

Electronic Supplementary Information

Efficient Light-Induced Production of Reactive Oxygen Species from a Far-Red ER-Targeting BODIPY Dye

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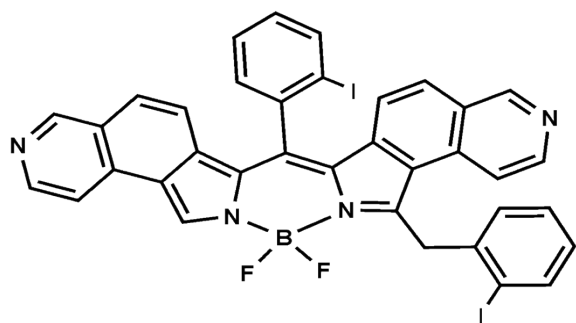
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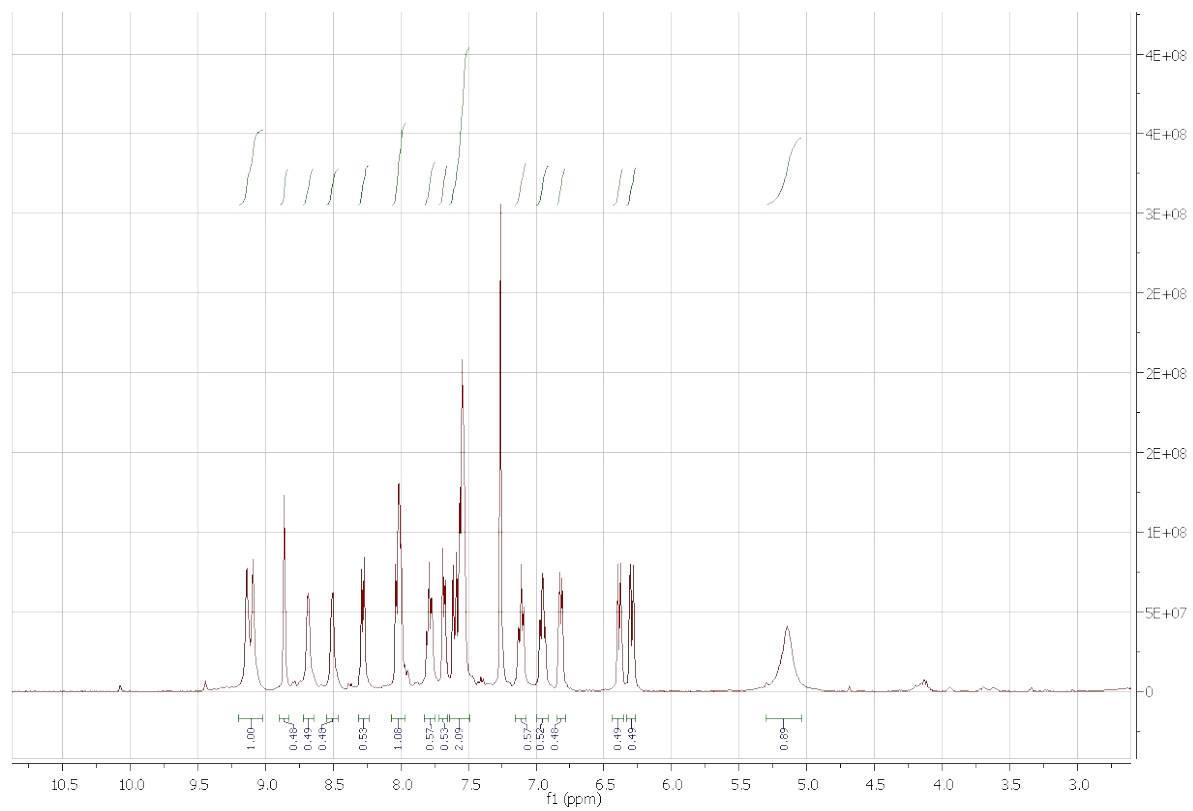
Characterization

