Electronic Supplementary Information:

The role of crystallinity of palladium nanocrystals in ROS generation and cytotoxicity induction

Yanxin Wu[1,#], Rongtao Liu[1,#], Jian Liu[1], Jianbo Jia[1], Hongyu Zhou[1]*, Bing Yan[1]

[1]Institute of Environmental Research at Greater Bay, Key Laboratory for Water Quality and Conservation of the Pearl River Delta, Ministry of Education, Guangzhou University, Guangzhou, Guangdong, 510006, China

[#]These authors contributed equally to this work.

***Corresponding author**

Hongyu Zhou (hyzhou001@gzhu.edu.cn)

The concentrations of Pd nanocrystals were calculated to maintain the equivalent for surface atoms of samples, according to *SI Eql(1-1)~ (1-6)*.

PdNCs	$N = 12m^2 - 24m + 14$	Eql(1-1)
PdNOs	$N = 4m^2 - 8m + 6$	Eql(1-2)
PdNTs	$N = 2m^2 - 4m + 4$	Eql(1-3)
PdNCTs	$N_{\{111\}} = \frac{3}{2}m^2 - 2m$	Eql(2-4)
		Eql(2-5)
	$N_{\{110\}} = \frac{1}{36}m^2 - \frac{2}{3}m + 8$	Eql(2-6)
	$N_{Total} = \frac{55}{36}m^2 - \frac{8}{3}m + 8$	

Calculations were performed by assuming that all the nanocrystals had perfect morphologies. m, defined as the number of atoms lying on an equivalent edge (corner atoms included). N, defined as the number of surface atoms.

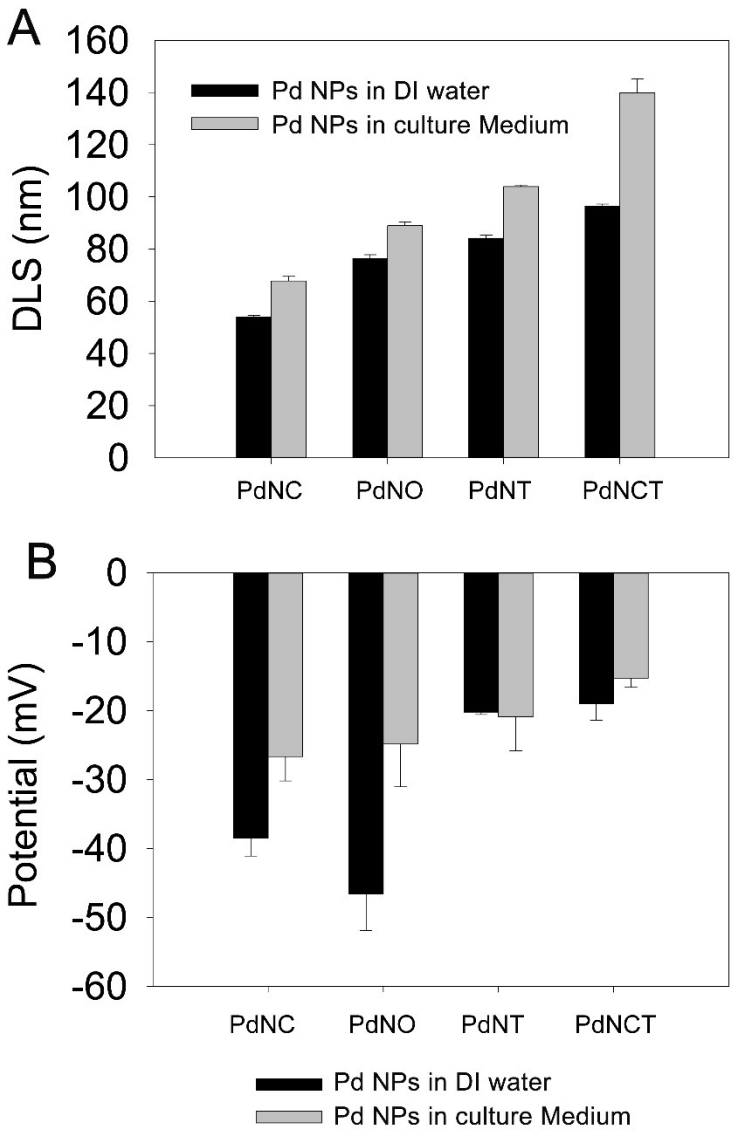

Fig. S1 DLS and zeta potential measurement of different Pd nanocrystals in deionized water or cell culture medium with 10% fetal bovine serum.

