Supporting Information

A paclitaxel-based supramolecular hydrogel loaded with mifepristone for the inhibition of breast cancer metastasis

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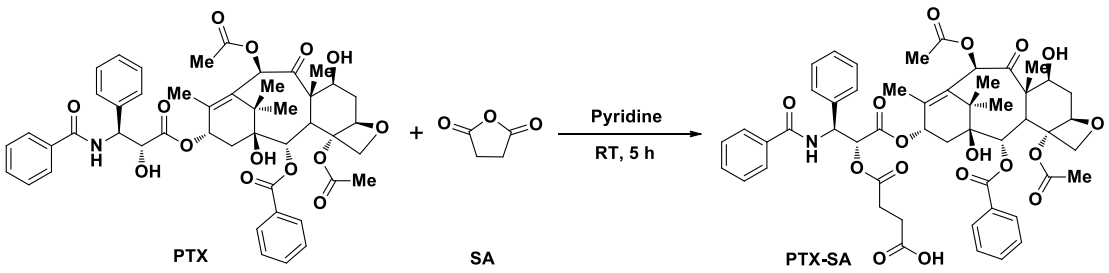
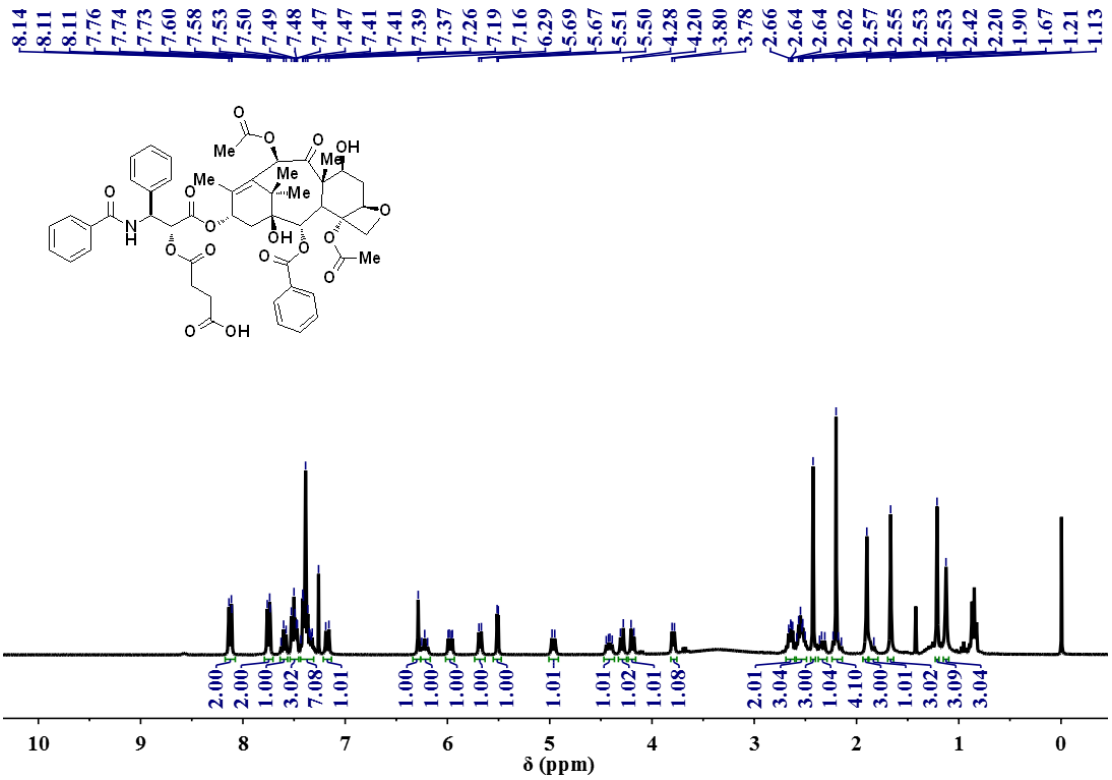
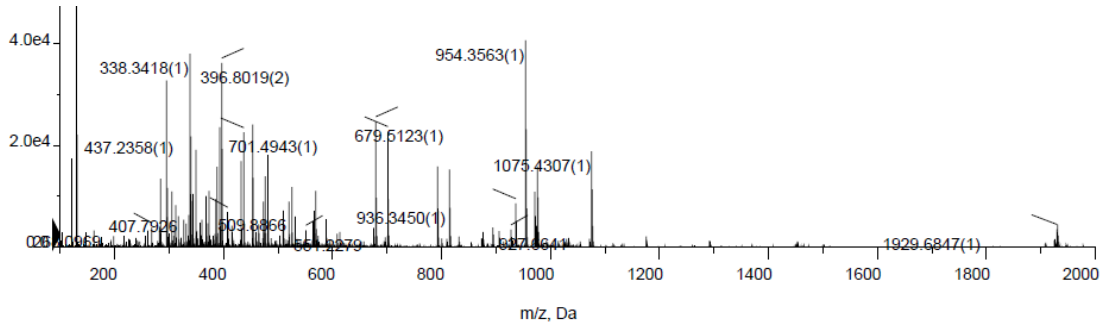