BDP-1I

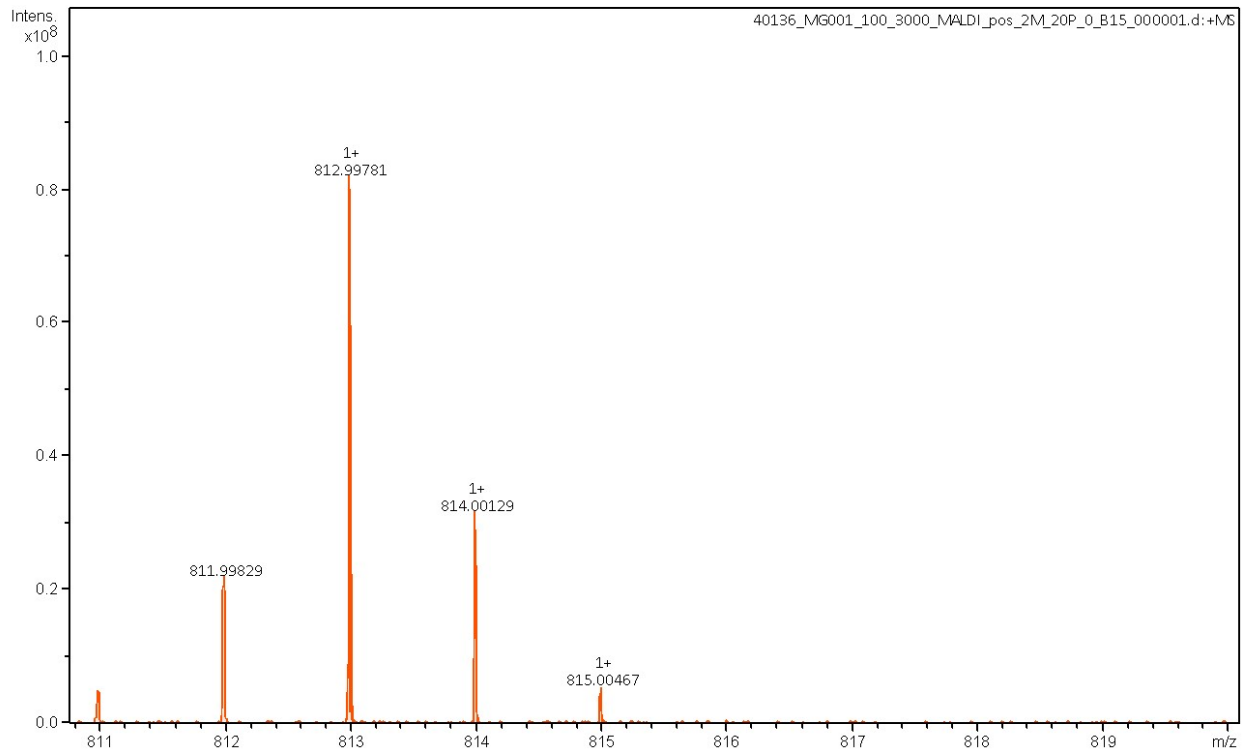


BDP-1I

^1H NMR (CDCl_3)



