Electronic Supplementary Material (ESI) for RSC Advances.


# Supporting information

## Carrier-free Nanomedicines Self-Assembled from Palbociclib Dimers and Ce6 for Enhanced Combined Chemo-Photodynamic Therapy of Breast Cancer

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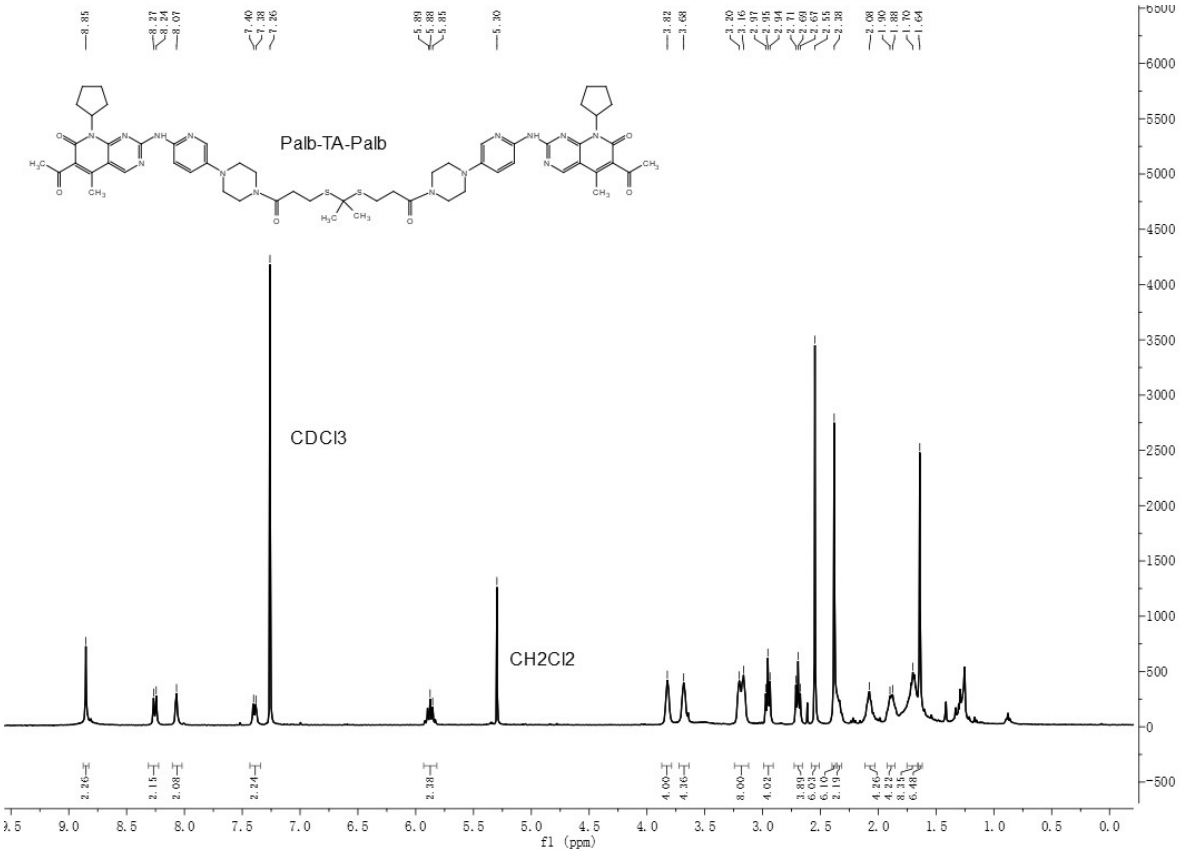


