Supplementary data

## Phenylboronic Acid-based Core-Shell Drug Delivery Platform Clasping 1,3-Dicarbonyl Compounds by A Coordinate Interaction

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**Scheme S1**. Graphical illustration for the formation of nano-construct through coordinate interaction between PBA of pPBA and 1,3-dicarbonyl of CUR.



**Figure S1**. A) Scheme for static quenching of PBA fluorescence by photoinduced electron transfer (PET) after mixing with 1,3-dicarbonyl. B) Quenching of PBA fluorescence after mixing with CUR.



Figure S2. XPS spectra for PBA and PBA with CUR.



**Figure S3**. <sup>1</sup>H NMR spectra of pPBA. Conjugation of PBA was calculated. The molar ratio of PBA to maleic anhydride was 160 PBA groups to 513 maleic anhydride groups.



**Figure S4**. A) Reaction scheme for the synthesis of pCTRL with pPBA. B) Fluorescence of PBA from pPBA, pCTRL and pMVEMA (equivalent of polymer backbone, ex at 300 nm). Removal of boron moiety was confirmed by monitoring PBA fluorescence.



**Figure S5**. Solubilizing CUR with pMVEMA. Severe aggregation of CUR was observed, implying that pMVEMA can not solubilize CUR.



Figure S6. Characterization of nano-constructs by the interaction between curcumin (CUR)

and PBA. A) Quenching effect of pPBA fluorescence depending on CUR ratio to PBA of pPBA. B) PDI value of nano-constructs depending on CUR ratio to PBA. C) Size distribution and D) colloidal stability of CCN. E) Z-average size and PDI values of CCN at 4 °C and room temperature for 30 days. F) Size distribution of CCN in PBS and CCN incubated in media (DMEM containing 10 % FBS) for 24 h.



**Figure S7**. Calculation of  $K_{eq}$ . A) Plotting  $K_{ARS}$  for PBA and ARS at pH 5.0 and 7.4. B) Benesi-Hilderbrand equation for the estimation of  $K_{eq}$ . C) Plotting  $K_{eq}$  for CUR and PBA at pH 5.0 and 7.4. Slopes mean  $K_{ARS}/K_{eq}$ .



**Figure S8**. A) Relative median fluorescence intensity (MFI) values for cellular uptake of CCN after treatment of endocytosis inhibitors; 1. the cells that were not treated with the inhibitors; 2. methyl-beta-cyclodextrin; 3. chlorpromazine; 4. genistein; 5. wortmannin; 6. incubating in 4 °C. B) Cytotoxicity of pPBA, CUR, and CCN to MC38 analyzed by MTT assay. C) Quantification of western blot results in Fig. 4C.



Figure S9. A) Hemolysis results of the samples. B) Body weight change after treatment of each sample. (n = 7). C) Representative images of tumor-bearing mice on day 1 and 10. D) Excised tumor images at day 10. E) Excised tumor weight at day 10. Data represent the mean  $\pm$  SE (\*P < 0.05, \*\*P < 0.01, \*\*\*P < 0.001).



**Figure S10**. A) Representative 1,3-dicarbonyl compounds used in the study. B) Structure of quinizarin. C) Quenching of PBA fluorescence after interaction with quinizarin (excitation at 300 nm).