HRMS



Electronic Spectroscopy

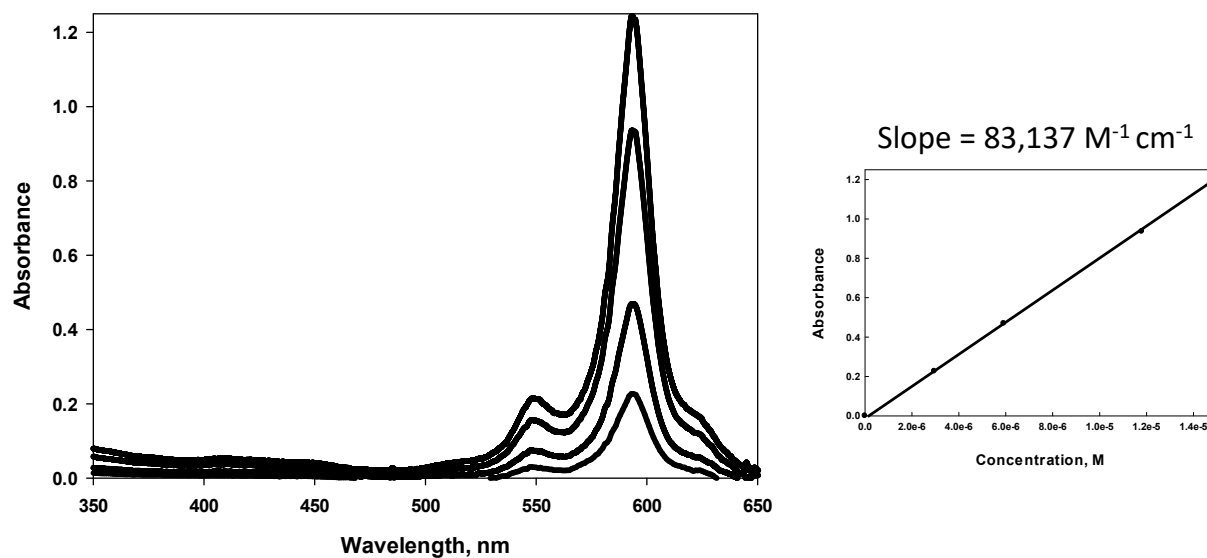
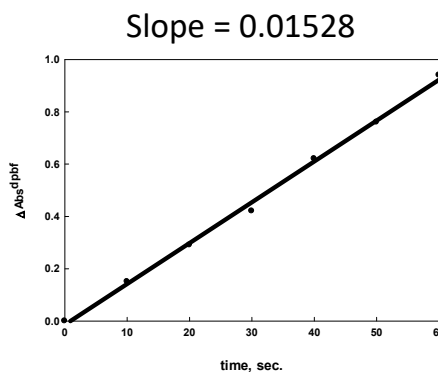
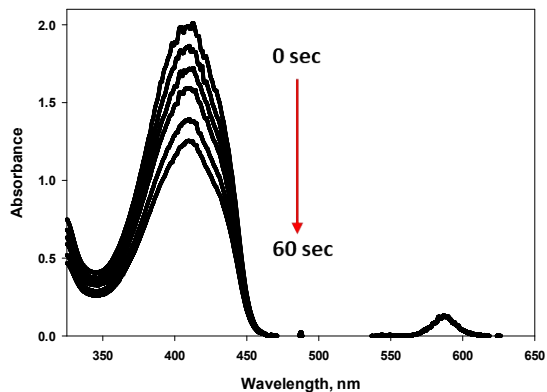


Figure S1: Beers-Law plot for **BDP-11** in DCM (298 K).

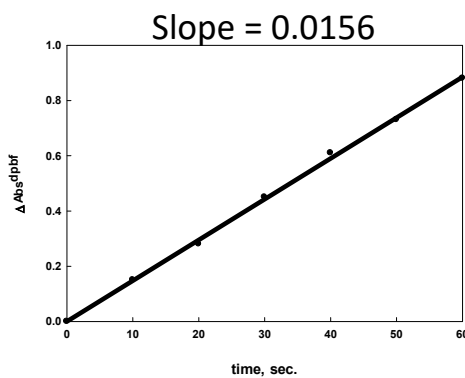
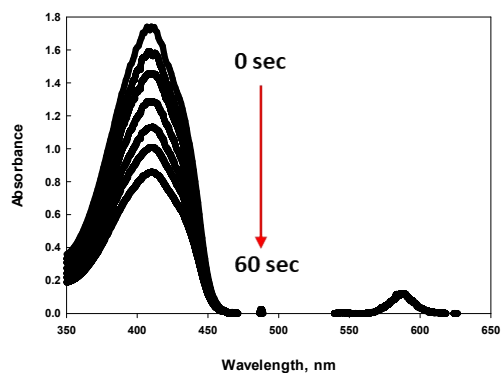
Singlet Oxygen Quantum Yield: DPBF studies

