

Electronic Supplementary Information (ESI)

of

**A multifunctional metal-organic framework based tumor targeting drug delivery system for cancer
therapy**

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Table S1. Zeta potential of different modified MIL-101.

Sample	Zeta potential (mV)
MIL-101-NH ₂ (Fe)	16.7±0.777
MIL-101-N ₃ (Fe)	21.7±0.462
DOX@MIL-101-N ₃ (Fe)	8.23±0.156
DOX@β-CD-SS-MIL-101	-18.9±0.346
DOX@PEG-RGD-β-CD-SS-MIL-101	-1.3±0.332

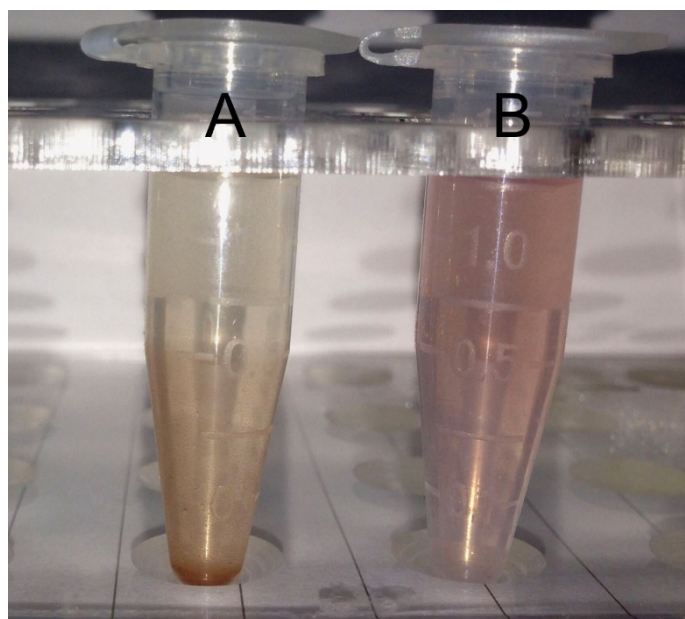


Fig. S1. Photographs of MIL-101-N₃(Fe) (A) and DOX@PEG-RGD- β -CD-SS-MIL-101 (B) dispersed in water for 24 hours. Nanoparticles were firstly ultrasonic dispersion in water at a concentration of 0.2 mg/mL. The clear colloidal suspensions were then left at dark before the photographs were taken.

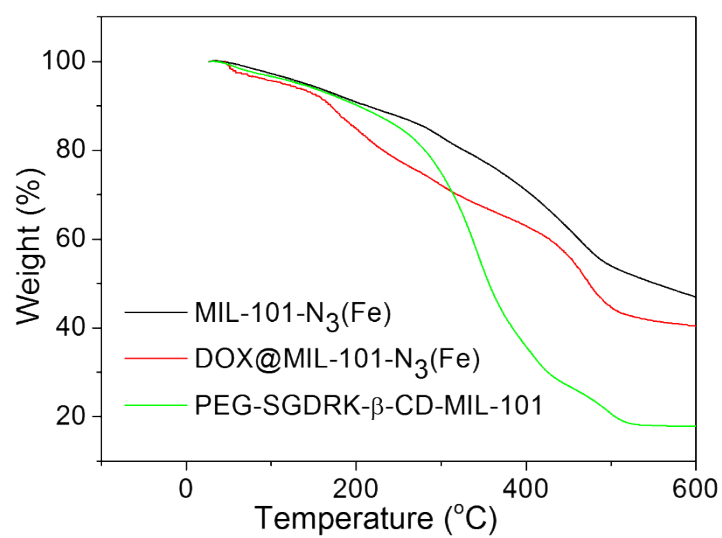


Fig. S2 TGA curves of different nanoparticles: MIL-101-N₃(Fe) (black line), DOX@MIL-101-N₃ (red line), and DOX@PEG-RGD-β-CD-SS-MIL-101 (green line).

