Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.

Supporting Information

Topology Dictates Function: Controlled ROS Production and Mitochondria Accumulation via Curved Carbon Materials

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Table S1. The determination of the complex ratio between γ-CD and Cor in the purified inclusion complex. The peak at 4.9 ppm (γ-CD) and 8.0 ppm (Cor) was selected for comparison. An integral area ratio at 1.6 (γ-CD:Cor) indicates the formation of a 2:1 γ-CD:Cor complex.

#	**Feeding Ratio** (γ-CD:Cor)	**Integral Area Ratio** (γ-CD:Cor)	**Complexing Ratio** (γ-CD:Cor)
1	1:1	1.61	2:1
2	2:1	1.57	2:1
3	4:1	1.56	2:1
4	6:1	1.63	2:1
5	8:1	1.67	2:1

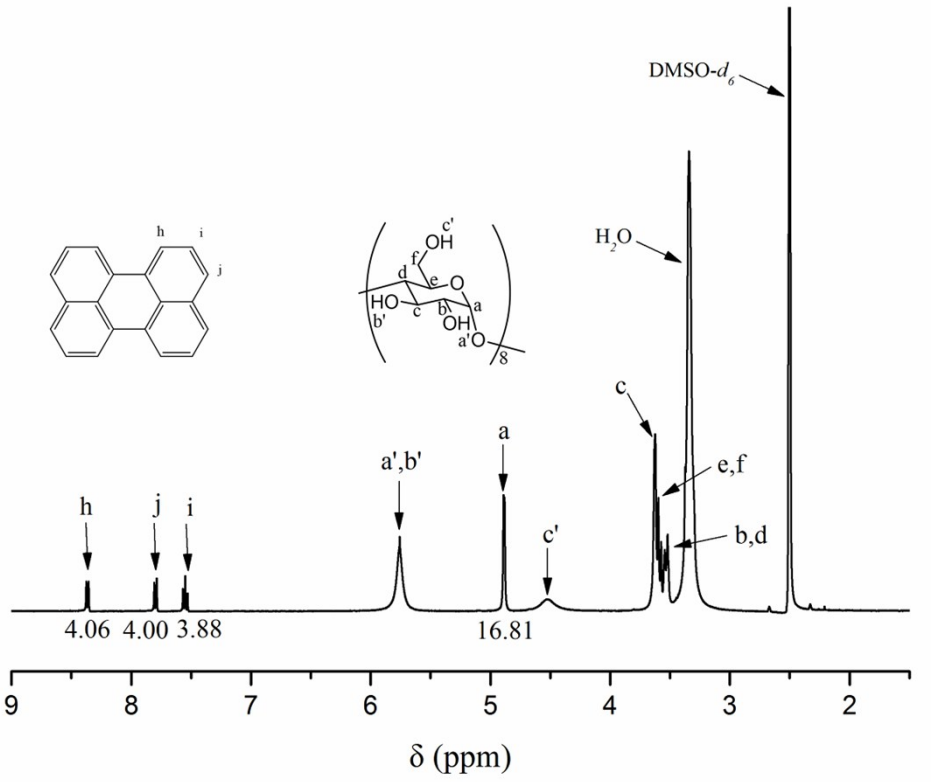


Figure S1. ^{1}H NMR spectrum of γ-CD/Per complex in DMSO-d_6. The ratio of integral area of the corresponding peak at positon i, j, h (Per) and position a (γ-CD) indicates the formation of a 2:1 (γ-CD:Per) inclusion complex.