DPBF Results for BDP-1I

Run 1



Run 2



Run 3

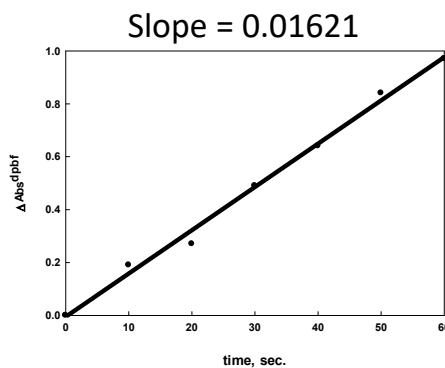
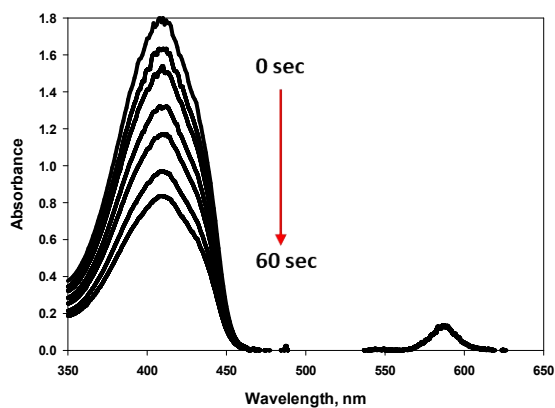
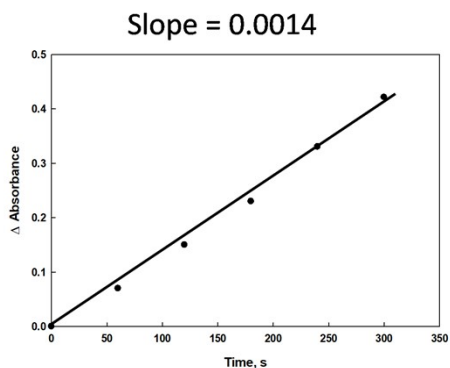
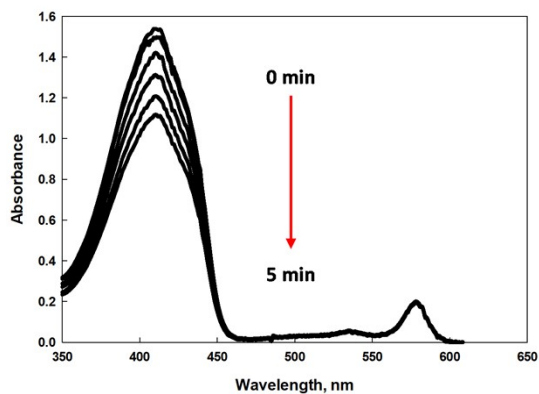


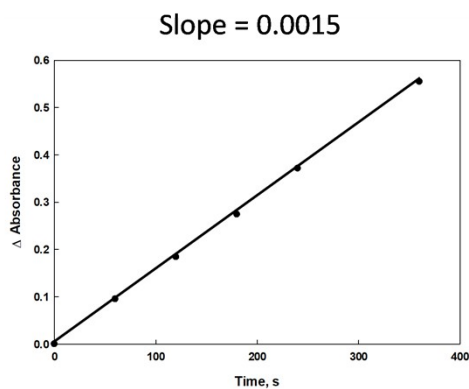
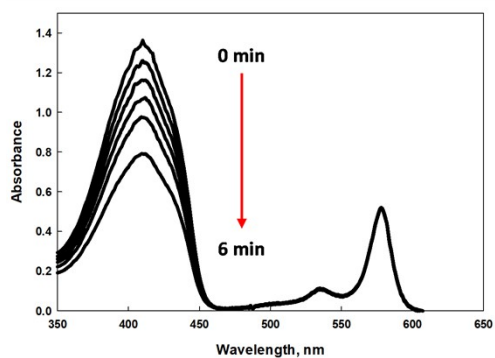
Figure S2. Acetonitrile DPBF and BDP-1I solutions irradiated with a 300 W mercury arc lamp equipped with a 550 nm long band-pass filter.