**Fig. S1** The $^{1}$H NMR spectrum of **Palb-TA-Palb.**

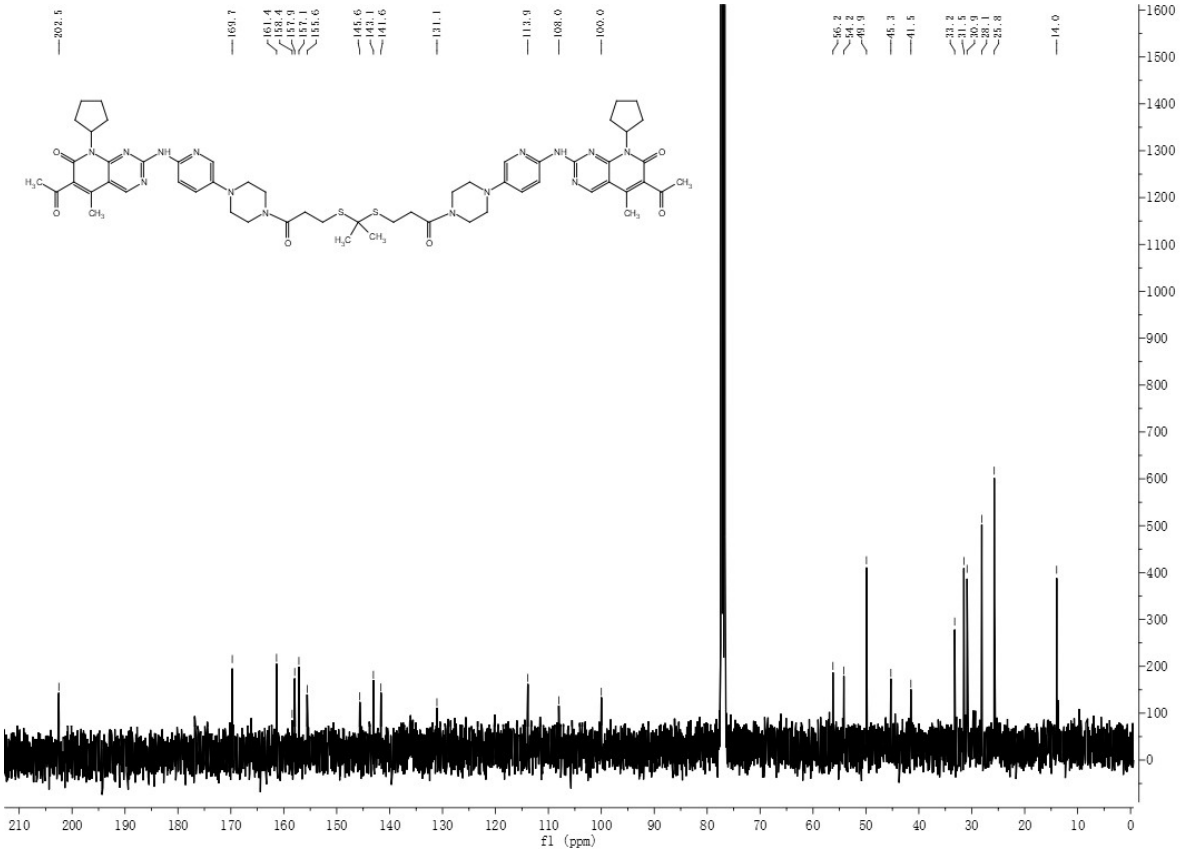


**Fig. S2** The $^{13}$C NMR spectrum of **Palb-TA-Palb.**

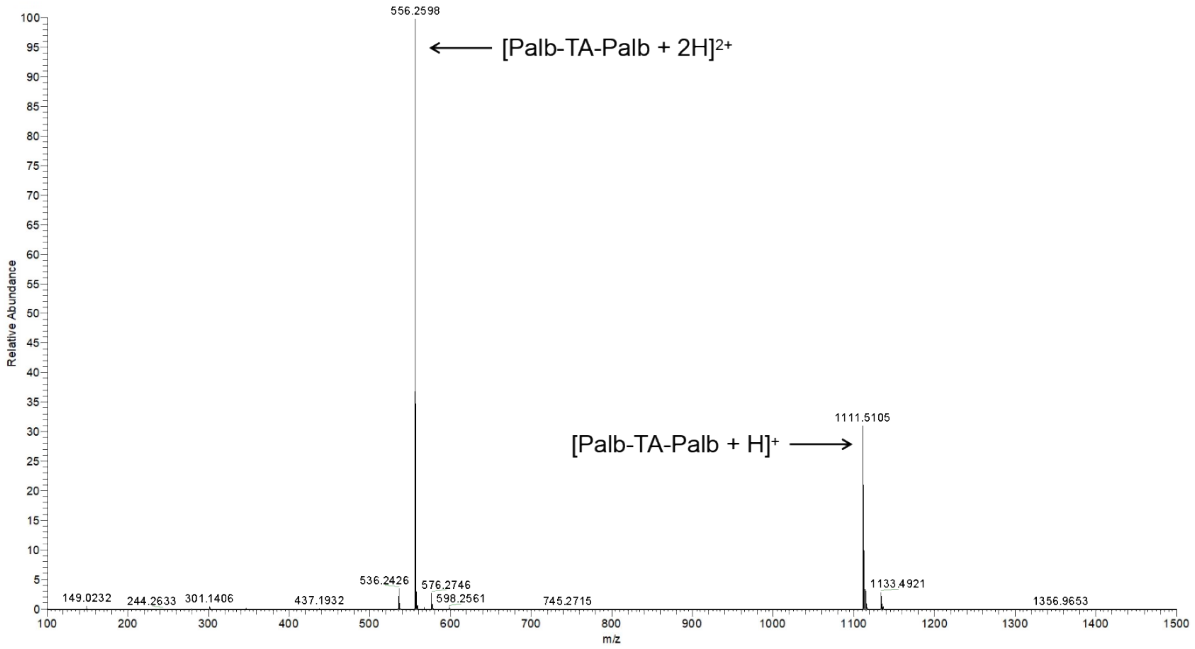


**Fig. S3** The mass spectrum of **Palb-TA-Palb.**

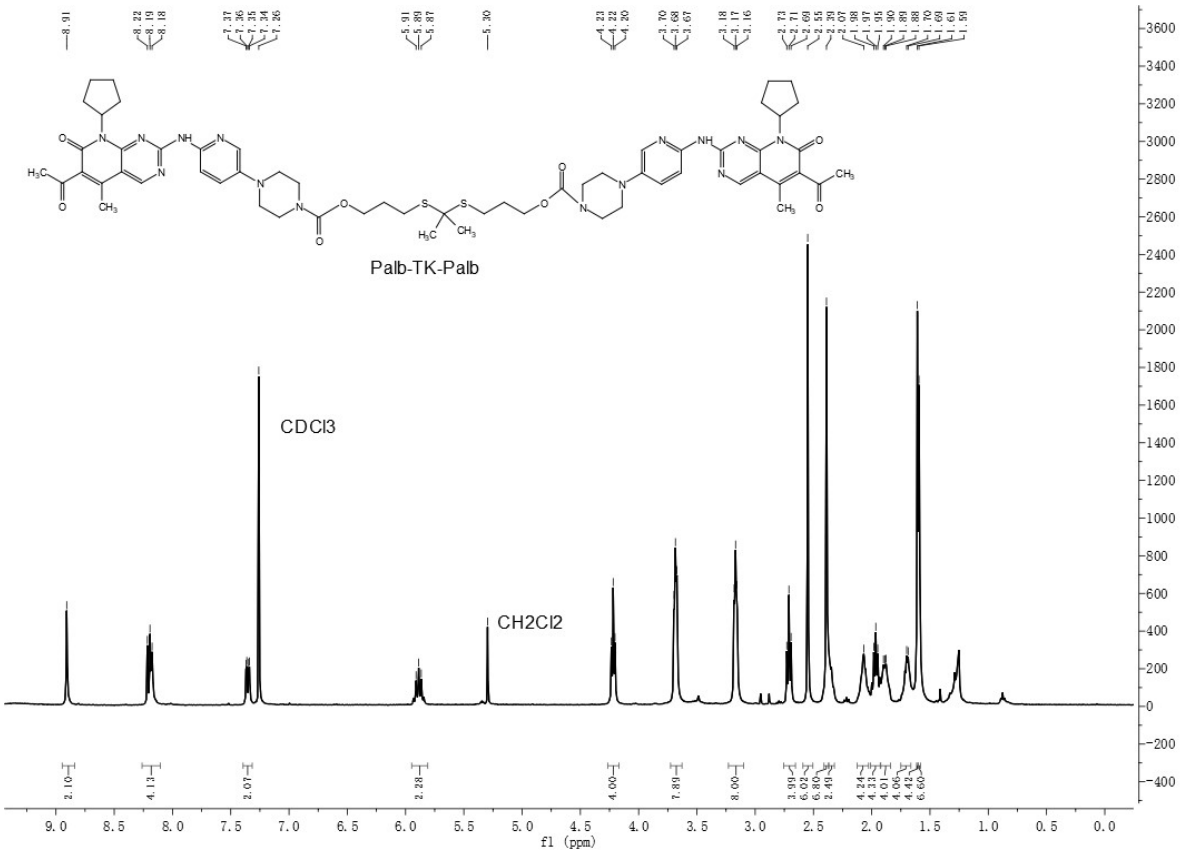