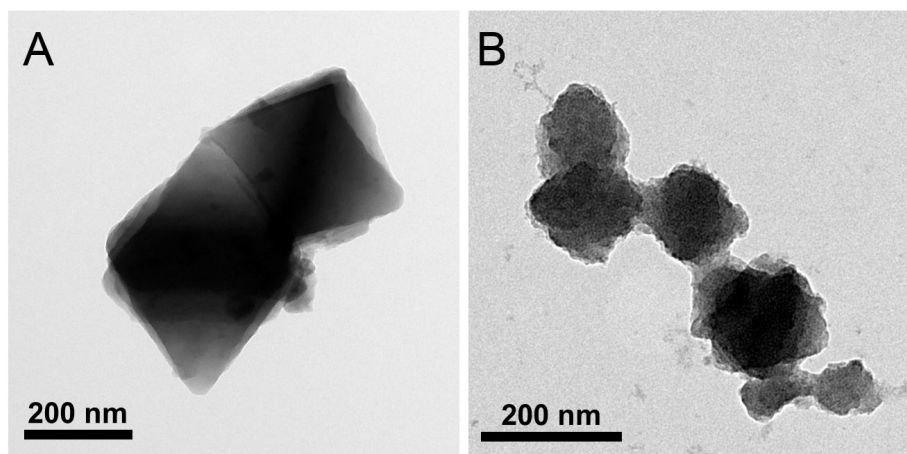


Fig. S3 (A) TEM image of surface modified DOX loaded TTMOF incubated in 5 mM PBS for 2 days. (B) TEM image of non-modified DOX modified MIL-101-N₃(Fe) incubated in 5 mM PBS for 2 days.

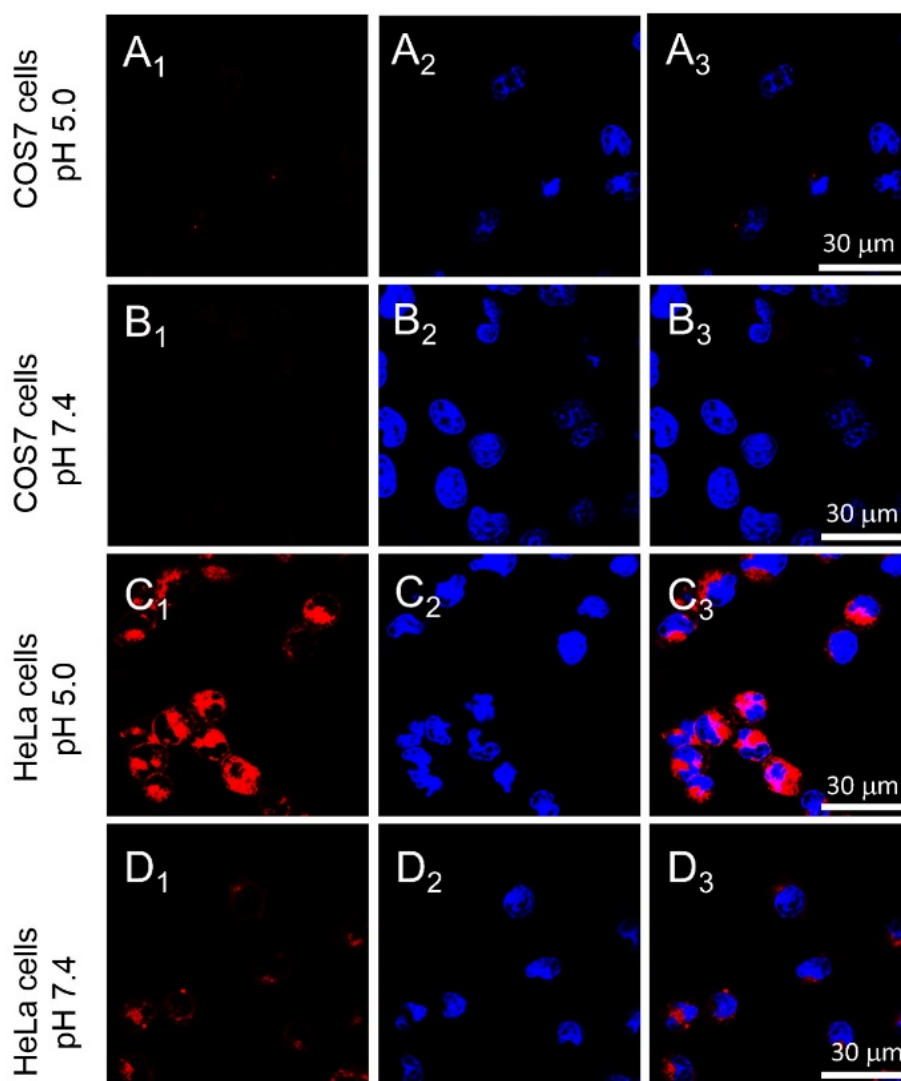


Fig. S4 CLSM images of COS7 cells incubated with DOX loaded TTMOF at pH 5.0 (A₁-A₃) or pH 7.4 (B₁-B₃) for 90 min, and HeLa cells incubated with the DOX loaded TTMOF at pH 5.0 (C₁-C₃) or pH 7.4 (D₁-D₃) for 90 min. (A₁, B₁, C₁, D₁): Red fluorescence images of DOX; (A₂, B₂, C₂, D₂): Blue fluorescence images of nuclei; (A₃, B₃, C₃, D₃): The merge images of blue and red fluorescence.