Figure S1 Synthesis route for succinic anhydride-modified paclitaxel compound (PTX-SA).



^{1}H NMR (300 MHz, $CDCl_3$) δ 8.17 – 8.07 (m, 2H), 7.79 – 7.71 (m, 2H), 7.60 (t, *J* = 7.3 Hz, 1H), 7.54 – 7.45 (m, 3H), 7.44 – 7.31 (m, 7H), 7.17 (d, *J* = 9.3 Hz, 1H), 6.29 (s, 1H), 6.22 (t, *J* = 8.6 Hz, 1H), 5.97 (dd, *J* = 9.3, 3.3 Hz, 1H), 5.68 (d, *J* = 7.0 Hz, 1H), 5.51 (d, *J* = 3.4 Hz, 1H), 4.96 (d, *J* = 7.9 Hz, 1H), 4.42 (dd, *J* = 10.8, 6.7 Hz, 1H), 4.29 (d, *J* = 8.4 Hz, 1H), 4.19 (d, *J* = 8.5 Hz, 1H), 3.79 (d, *J* = 7.0 Hz, 1H), 2.69 – 2.60 (m, 2H), 2.59 – 2.49 (m, 3H), 2.42 (s, 3H), 2.37 – 2.29 (m, 1H), 2.24 – 2.14 (m, 4H), 1.90 (s, 3H), 1.88 – 1.79 (m, 1H), 1.67 (s, 3H), 1.21 (s, 3H), 1.13 (s, 3H).

Figure S2 ^{1}H NMR spectrum of succinic anhydride-modified paclitaxel compound (PTX-SA).



HRMS: calc. M = 953.3470, obsvd. $(M + H)^+$ = 954.3563.

Figure S3 HRMS spectrum of succinic anhydride-modified paclitaxel compound (PTX-SA).

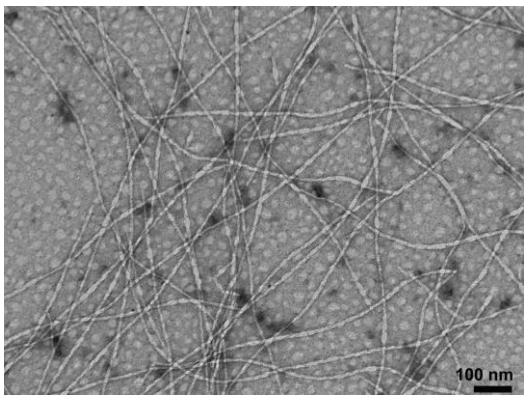


Figure S4 TEM image of paclitaxel hydrogel (P-nano).