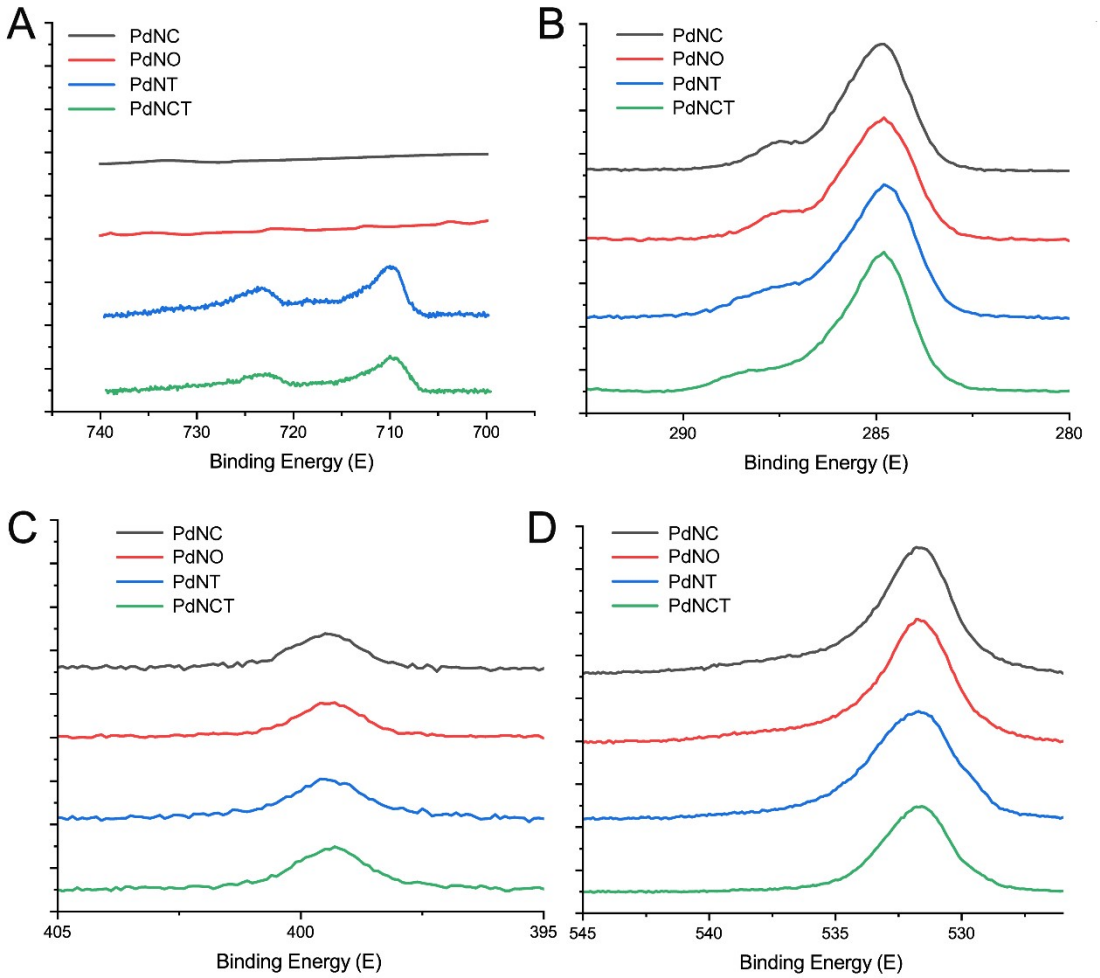

Fig. S2 XPS characterizations of different Pd crystals. (A) Fe2p, (B) C1s, (C) N1s, and (D) O1s high solution XPS spectra.

