ARTICLE

DPD simulations on morpholo-gies and struc-tures of blank PLGA-*b*-PEG-*b*-PLGA polymeric micelle and Docetaxel-loaded PLGA-*b*-PEG-*b*-PLGA polymeric micelle

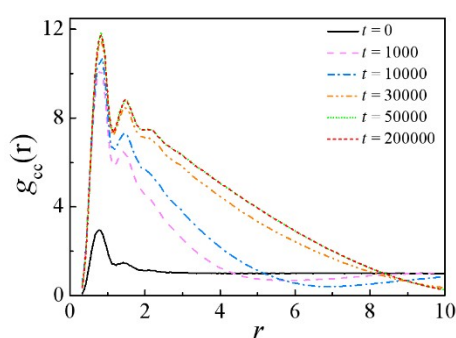Mengyao Wang,[1] Ye Lin,[1] Jianxu Gao,[1] and Dongmei Liu,*[1]

Fig. S1 The radial distribution functions between beads of the blank PLGA$_3$-*b*-PEG$_7$-*b*-PLGA$_3$ micelles at different simulation times.
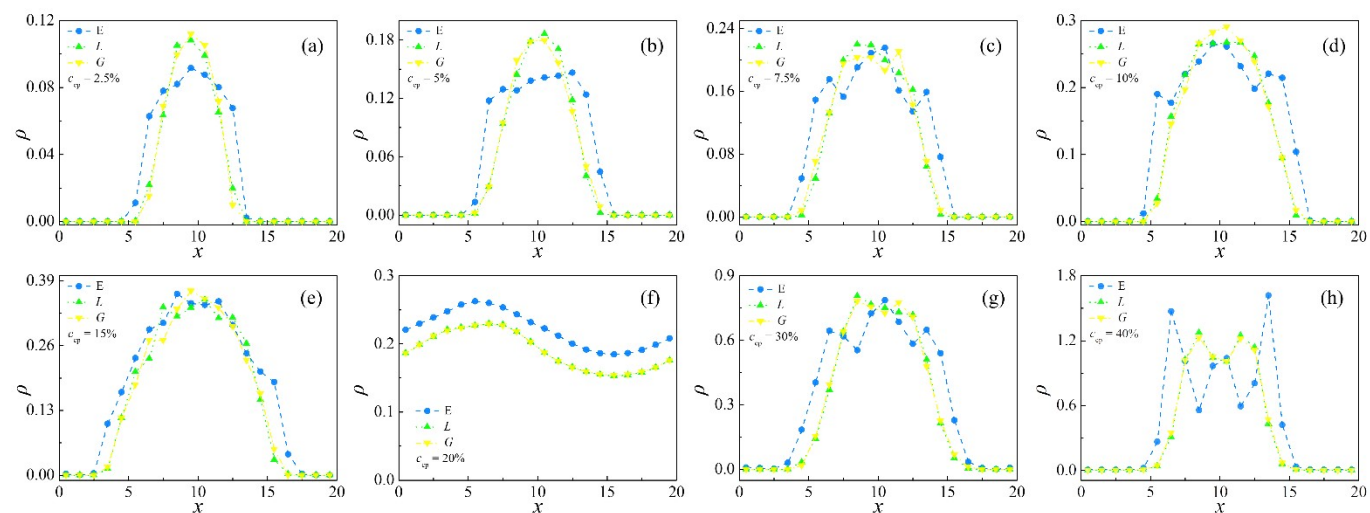

Fig. S2 Density profiles of E, L and G beads of the blank PLGA$_3$-*b*-PEG$_7$-*b*-PLGA$_3$ micelles as a function of copolymer concentration.
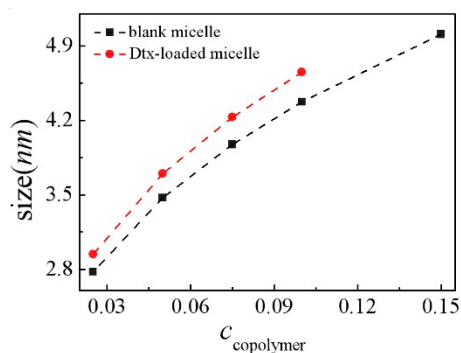
Fig. S3 The size of the blank and Dtx-loaded PLGA$_3$-*b*-PEG$_7$-*b*-PLGA$_3$ micelles as a function of the copolymer concentration.
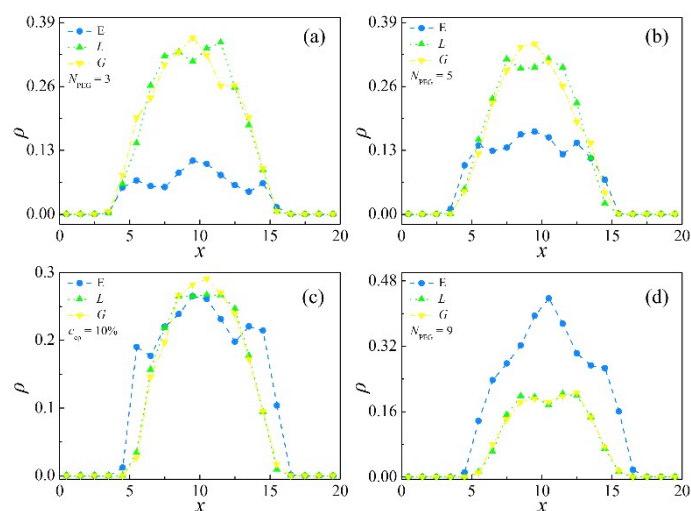