**Fig. S4** The $^{1}$H NMR spectrum of **Palb-TK-Palb.**

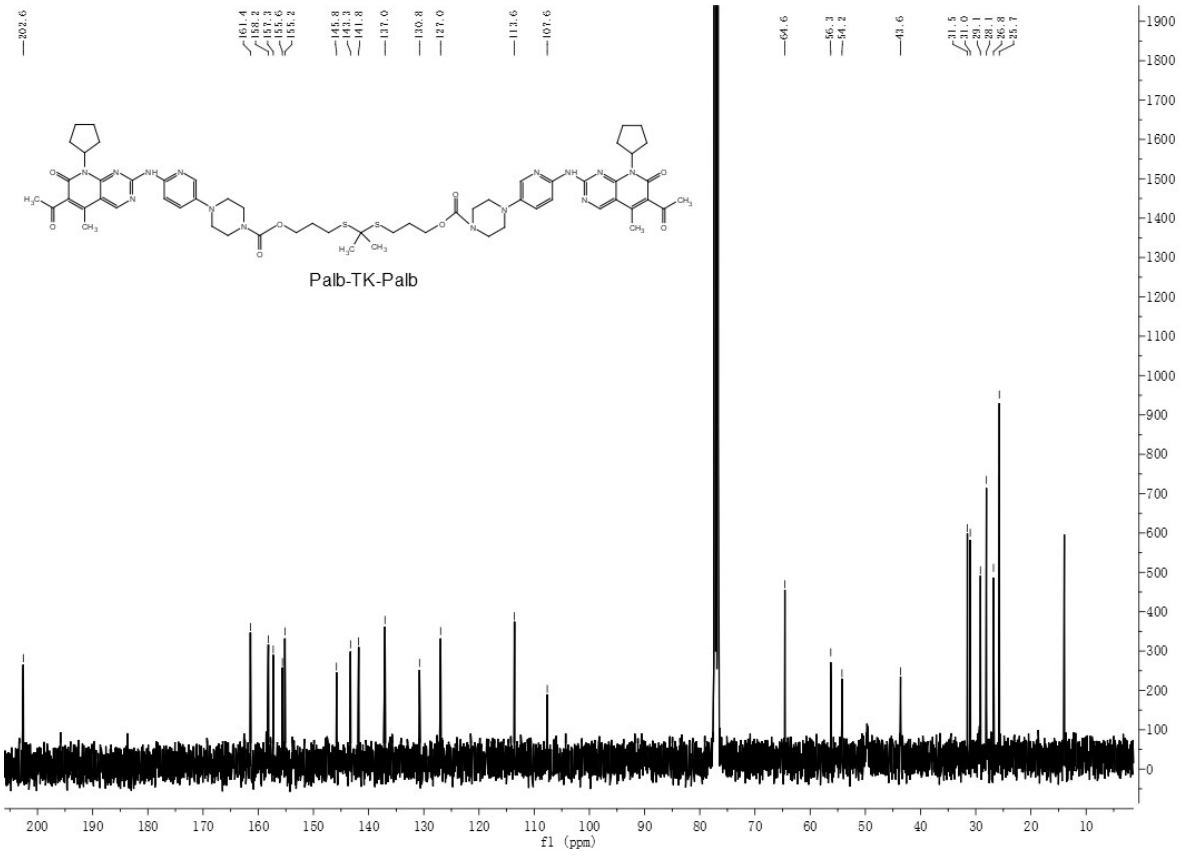


**Fig. S5** The $^{13}C$ NMR spectrum of **Palb-TK-Palb.**

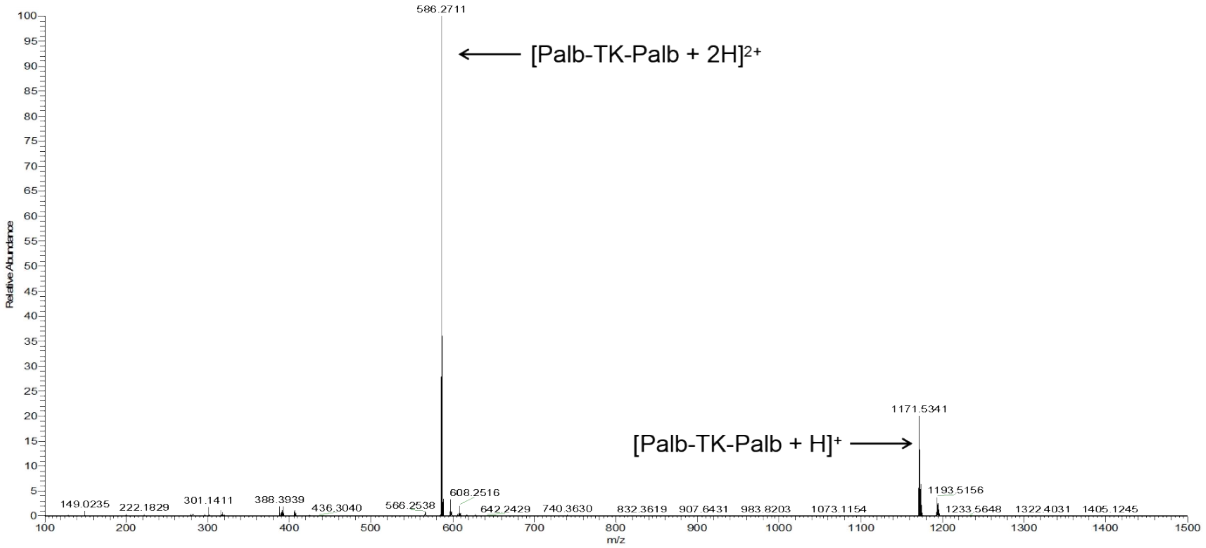


**Fig. S6** The mass spectrum of **Palb-TK-Palb.**

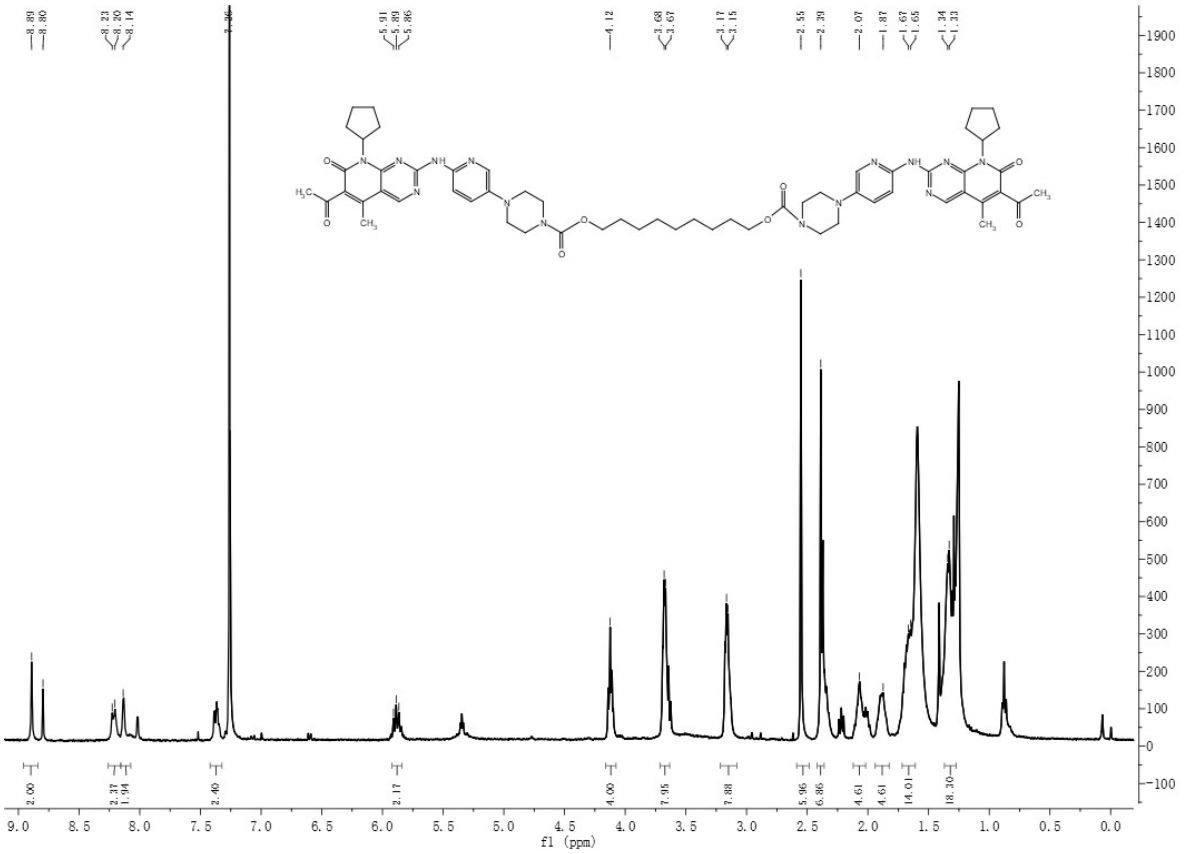

**Fig. S7** The $^{1}$H NMR spectrum of **Palb-CC-Palb.**

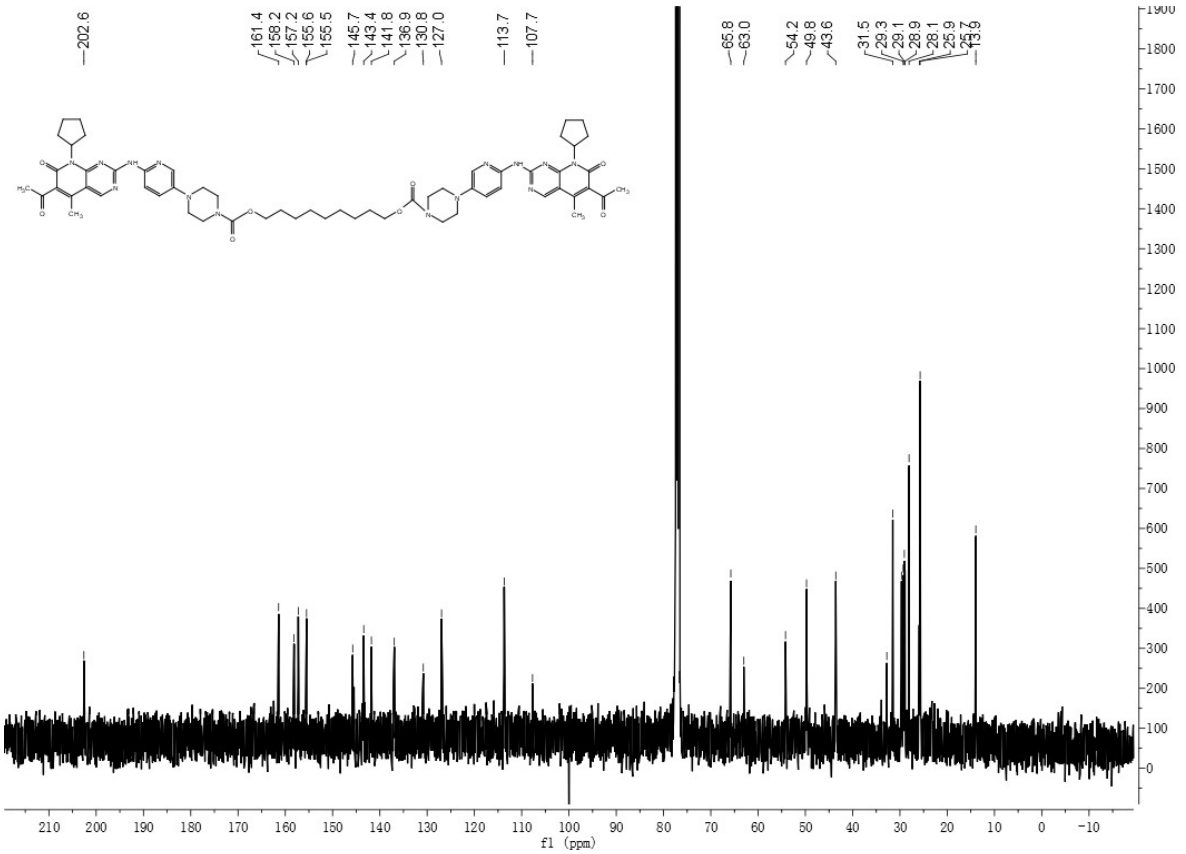