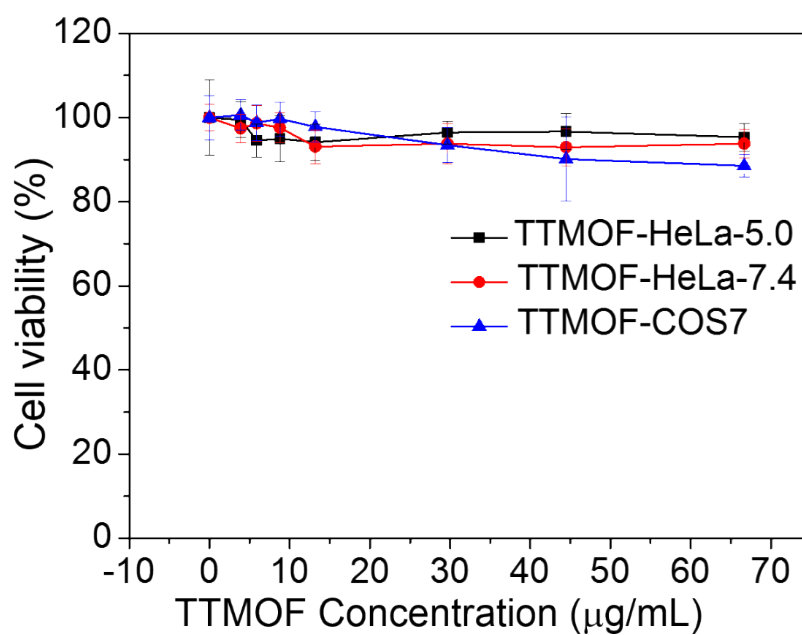


Fig. S5 Cell viability of HeLa cells after incubated with empty TTMOF at different dose at pH 5.0 (black), and pH 7.4 (red); and cell viability of COS7 cells incubated with empty TTMOF at pH 7.4 (blue).