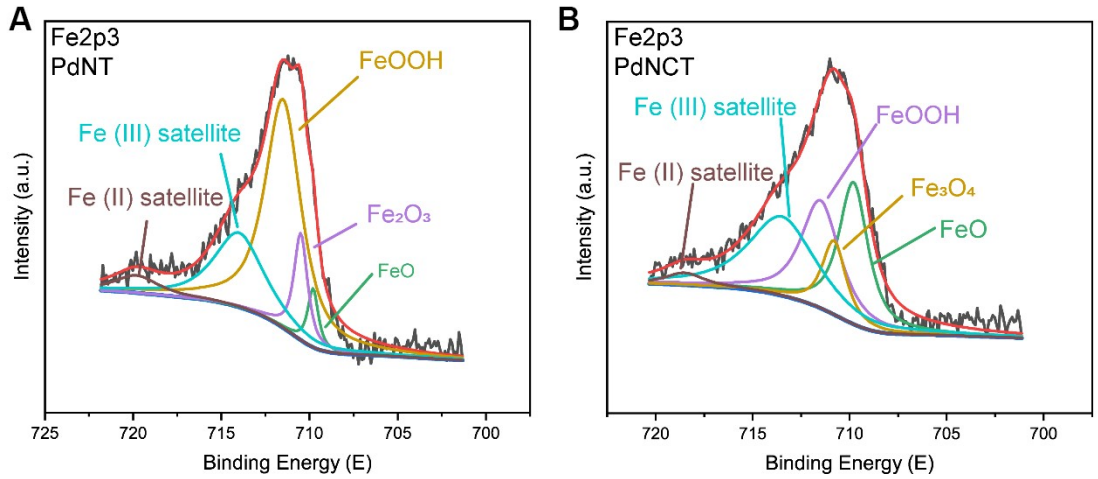

Fig. S3 High-resolution XPS Fe2p3 spectra of (A) PdNT and (B) PdNCT.