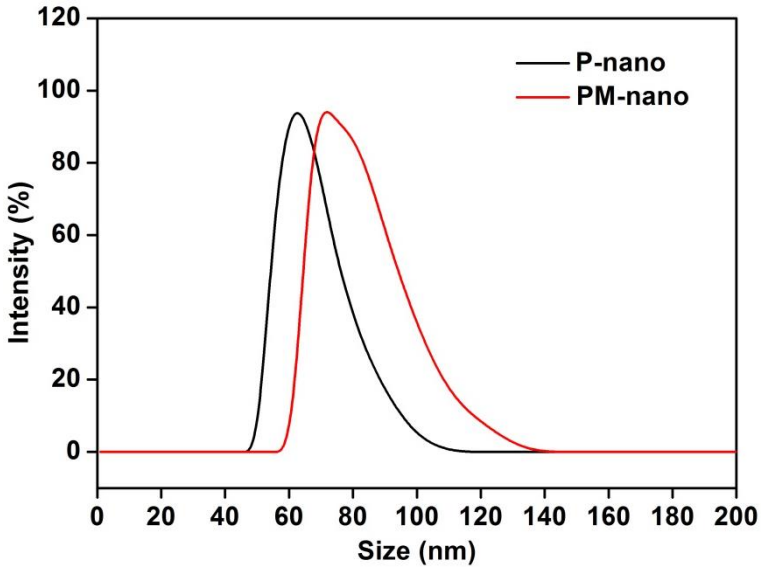


Figure S5 Hydrodynamic size distribution of nanofibers. P-nano, paclitaxel (PTX) hydrogel; PM-nano, PTX-conjugated and mifepristone (MIF)-loaded hydrogel.

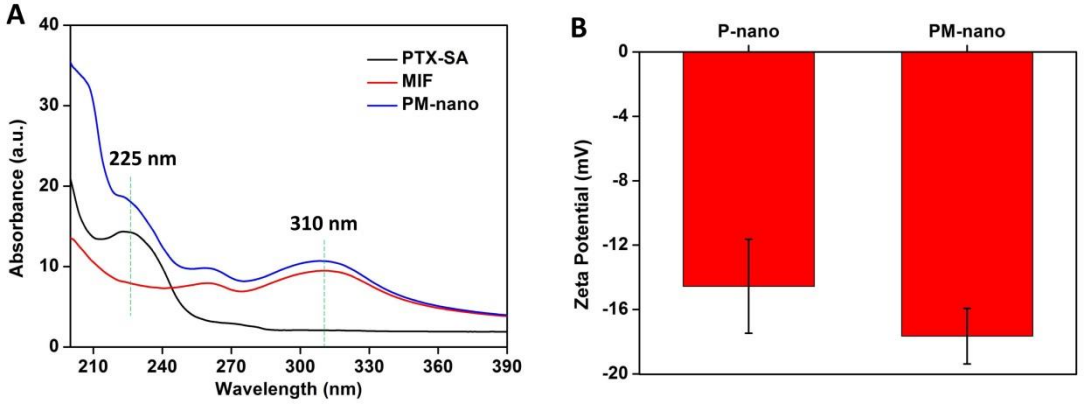


Figure S6 UV–vis absorption spectra and zeta potential. (A), UV–vis absorption spectra of succinic anhydride-modified paclitaxel compound (PTX-SA), mifepristone (MIF), and PTX-conjugated and MIF-loaded hydrogel (PM-nano). (B), Zeta potential of PTX hydrogel (P-nano) and PM-nano.