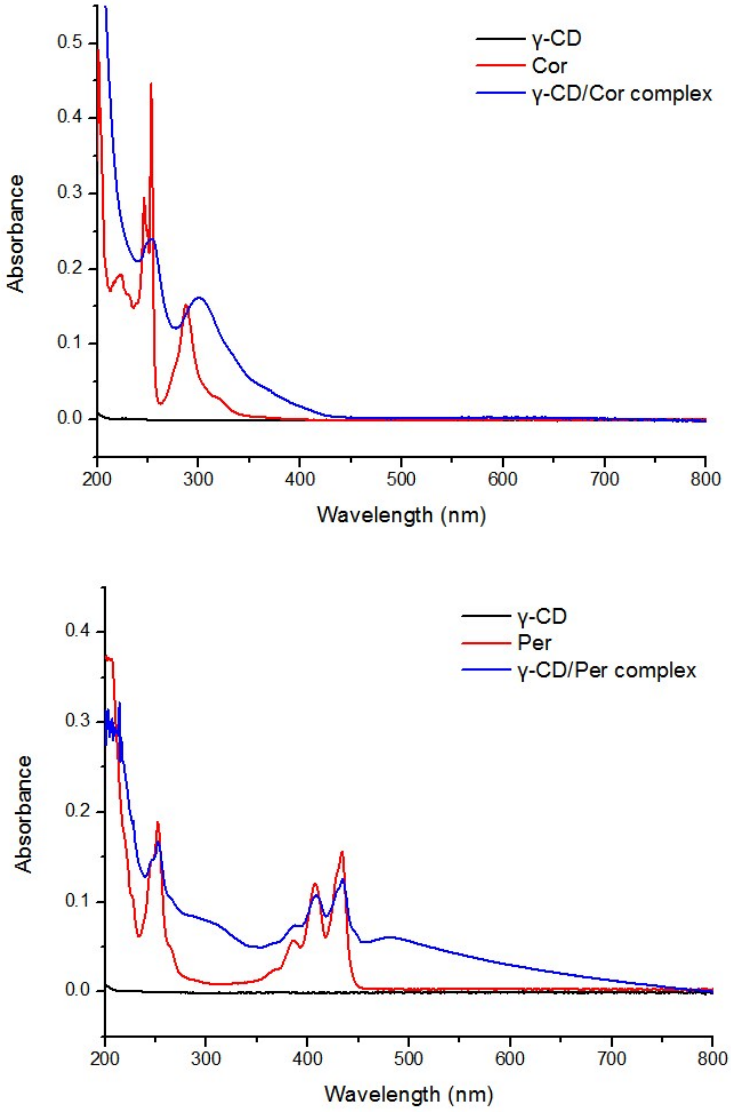


Figure S2. The adsorption spectra of γ-CD/Cor complex (*top*), γ-CD/Per complex (*bottom*), and the corresponding controls (γ-CD, Cor and Per). The concentration of all samples was set at 4 μM and the solvent was a mixture of ethanol and water (1:1, v/v).