**Fig. S8** The $^{13}$C NMR spectrum of **Palb-CC-Palb.**

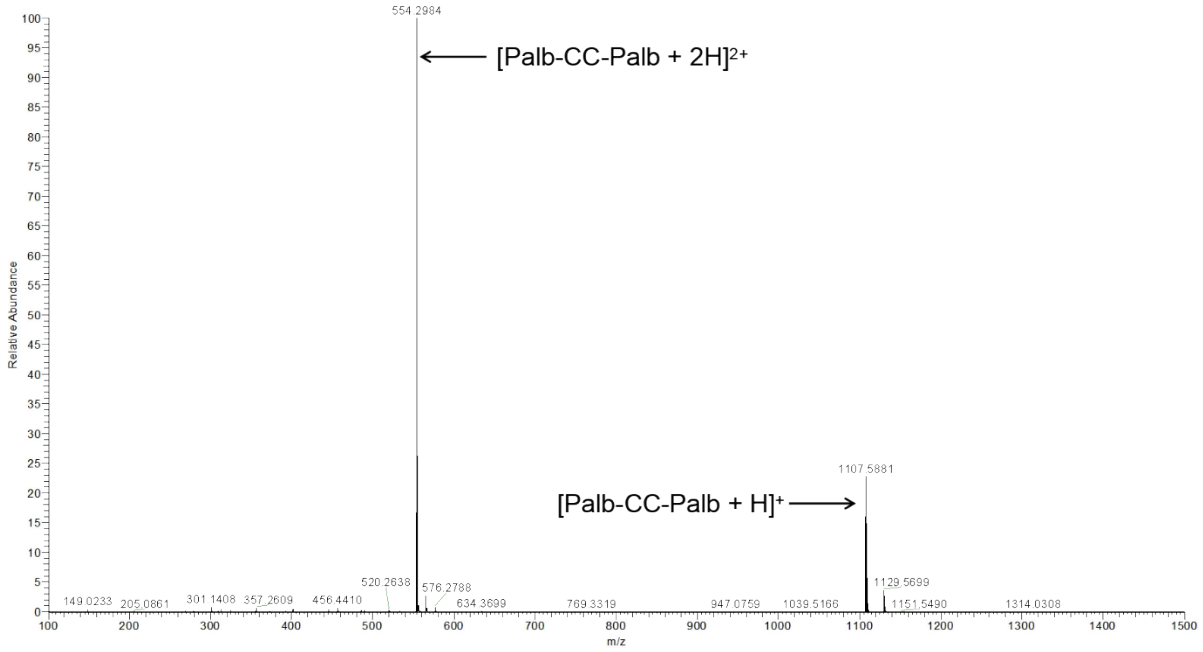


**Fig. S9** The mass spectrum of **Palb-CC-Palb.**

**Table S1.** Size, PDI and Count Rate of **TPP-TK-PPa NP**s with different weight content of DSPE-PEG2000