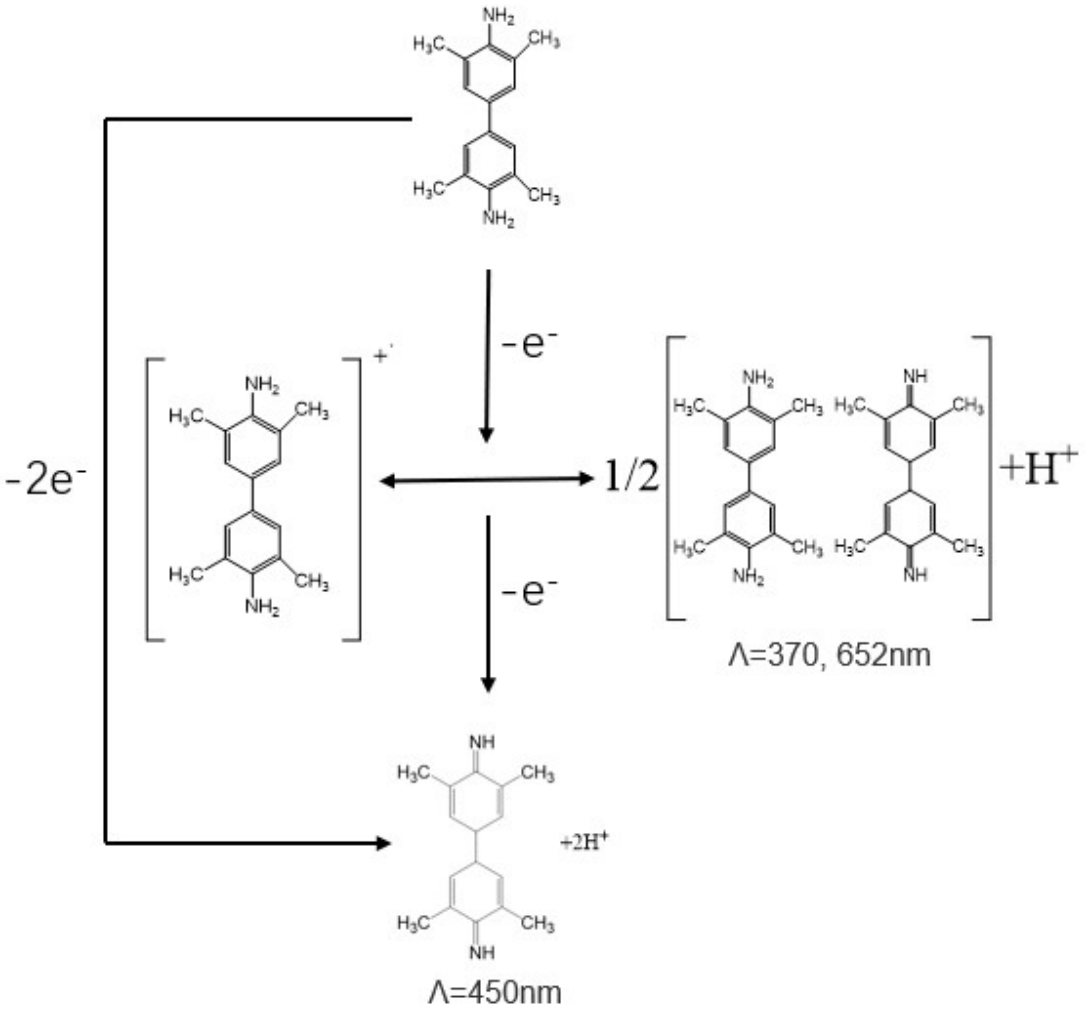

Fig. S4 Luminescence mechanism of TMB probe

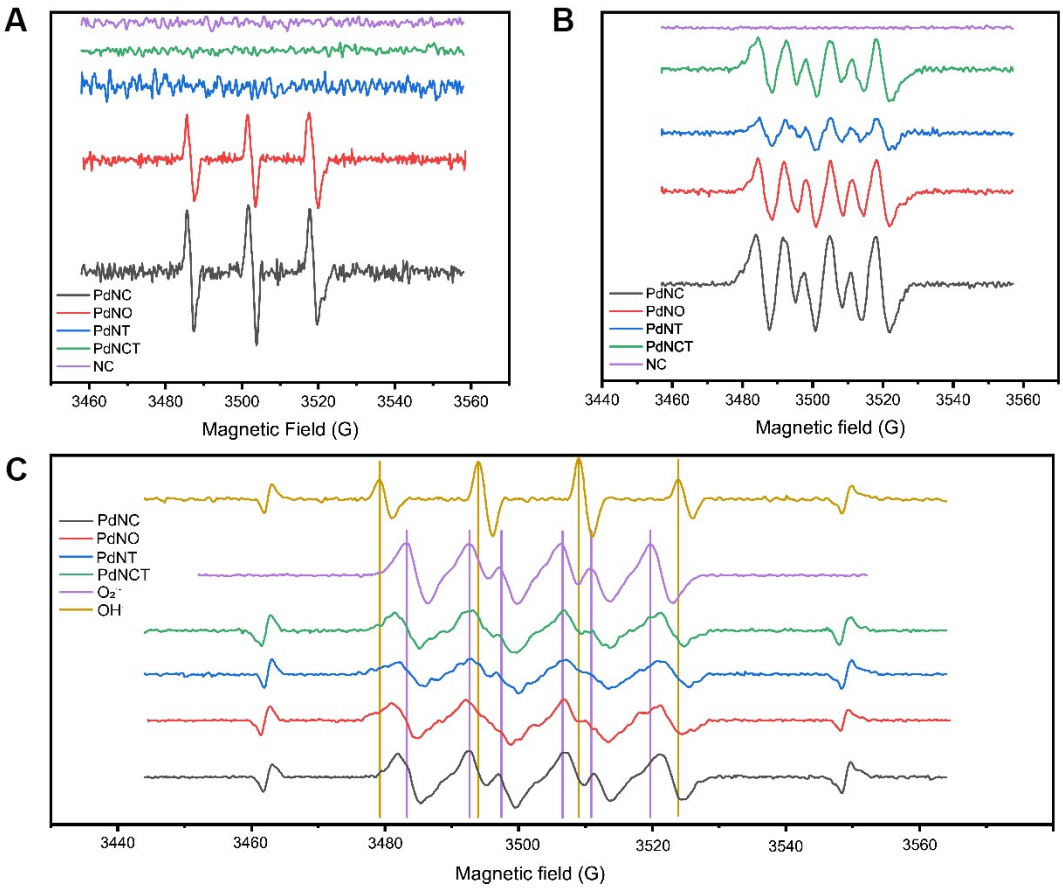

Fig. S5 ESR measurements. (A) ESR spectra of the samples after mixing 4-oxo-TMP solution with Pd nanocrystals to detect $^1O_2$ (B) ESR spectra of samples containing BMPO, DPTA, and Pd