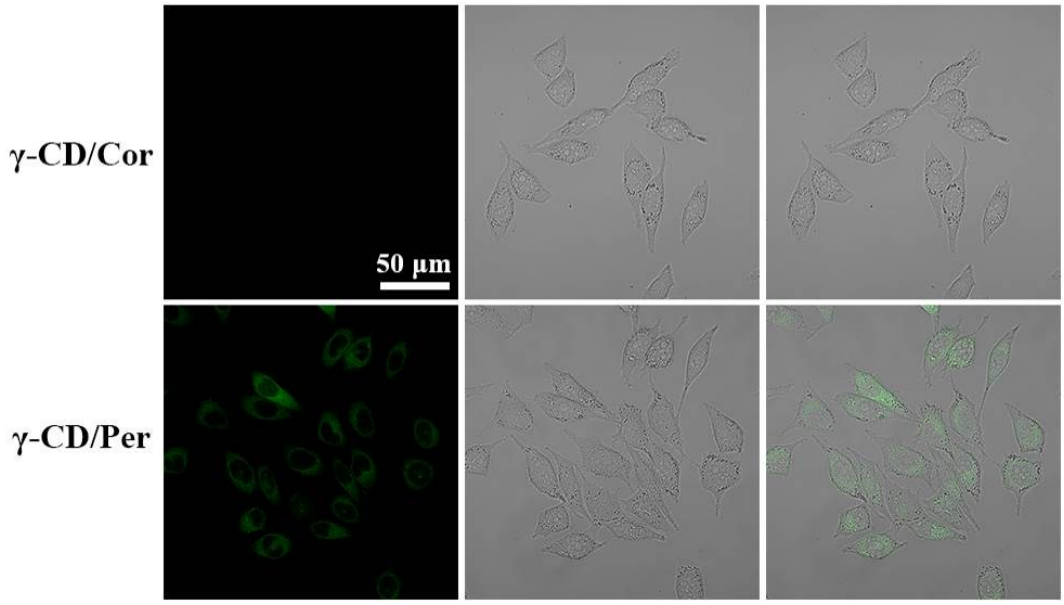
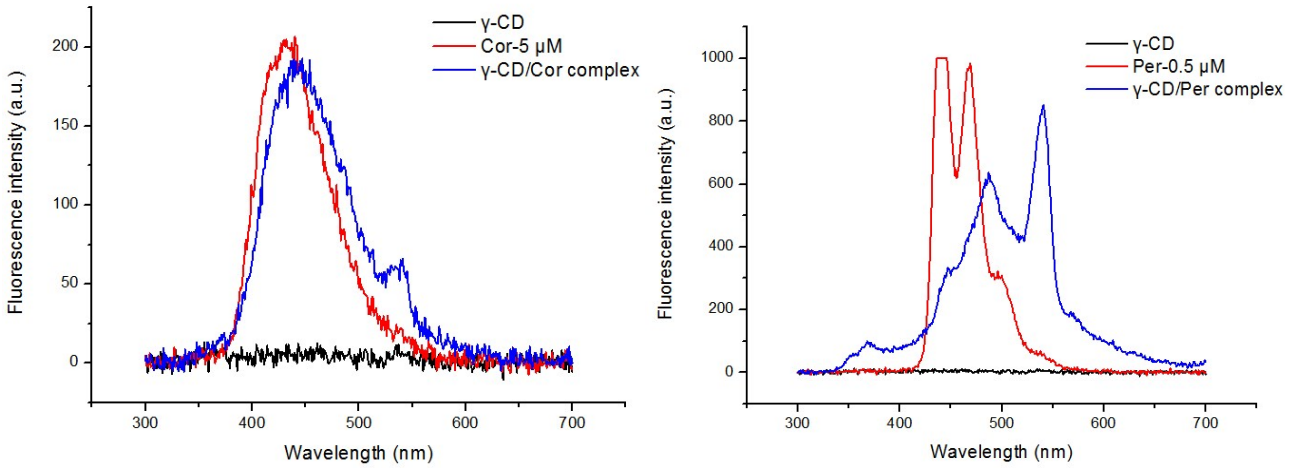
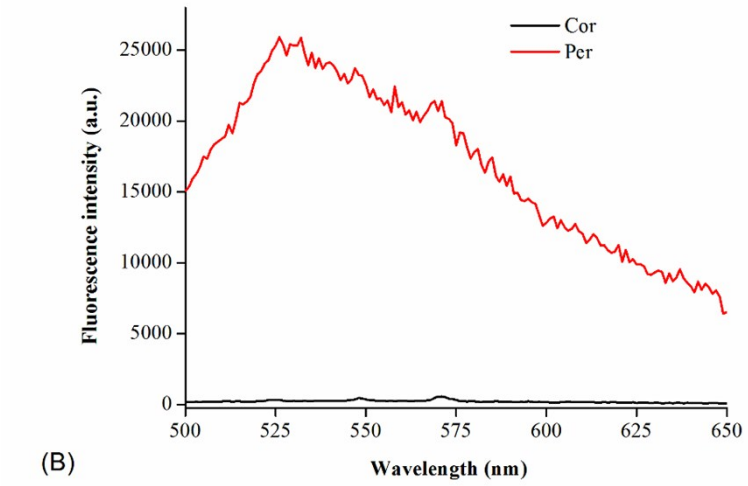


Figure S3. The confocal laser scanning microscope images of PC-3 cells treated by either γ-CD/Cor or γ-CD/Per inclusion complex. The reactive oxygen species (ROS)-sensitive probe (DCFH-DA) was not present. The left column was the images of cells excited at 488 nm that was the wavelength for the excitation of DCFH-DA. The middle column was the brightfield images and the right column was the merged images of the first two columns. These indicated that γ-CD/Per exhibited inherent fluorescence when being excited at 488 nm, whereas γ-CD/Cor didn't display fluorescence under the same condition.



(A)



(B)

Figure S4. (A) The emission spectra of gama-cyclodextrin (γ-CD, 5 μM in water), corannulene (Cor, 5 μM in acetonitrile), perylene (Per, 0.5 μM in acetonitrile), γ-CD/Cor (5 μM in water) and γ-CD/Per (0.5 μM in water) complexes. The excitation wavelength was 252 nm. (B) The emission spectra of corannulene (Cor, 100 μM) and perylene (Per, 100 μM) in acetonitrile. Both were excited at 488 nm that was the wavelength for exciting the reactive oxygen species-specific probe (DCFH-DA). All the analysis was performed at 25°C.

