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Fig. S1. The molecular dynamics simulations of DHA NPs self-assembly. The DHA self-assembly into DHA NPs were mainly via hydrophobic interactions (gray sticks) and hydrogen bond interactions (blue sticks).



Fig. S2. (A)Zeta potentials of DHA and DHA NPs. (B) Changes of hydrodynamic

diameter and PDI of DHA NPs stored in PBS with FBS (10%) for 24 h. Data are expressed as mean \pm SD (n = 3). (C) Changes of hydrodynamic diameter and PDI of DHA NPs stored in water for 7 days measured by DLS. (D) Cumulative drug release profiles of DHA NPs in different PBS solutions. Data are expressed as mean \pm SD (n = 3).



Fig. S3. FCM analysis of cells incubated with DHA NPs at 37 °C for 0.5, 2, and 4 h.



Fig. S4. CLSM images of HepG2 cells incubated with different concentrations of DHA NPs for 4 h at 37 °C. All scale bars are 20 μ m.



Fig. S5. CLSM images of HepG2 cells incubated with DHA NPs at 37 °C and 4 °C for 4 h. All scale bars are 20 μ m.



Fig. S6. Morphological apoptosis by staining with Hoechst 33258 in HepG2 cells treated with different concentrations of DHA NPs. All scale bars are $20 \,\mu$ m.



Fig. S7. Principal component analysis (PCA) of HepG2 cells based on untreated control group (C) and DHA NPs treatment group (NPs).



Fig. S8. FCM analysis of ROS generation of HepG2 cells in A) control group and B) DHA NPs treatment group.



Fig. S9. Representative photographs of mice in different groups after various treatments.



Fig. S10. H&E staining images of the major organs (heart, liver, spleen, lung and kidney) of mice from each group at day 12. Scale bars: $100 \mu m$.



Fig. S11. Ki67 staining images of tumor slices in different groups. Scale bars, $100 \,\mu\text{m}$.



Fig. S12. TUNEL staining images of tumor slices in different groups. Scale bars, 100 μ m.