nanocrystals. (C) ESR spectra of samples including DMPO, Pd nanocrystals – H_2O_2 system with the Mn^{2+} marker.

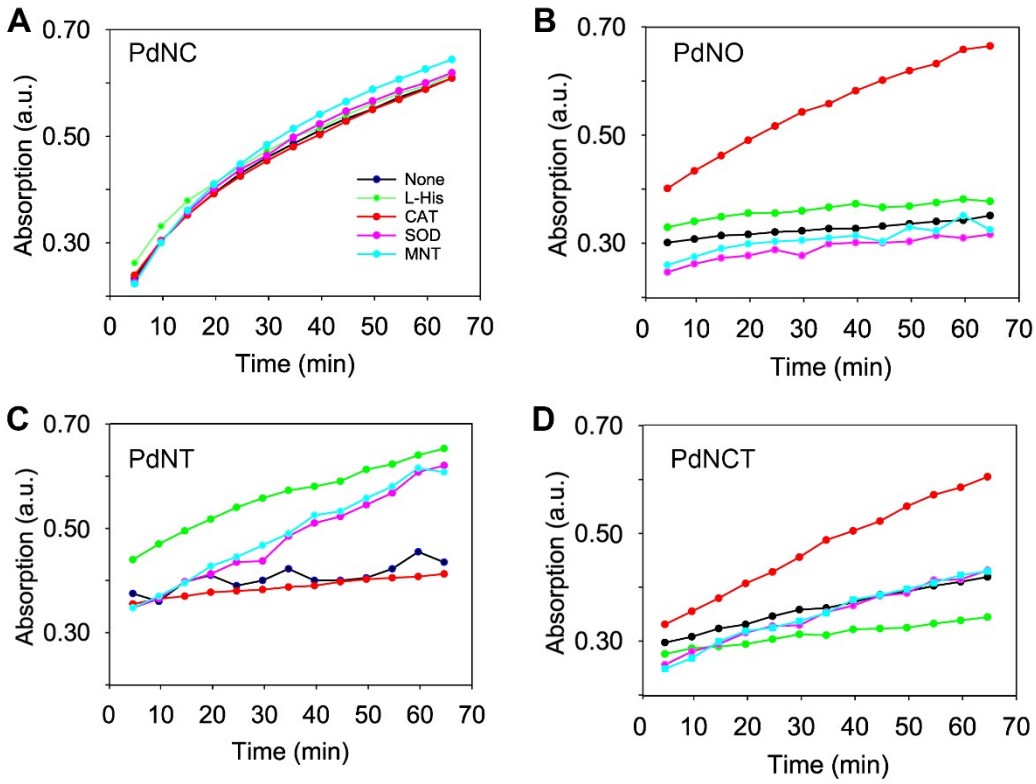

Fig. S6 The single-electron oxidation product at 652nm when TMB mixed with different crystals and ROS scavengers. (A) PdNCs, (B) PdNOs, (C) PdNTs, (D) PdNCTs.