| **Samples** | **NP-1** | **NP-2** | **NP-3** | **NP-4** | **NP-5** | **NP-6** | **NP-7** |
|---|---|---|---|---|---|---|---|
| **Content of DSPE-PEG2000** | 0 | 10% | 15% | 20% | 25% | 27.5% | 30% |
| **Size (nm)** | - | - | 165.3 | 223.4 | 140.0 | 69.4 | 172.5 |
| **PDI** | - | - | 0.318 | 0.231 | 0.295 | 0.212 | 0.264 |
| **Count rate (kcps)** | - | - | 211 | 238 | 293 | 295 | 222 |

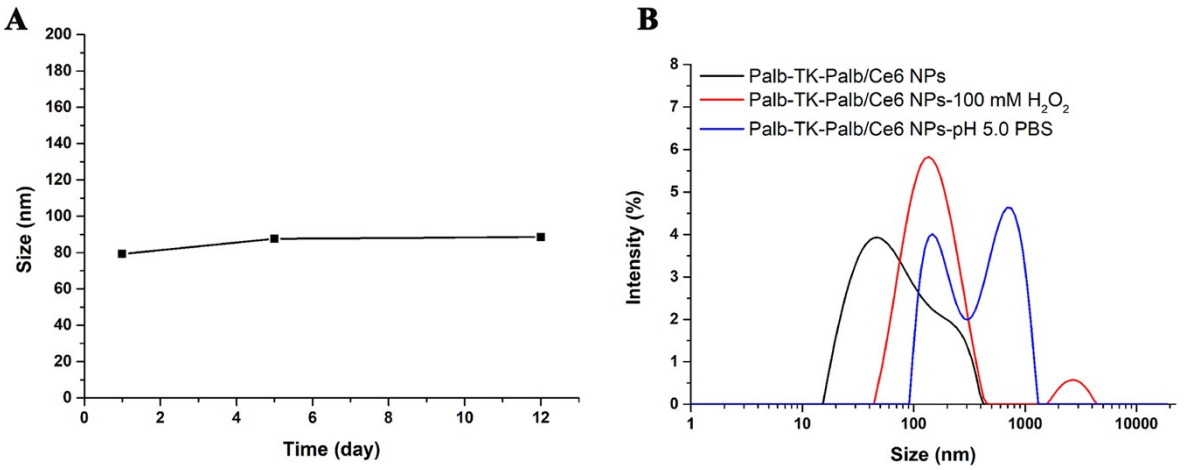


**Fig. S10** (A) Mean particle sizes of **Palb-TK-Palb/Ce6 NPs** at different time points. Data represent mean ± SD (n = 3). (B) The size distribution of **Palb-TK-Palb/Ce6 NPs** treated with 100 mM $H_2O_2$ or pH = 5.0 PBS for 48 h.