Fig. S4 Density profiles of E, L and G beads of the blank PLGA$_3$-*b*-PEG$_7$-*b*-PLGA$_3$ micelles as a function of the PEG block length.
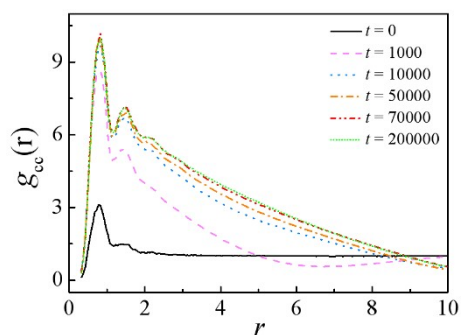

Fig. S5 The radial distribution functions between beads of the Dtx-loaded PLGA$_3$-*b*-PEG$_7$-*b*-PLGA$_3$ micelles at different simulation times.
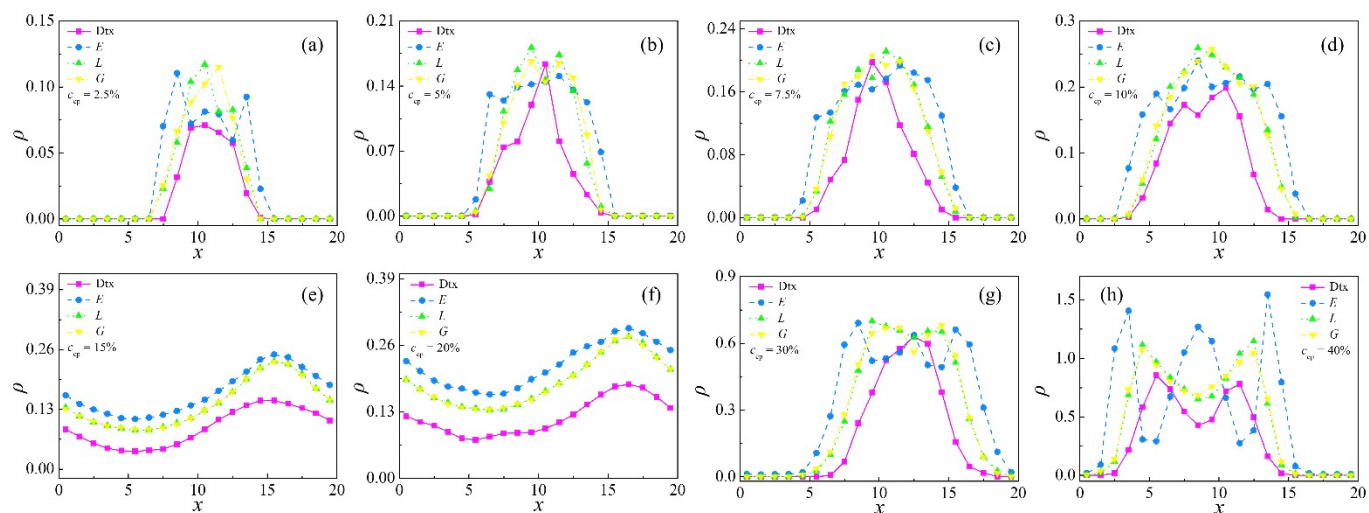
Fig. S6 Density profiles of E, L and G beads of the PLGA$_3$-b-PEG$_7$-b-PLGA$_3$ copolymers and Dtx beads as a function of copolymer concentration.
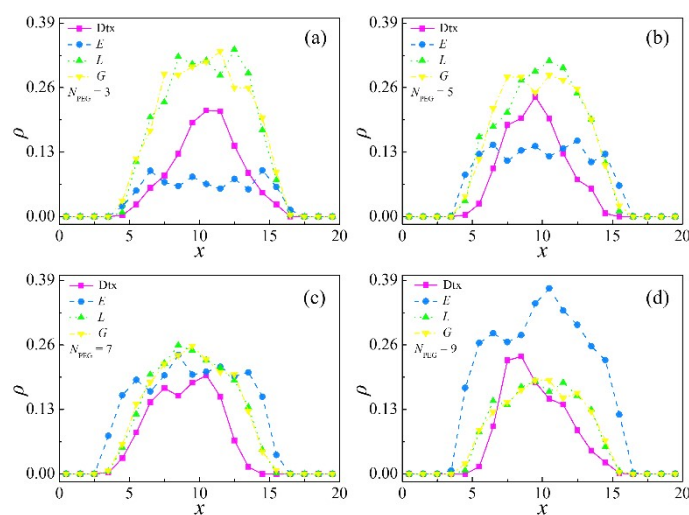