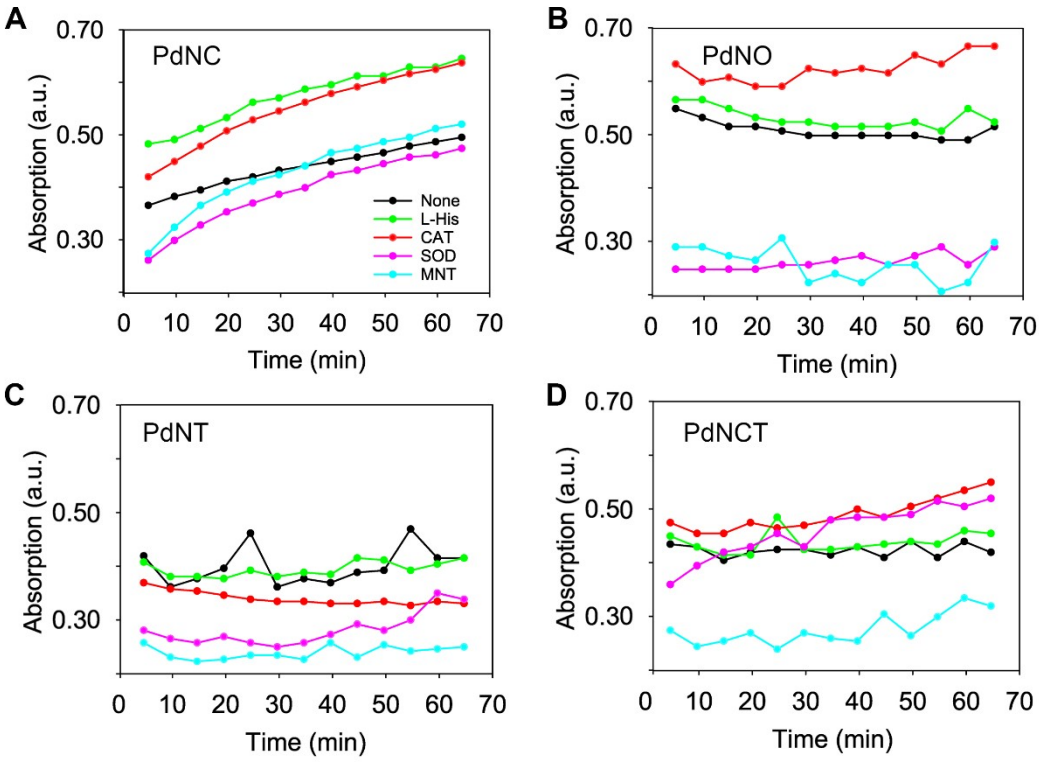

Fig. S7 The completed oxidation product at 450nm when TMB mixed with Pd nanocrystals and different ROS scavengers. (A) PdNCs, (B) PdNOs, (C) PdNTs, (D) PdNCTs.