DPBF results for BDP-1

Run 1



Run 2



Run 3

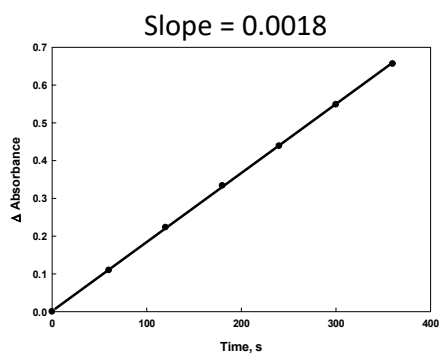
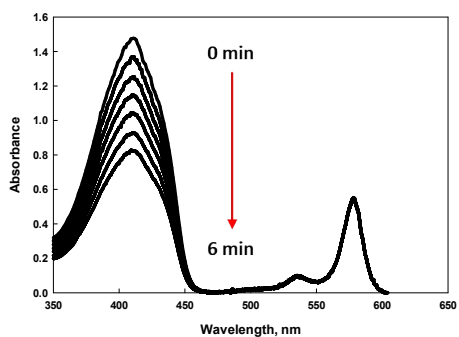
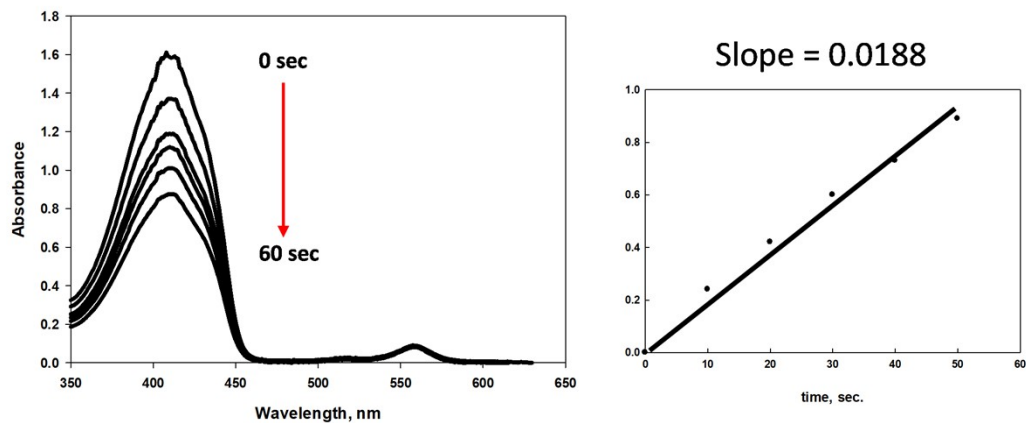


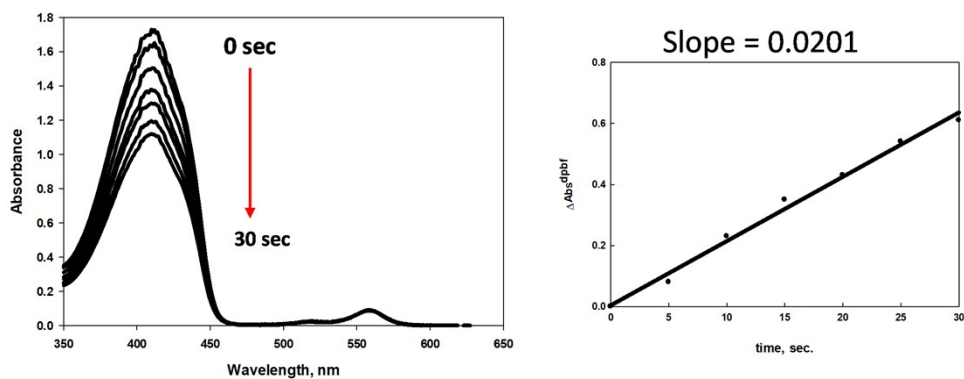
Figure S3. Acetonitrile DPBF and BDP-1 solutions irradiated with a 300 W mercury arc lamp equipped with a 550 nm long band-pass filter.