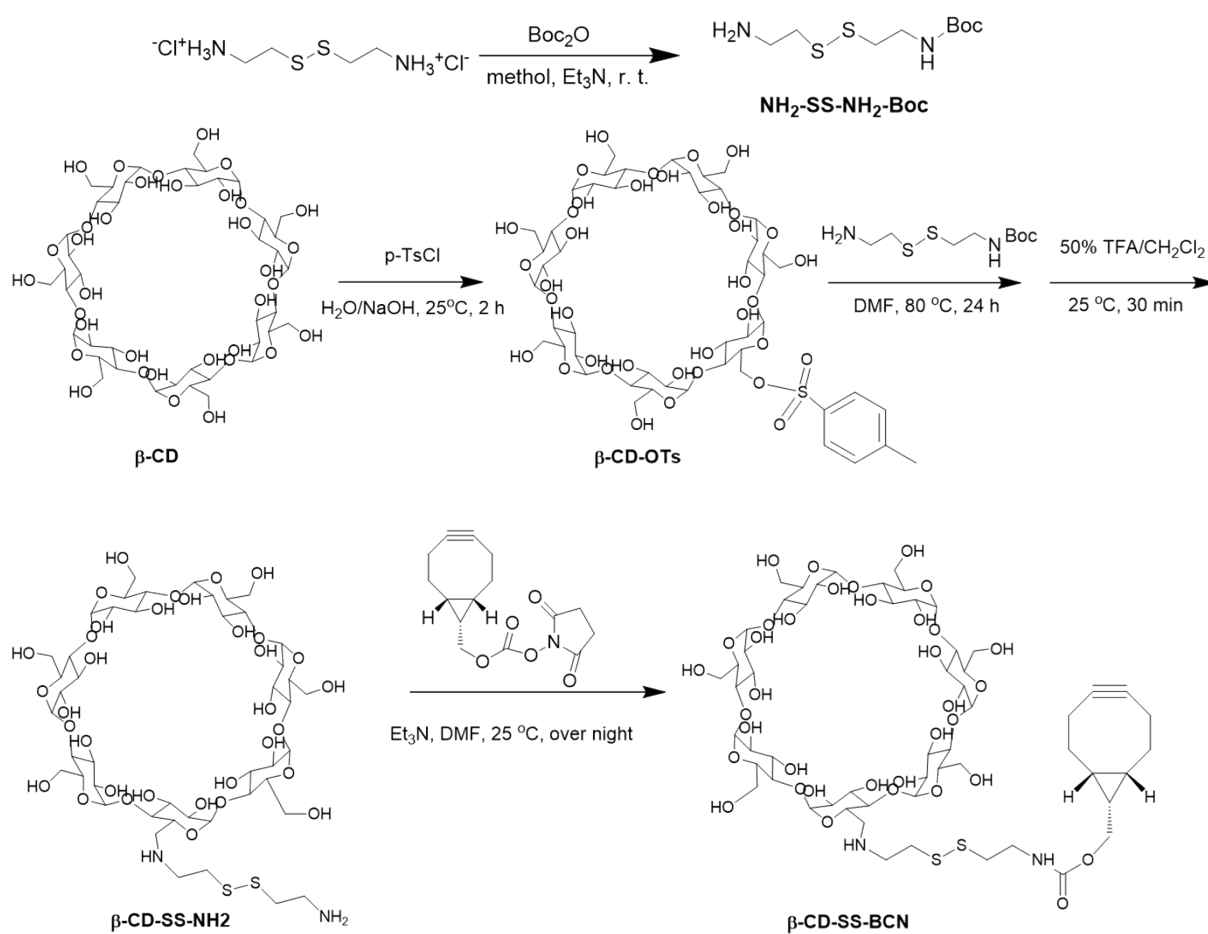


Fig. S6 Synthesis procedure of bicyclononyne functionalized $\beta\text{-CD}$ ($\beta\text{-CD-SS-BCN}$).

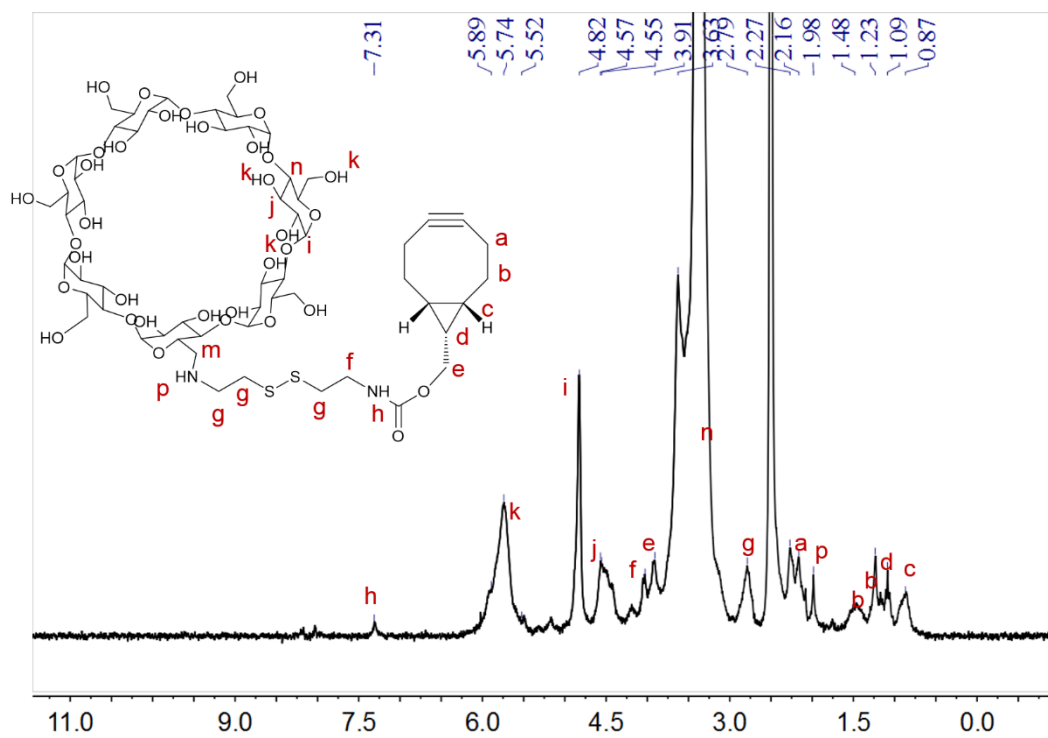


Fig. S7 ¹H NMR spectrum of β-CD-SS-BCN.