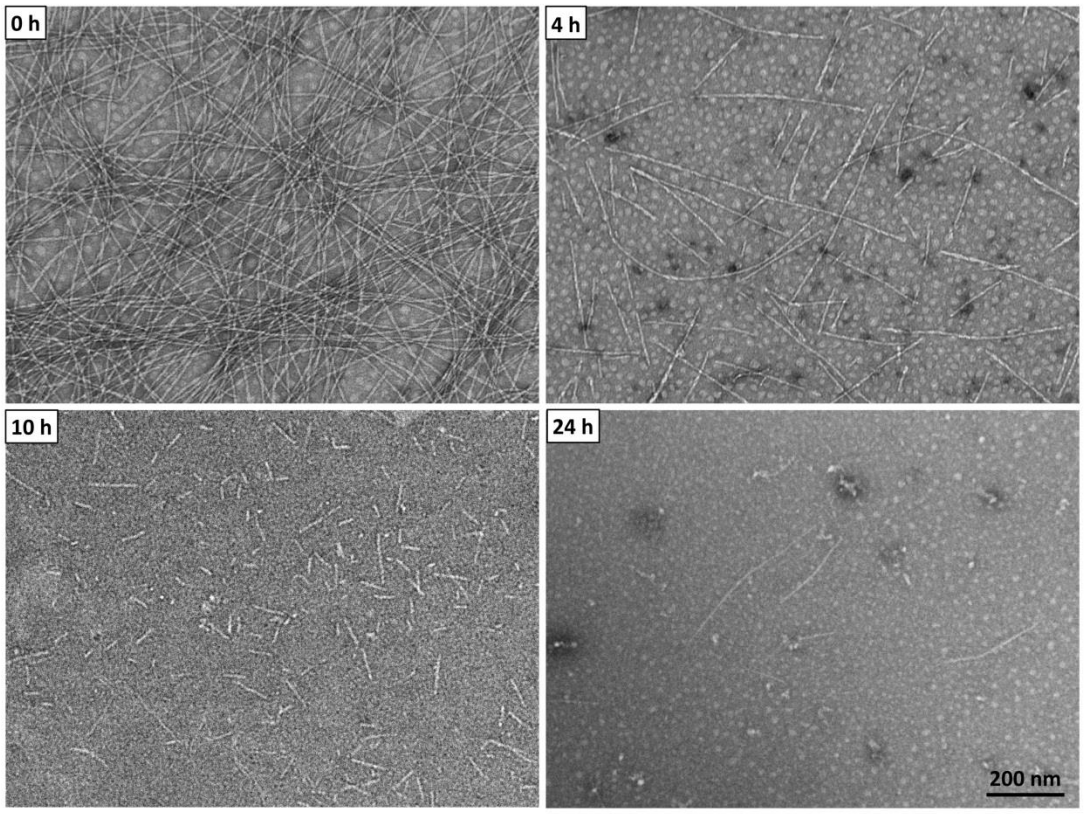


Figure S7 TEM images of paclitaxel (PTX)-conjugated and mifepristone (MIF)-loaded hydrogel (PM-nano) after 0 h, 4 h, 10 h or 24 h of incubation with serum.

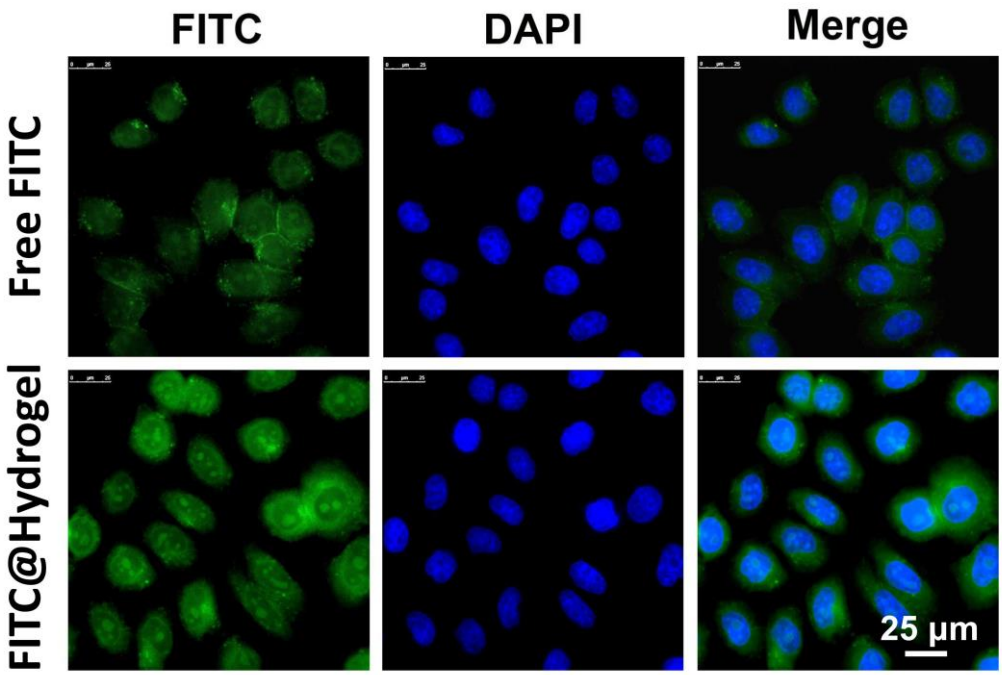


Figure S8 Fluorescence images of MCF-7 cells treated with free FITC or FITC-loaded hydrogel (FITC@Hydrogel) after a 4 h of incubation with an equivalent FITC concentration (10 μg/mL).