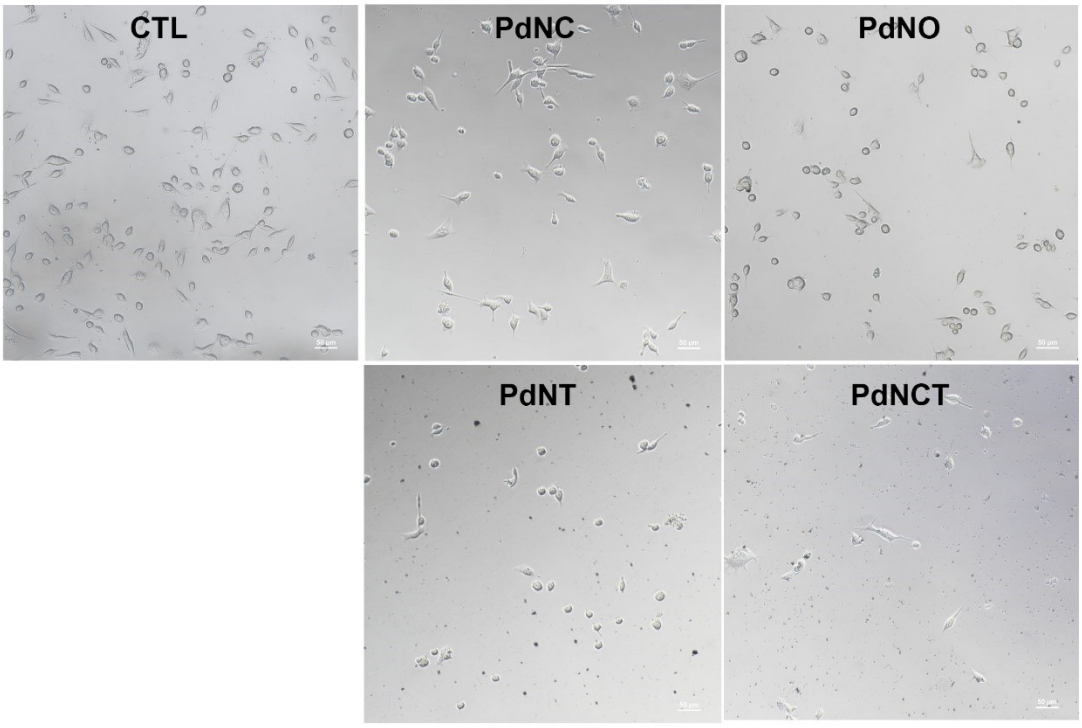

Fig. S8 Representative photographs of GES-1 cells treated with culture medium (CTL) or different Pd nanocrystals at 7 μg/mL for 24 h.

