Supporting Information

Nanolipid formulations of benzoporphyrin derivative: Exploring the dependence of nanoconstruct photophysics and photochemistry on their therapeutic index in ovarian cancer cells

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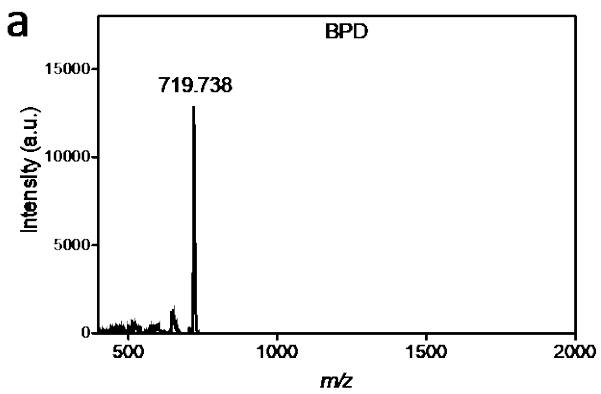
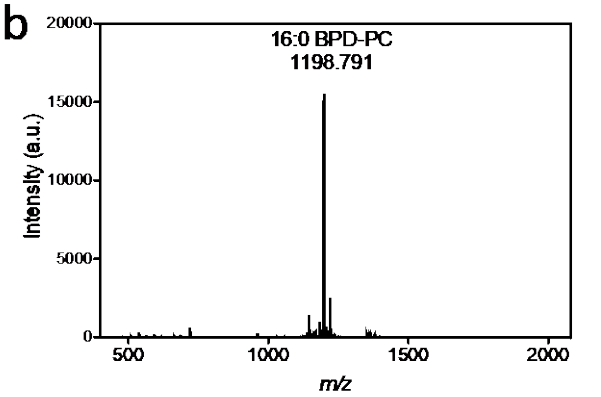
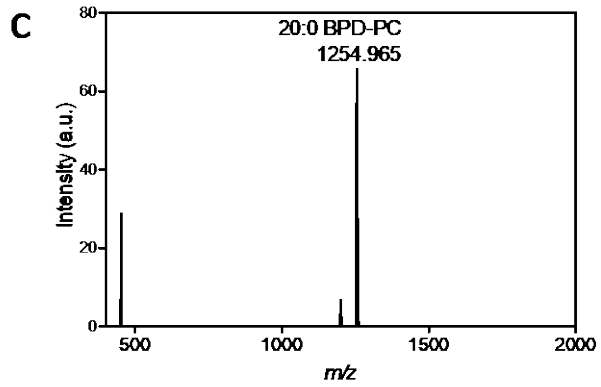
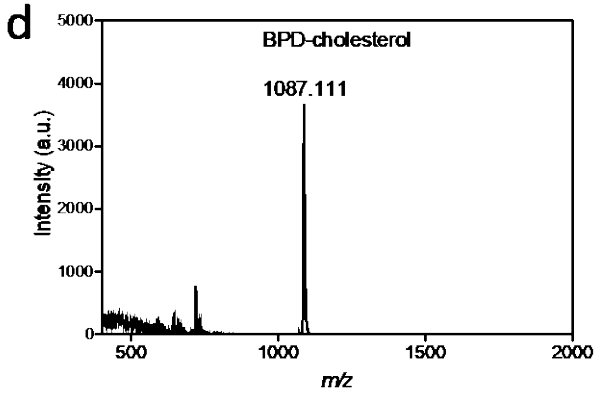
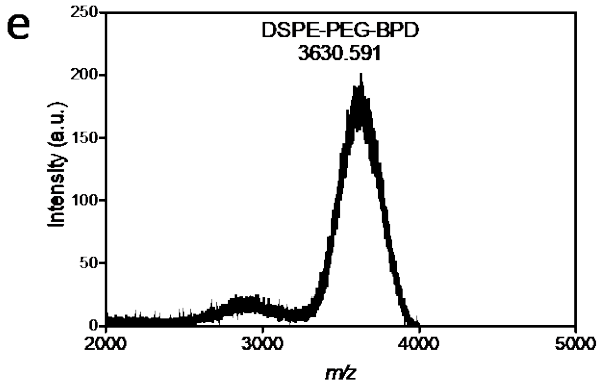
SUPPLEMENTARY RESULTS











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Molecule	Observed Mass (m/z)	Expected Mass (g/mol)
BPD	719.738	718.79
16:0 BPD-PC	1198.791	1196.41
20:0 BPD-PC	1254.965	1252.52
BPD-cholesterol	1087.111	1087.43
DSPE-PEG-BPD	3630.591	3479.25

Figure S1. MALDI-MS spectra of BPD (a) and its lipidated variants conjugated to 16:0 PC (b), 20:0 PC (c) cholesterol (d) and DSPE-PEG$_{2000}$ (e). (f) A summary of the expected m/z values of the BPD variants and their expected molecular weights in g/mol, as determined by ChemDraw Professional v15.1.