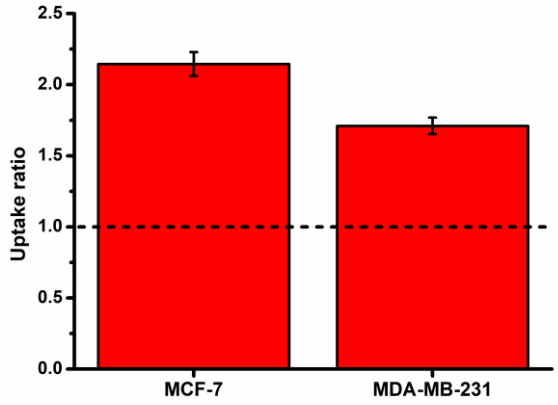


Figure S9 Cellular uptake ratio of FITC-loaded hydrogel (FITC@Hydrogel) to free FITC determined by Image J software based on the average fluorescence intensity of MCF-7 and MDA-MB-231 cells after a 4 h of incubation.

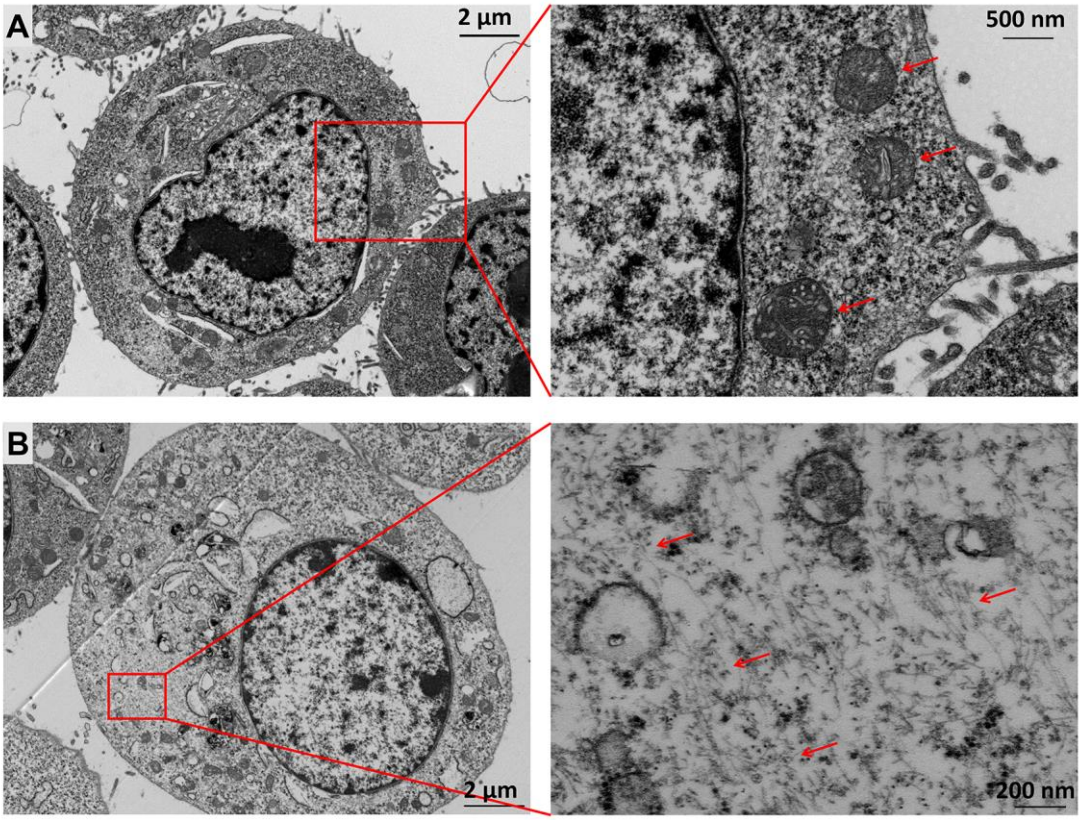


Figure S10 TEM images of the nanofibers (red arrows) in the lysosome (A) and the cytoplasm (B) after a 4 h of co-incubation of 4T1 cells with paclitaxel (PTX)-conjugated and mifepristone (MIF)-loaded hydrogel (PM-nano).