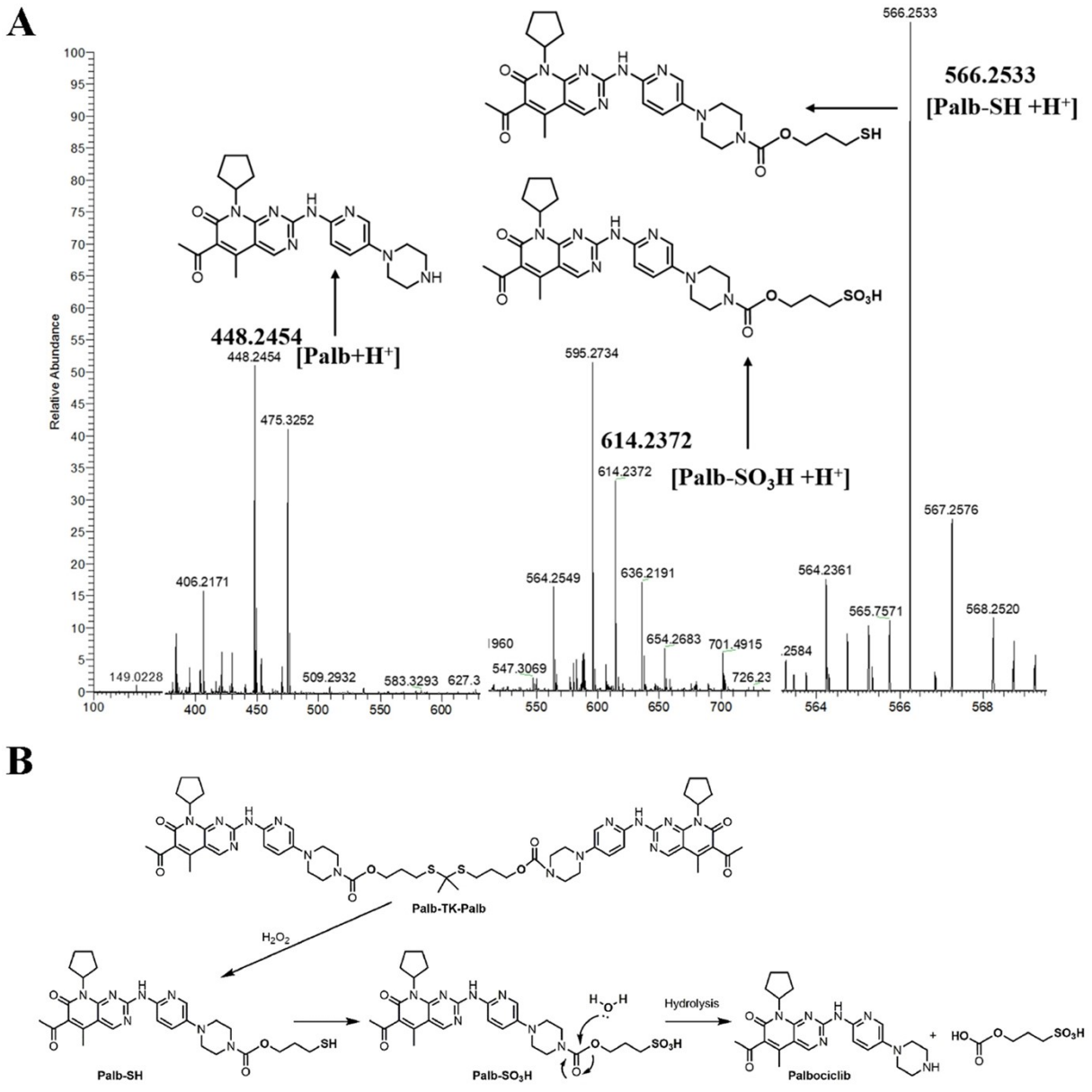

**Fig. S11** The combined HR-MS (ESI) of **Palb-TK-Palb** after after 200 mM $H_2O_2$ incubation for 48 h (A). The proposed light-triggered degradation mechanism of **Palb-TK-Palb** (B).

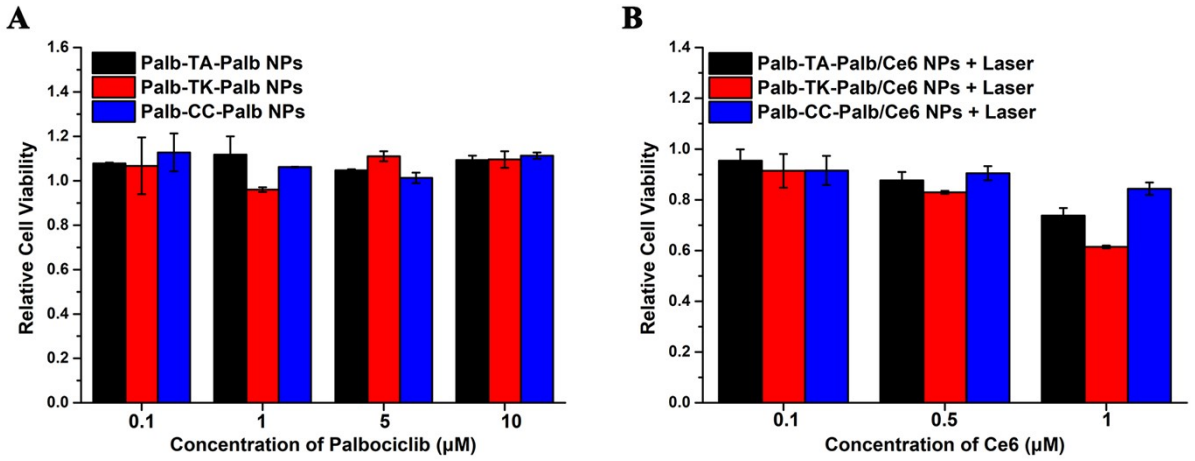


**Fig. S12** Cytotoxicity of various formulations against MDA-MB-231 cells without (A) and with (B) 660 nm laser irradiations (20 mW/cm$^2$, 1 min) after incubation for 24 h.