DPBF Results for Rose Bengal (RB)

Run 1



Run 2



Run 3

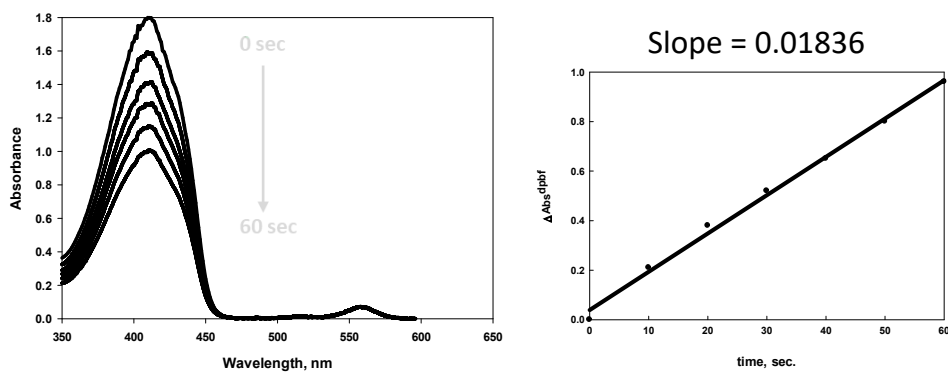
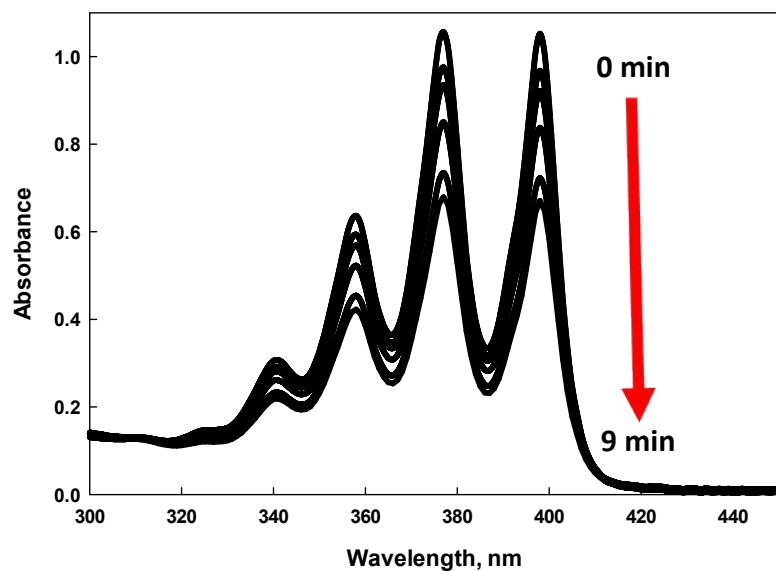


Figure S4. Acetonitrile DPBF and RB solutions irradiated with a 300 W mercury arc lamp equipped with a 550 nm long band-pass filter. Irradiation time for run 1 was 0-30 sec, while runs 2 and 3 were irradiated for a total of 60 sec.