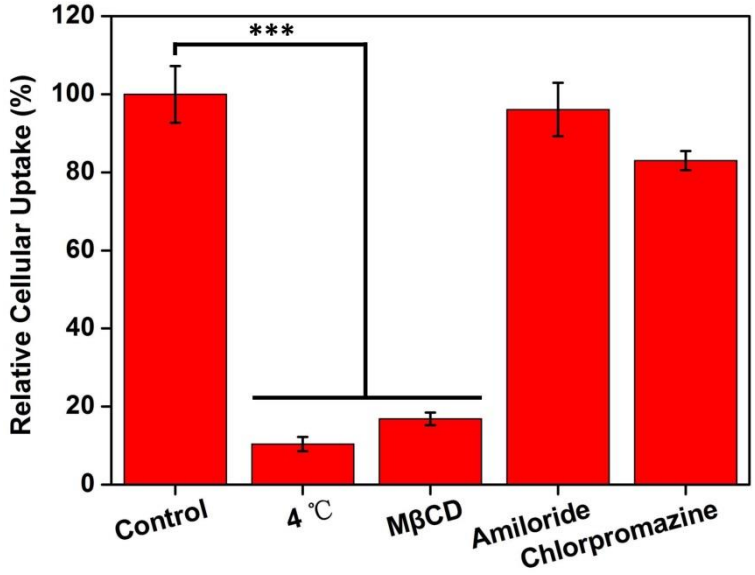


Figure S11 Relative cellular uptake amount of paclitaxel (PTX)-conjugated and mifepristone (MIF)-loaded hydrogel (PM-nano) in 4T1 tumor cells with different treatments. *** $P < 0.001$. MβCD, methyl-β-cyclodextrin.

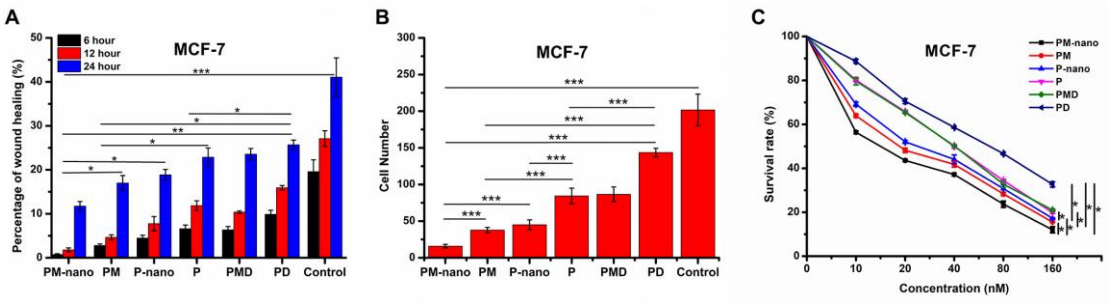


Figure S12 Effects on the biological functions of MCF-7 cells. (A), Quantification analysis of the scratch-wounds of MCF-7 cells before and after 24 h of treatment with various materials. (B), Quantification analysis of the invaded MCF-7 cells after various treatments. (C), Cytotoxicity of various materials against MCF-7 cells evaluated by MTT assays. * $P < 0.05$, ** $P < 0.01$， *** $P < 0.001$. P, paclitaxel; PD, paclitaxel + dexamethasone; PM, paclitaxel + mifepristone; PMD, paclitaxel + mifepristone + dexamethasone; PM-nano, paclitaxel-conjugated and mifepristone-loaded supramolecular hydrogel; P-nano, paclitaxel hydrogel.