified O-carboxymethyl chitosan nanoparticles	Paclitaxel	14.9 %	83.7 %	1
Maya et al	Cetuximab conjugated O-carboxymethyl chitosan nanoparticles	Paclitaxel	----------	75.0 %	2
Tran et al.	self-assembled gelatin–oleic acid nanoparticles	Telmisartan	9.05 %	90.5 %	3
Emami et al.	succinate-chitosan-polyethylene glycol-folic acid	Paclitaxel	28.2 %	82.5 %	4
Koo et al.	oligomer-conjugated glycol chitosan nanoparticles	Paclitaxel	24.2 %	78.4 %	5
Wang et al.	Amphiphilic carboxymethyl chitosan-quercetin	Paclitaxel	25.37 %	64.24 %	6
In this Work	OCMC@MMA NPs/CDs	Telmisartan	28.2 %	82.9 %	--

Reference:

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