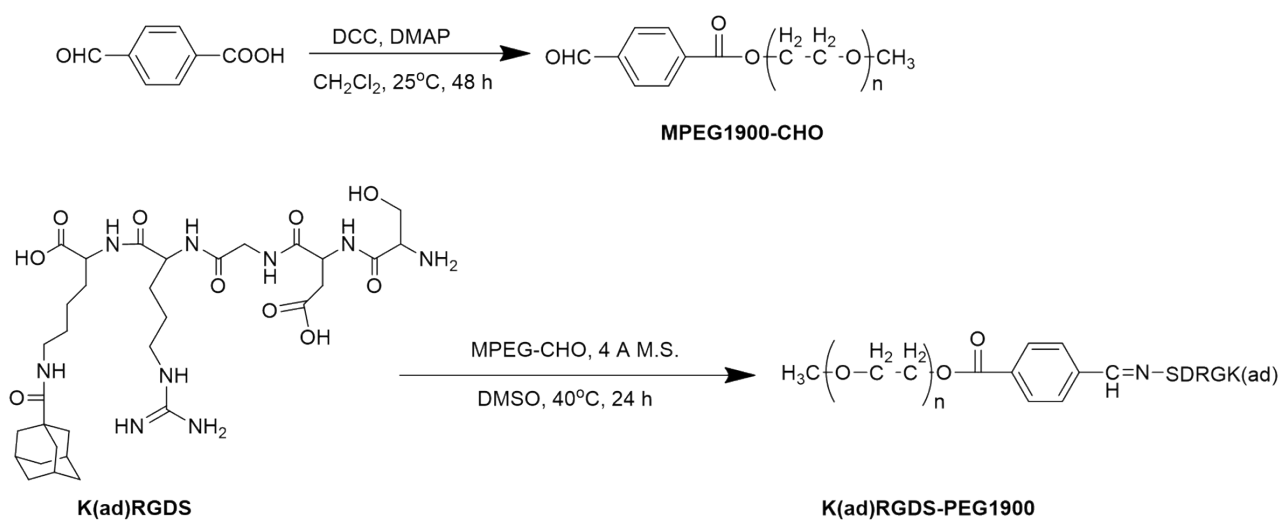


Fig. S8 Synthesis procedure of K(ad)RGDS-PEG1900.