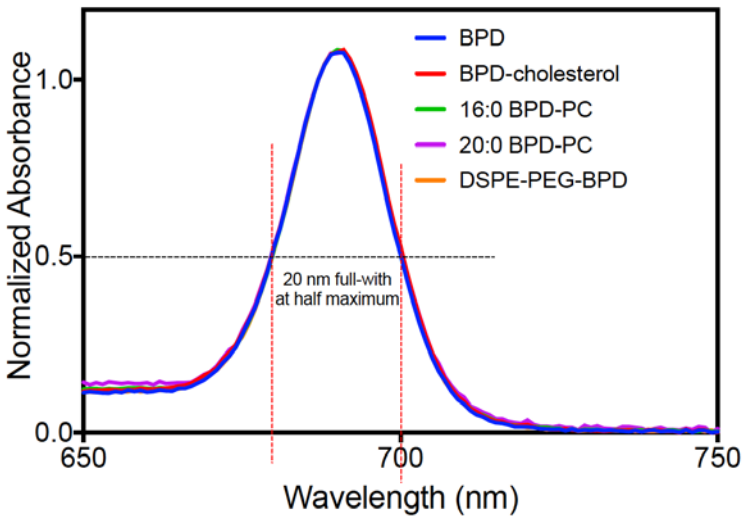

Figure S2. Normalized absorption spectra of the Q-band of BPD and its lipidated variants in DMSO showing no blue or red-shifting in the absorption maxima, and no broadening of the Q-band, as the full-width at half maximum is the same for all BPD variants.

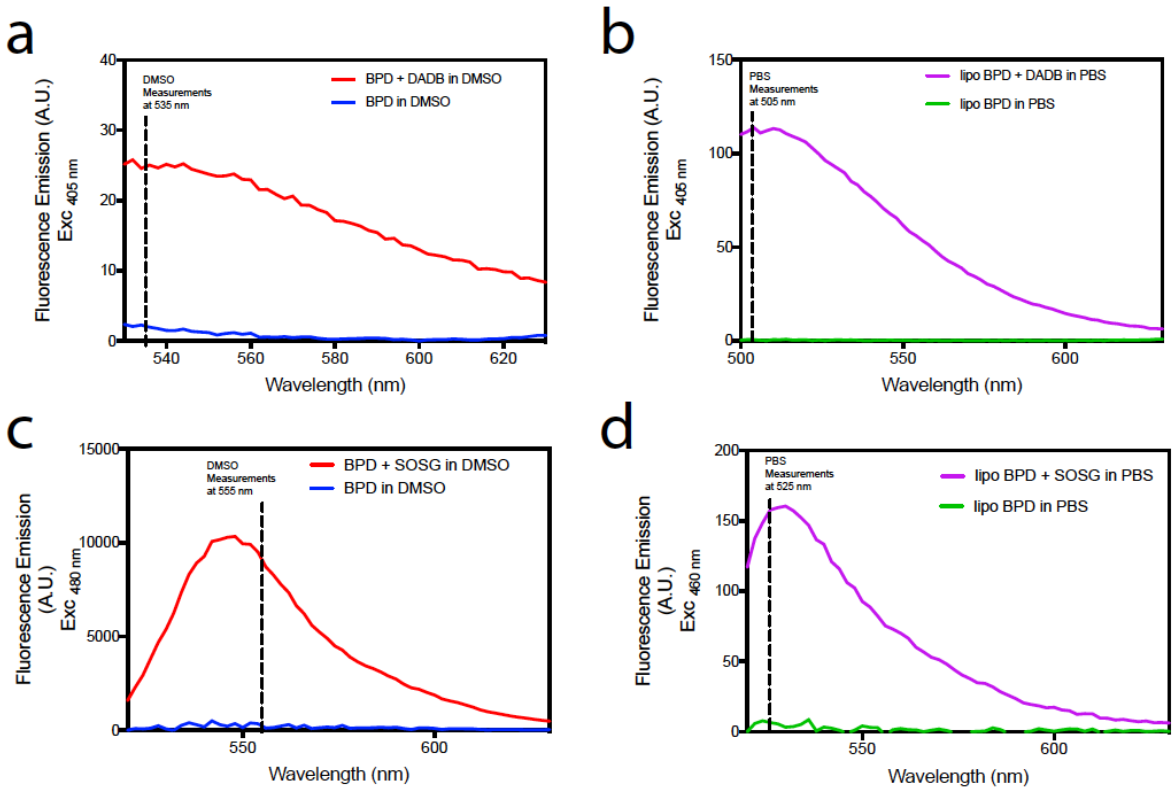

Figure S3. Fluorescence emission spectra of BPD in the absence and presence of DADB in DMSO (a), lipo BPD in the absence and presence of DADB in PBS (b), BPD in the absence and presence of SOSG in DMSO (c) and lipo BPD in the absence and presence of SOSG in PBS (d). The emission of BPD and lipo BPD is negligible at the wavelengths used to monitor singlet oxygen production (535 nm, 505 nm, 555 nm, 525 nm, respectively).