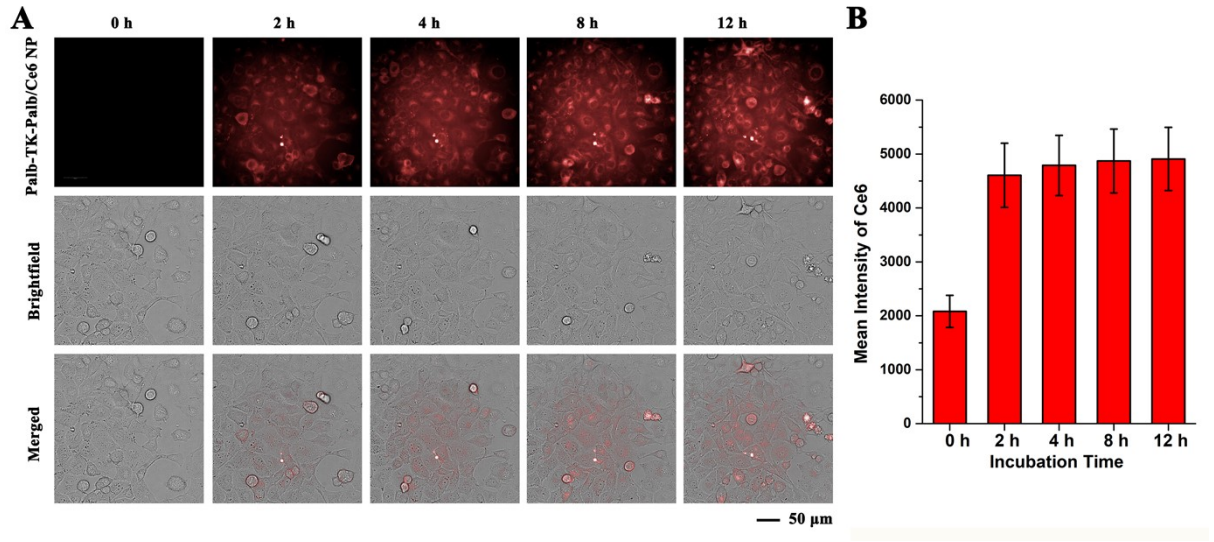


**Fig. S13** In vitro cellular uptake ability of **Palb-TK-Palb/Ce6 NPs** for different time. The images (A) and the relative intensity (A) of Ce6 were studied by high content analysis system-operetta CLS$^{TM}$.

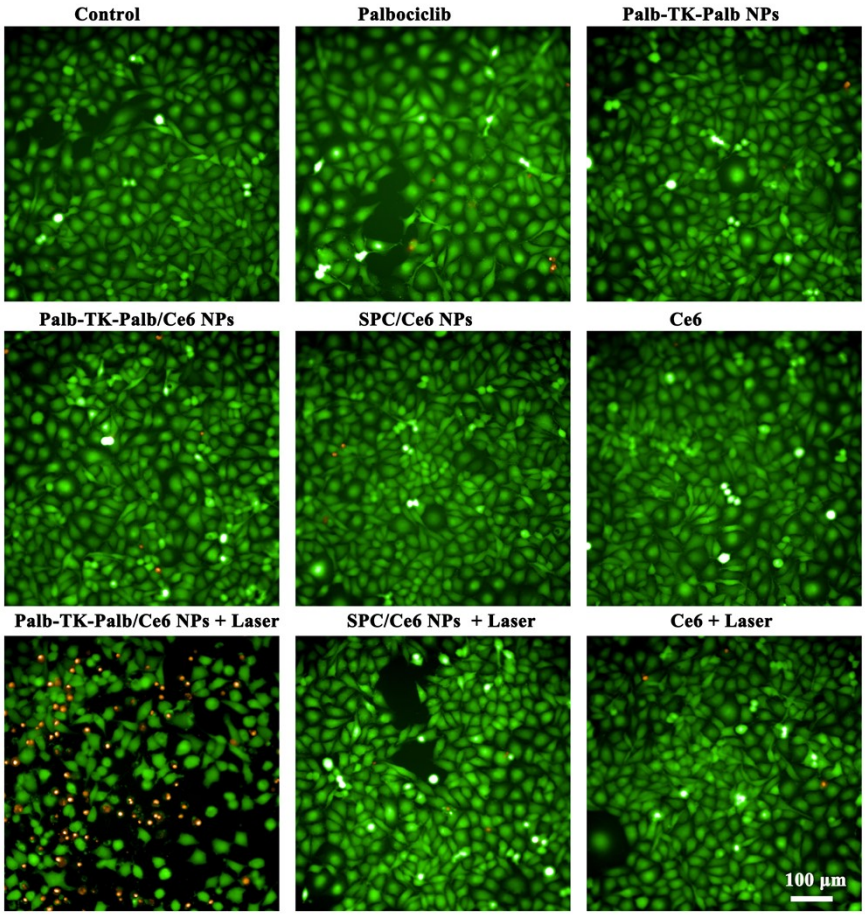


**Fig. S14** The live/dead staining of MDA-MB-231 cells treated with different formulations. Calcein-AM was used to stain live cell (green). PI was used to stain dead cells (yellow).