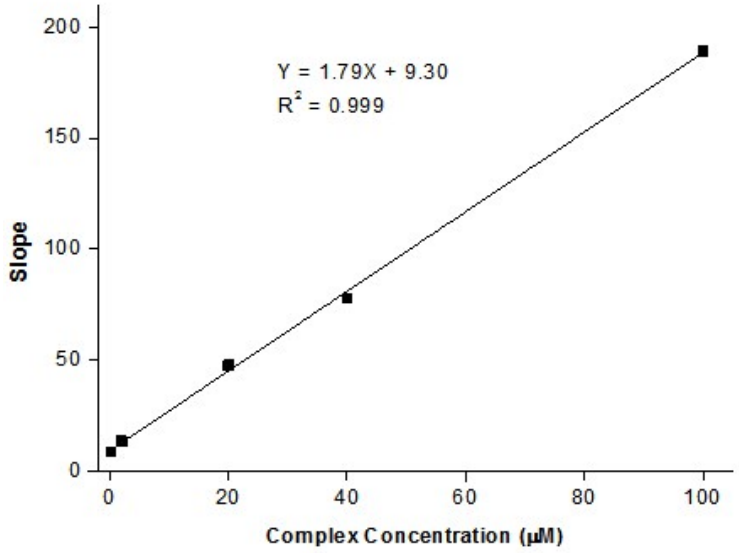


Figure S5. The plot of slope in Figure 2B against the γ-CD/Cor complex concentration.

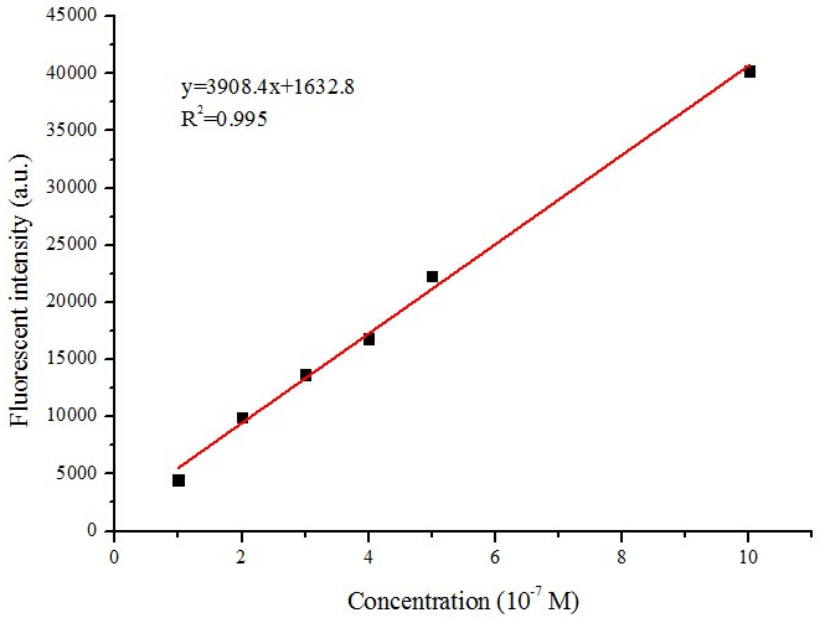


Figure S6. The fluorescence of reactive oxygen species (ROS)-sensitive probe (DCFH-DA) upon incubation with hydrogen peroxide (0.1-1.0 μM) at 25°C for 30 min in H_2O. The excitation wavelength was 485 nm and the signal was collected at 530 nm.

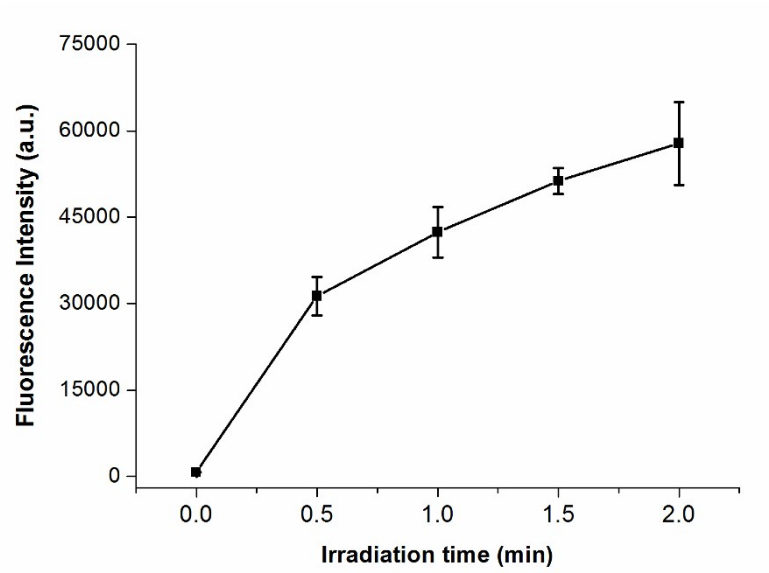


Figure S7. The fluorescence of activated DCFH-DA probe (5 μM) in PBS (25 mM, pH 7.2) upon the laser irradiation at 254 nm for up to 2 min (n = 3). The excitation and emission wavelength for detection was 485 nm and 530 nm, respectively.