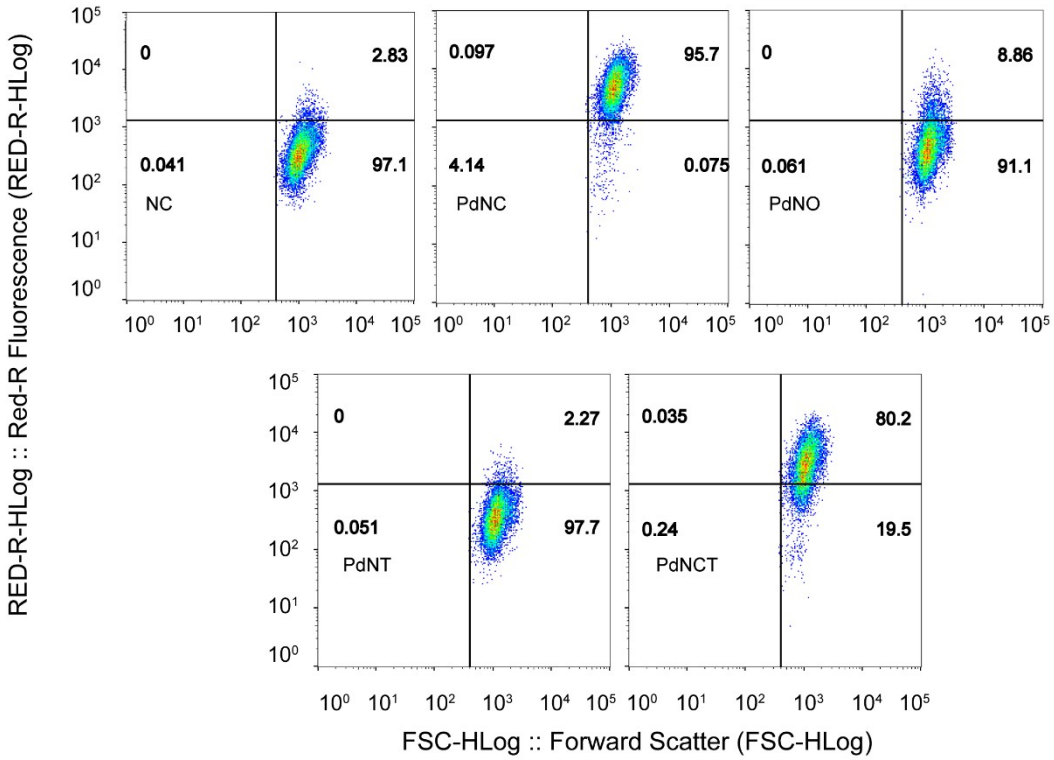

Fig. S9 HO-1 expression measurement though flow cytometry analysis. NC: Negative Control.

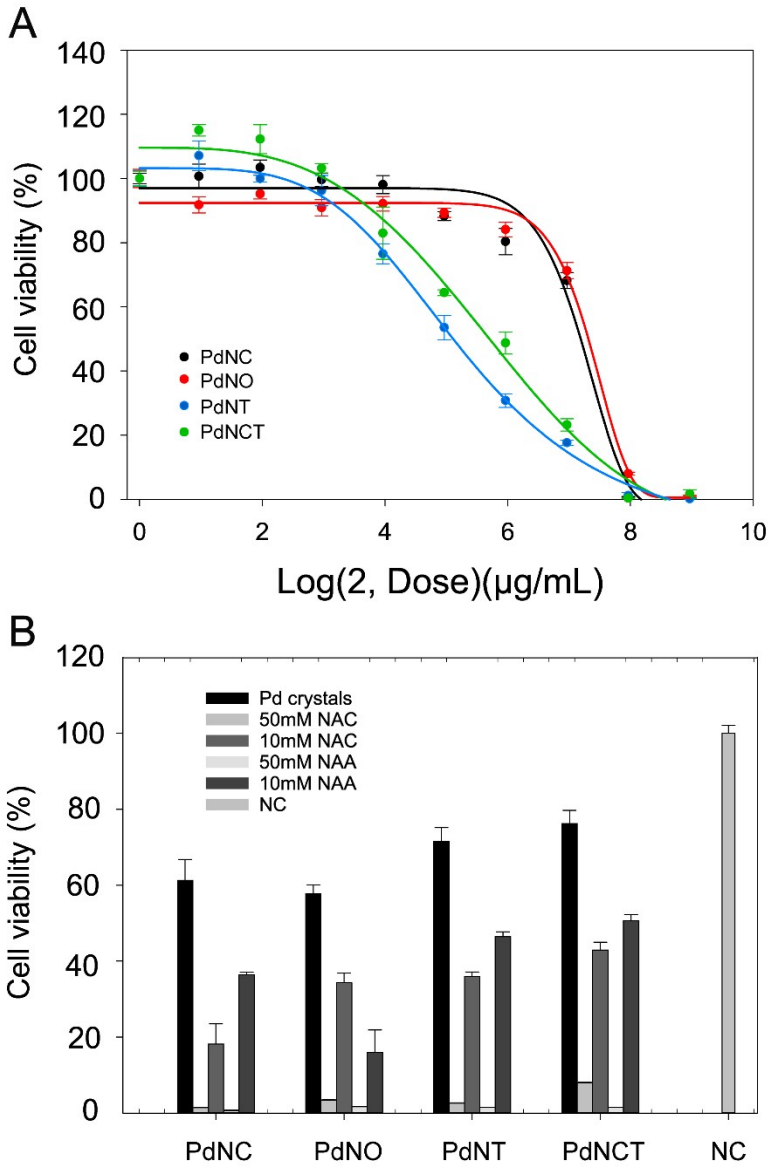

Fig. S10 Cell viability experiments of Pd crystals in MCF-7 cell lines. (A) Dose-response curves. (B) Pd crystals incubated with 50/10 mM NAC/NAA.