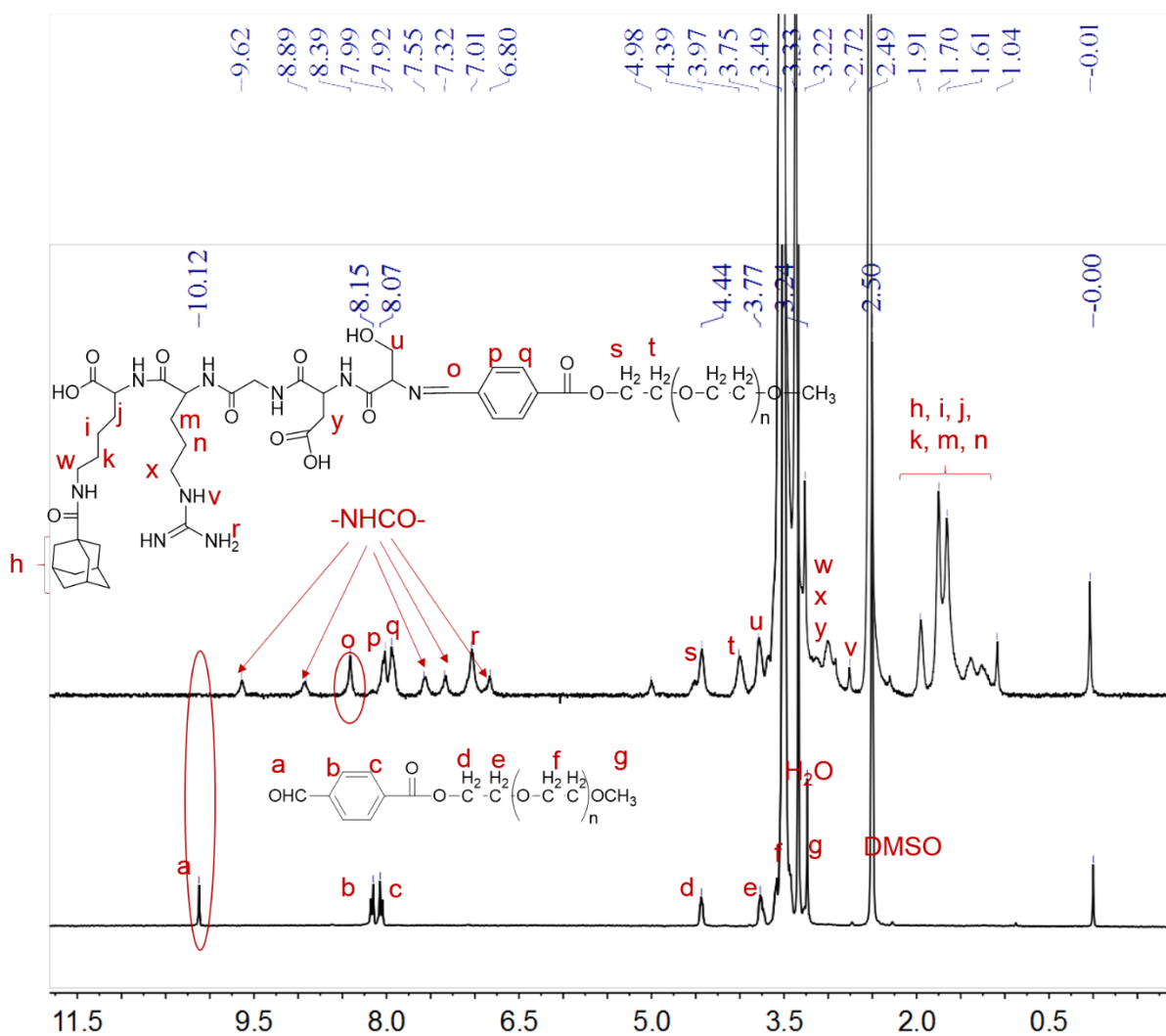


Fig. S10 $^1\text{H NMR}$ spectrum of MPEG-1900-CHO and K(ad)RGDS-PEG-1900.

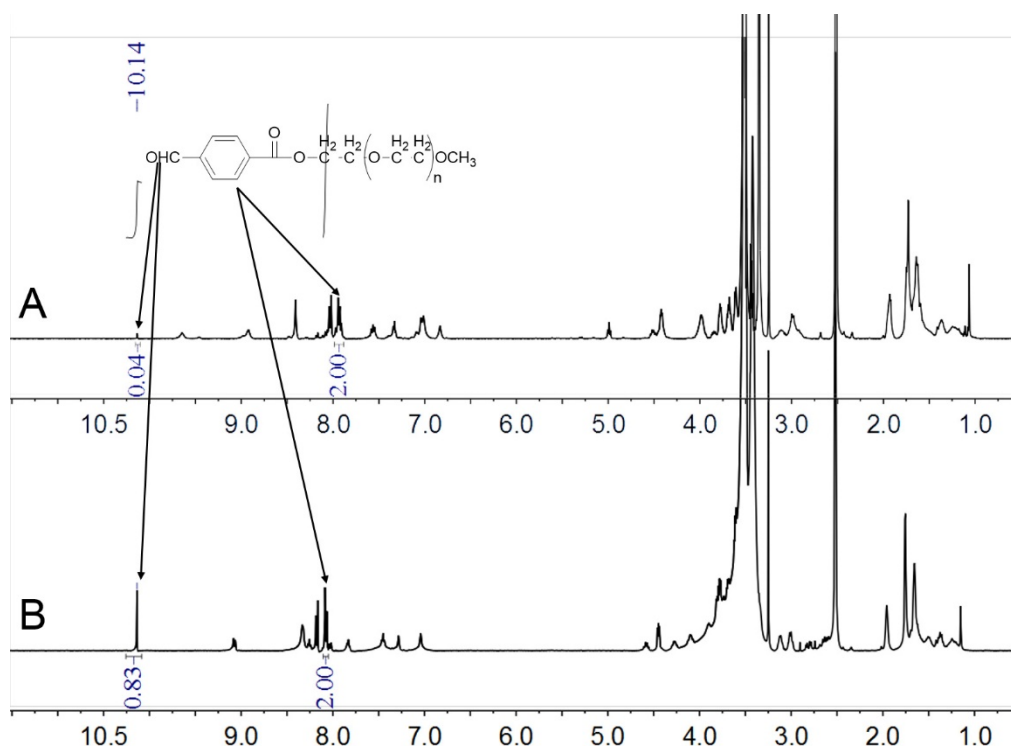


Fig. S11 ^1H NMR spectrums of K(ad)RGDS-PEG-1900 after incubated in PBS 7.4 (A) or ABS 5.0 (B) at 37 °C for 2 hours.