Fig. S7 Density profiles of E, L and G beads of the PLGA$_3$-b-PEG$_7$-b-PLGA$_3$ copolymers and Dtx beads as a function of the PEG block length.
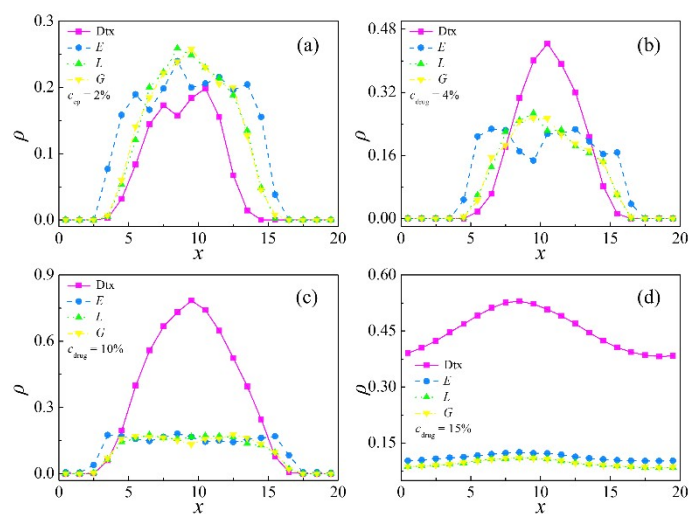

Fig. S8 Density profiles of E, L and G beads of the PLGA$_3$-b-PEG$_7$-b-PLGA$_3$ copolymers and Dtx beads as a function of the Dtx drug concentration.
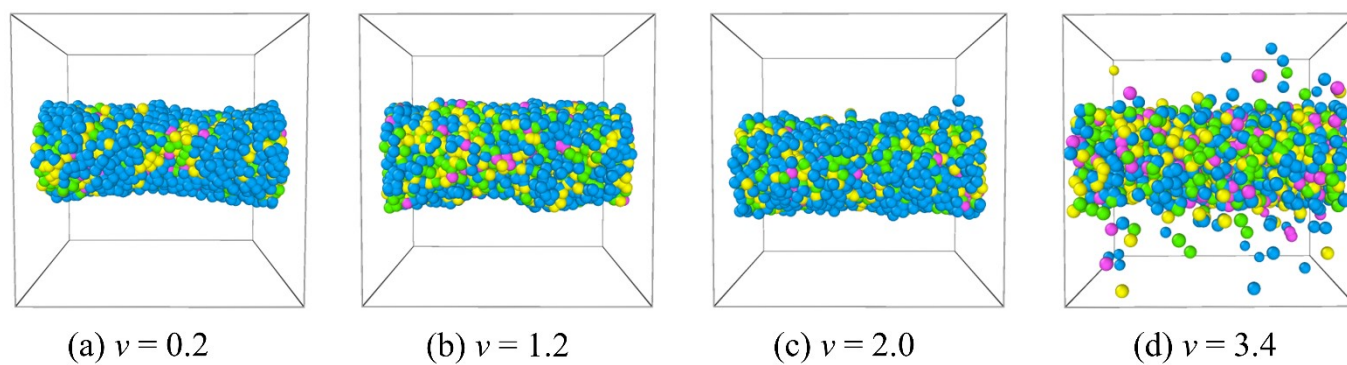
(a) $v = 0.2$ (b) $v = 1.2$ (c) $v = 2.0$ (d) $v = 3.4$

Fig. S9 Morphologies snapshpts of Dtx-loaded PLGA$_3$-b-PEG$_7$-b-PLGA$_3$ micelles under different shear rates v (v = 0.2, 1.2, 2.0, 3.4).