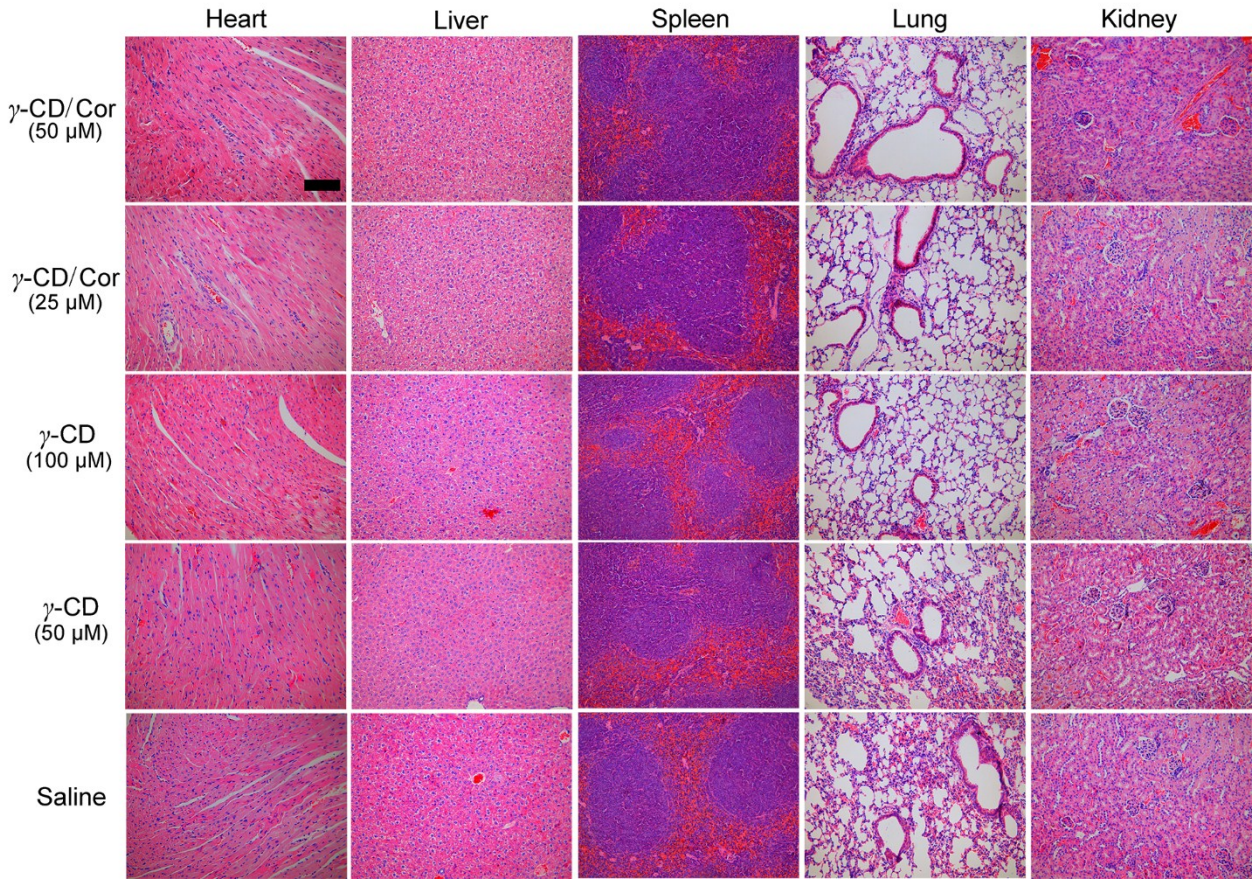


Figure S8. Hematoxylin and eosin staining of major organs of mice that were treated by γ-CD/Cor complex (25 and 50 μM). γ-CD and normal saline were employed as the control. All samples were intravenously injected and the analysis was performed 48 h post dose administration. Scale bar: 100 μm.