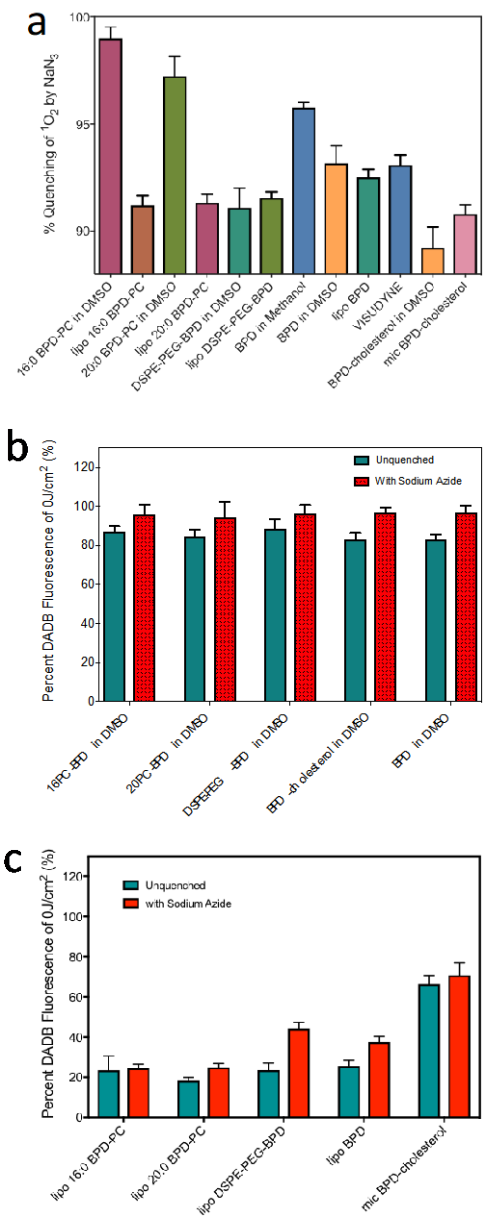

Figure S4. Quenching of singlet oxygen by sodium azide in the SOSG assay (a) and DADB assay (b, c) upon irradiation of BPD and its lipidated variants free in DMSO or entrapped in nanolipid formulations with 25 J/cm^2 of 690 nm light at 150 mW/cm^2. In the SOSG assay, percentage quenching by sodium azide is derived using the following equation:

$$100 - \left(\left(\frac{SOSG\ emission\ of\ unquenched\ sample - SOSG\ emission\ with\ NaN_3\ quenching}{SOSG\ emission\ of\ unquenched\ sample} \right) x\ 100 \right)$$

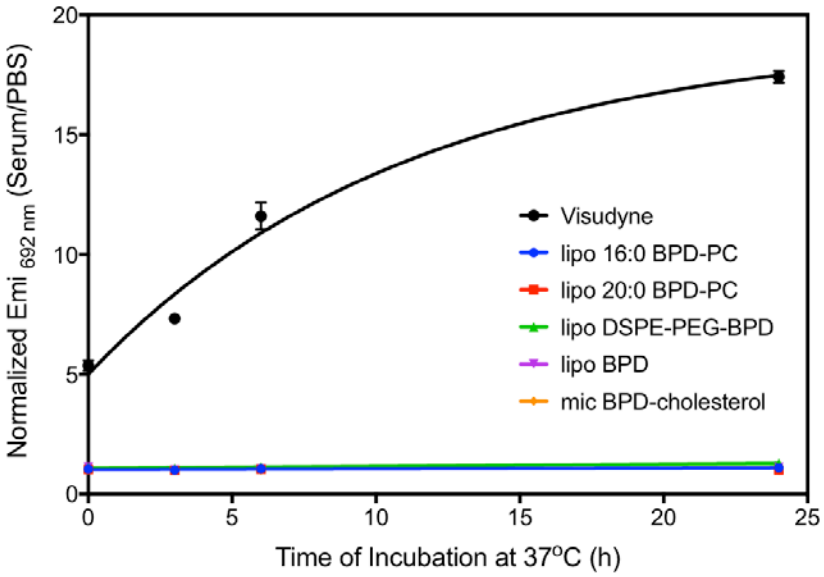

Figure S5. Dequenching of BPD and its lipidated variants entrapped in nanolipid formulations when incubated in serum-containing medium at 37°C over 24 hours. Rapid and substantial dequenching of BPD from Visudyne indicates immediate dissociation of BPD from the nanolipid construct that is sustained over the 24 hour incubation period.