ABDA $^1\text{O}_2$ Quantum Yield Measurement

RB ABDA Run 1



RB ABDA run 2

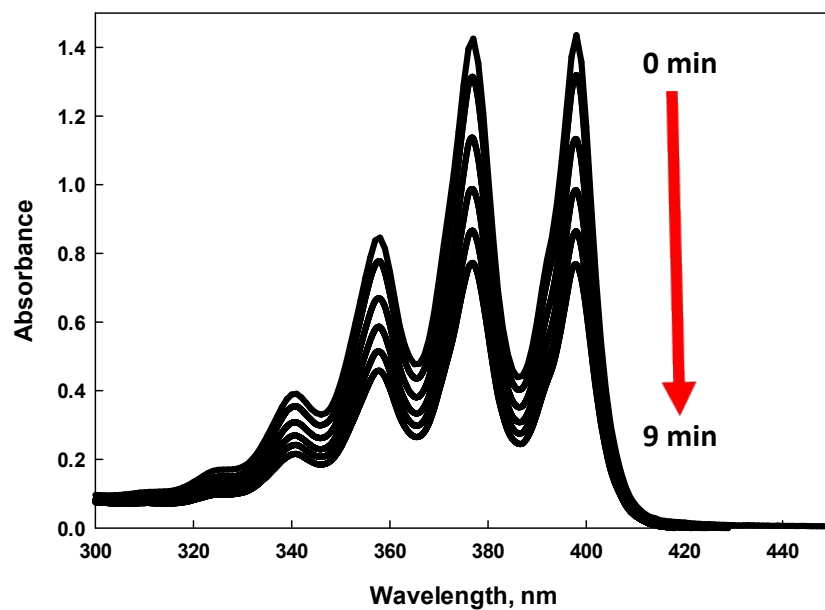
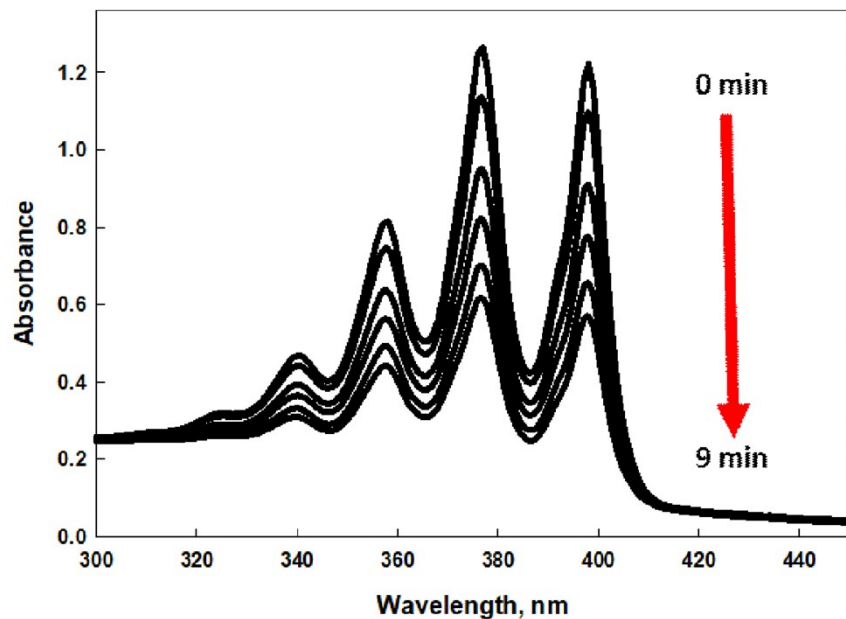


Fig. S5. Electronic spectra of acetonitrile solution of the singlet oxygen scavenger (ABDA) and RB after irradiation with 300 W lamp equipped with a 550 nm long band-pass filter.

BDP-1I ABDA Run 1



BDP-1I ABDA Run 2

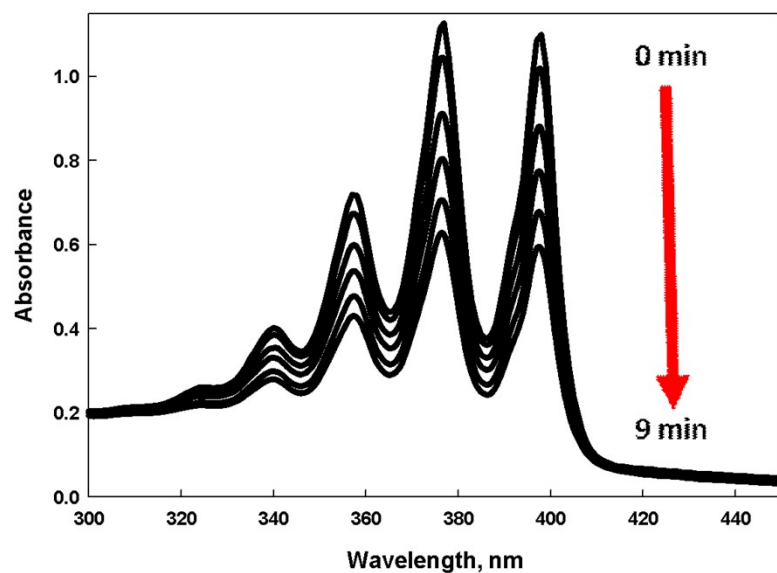
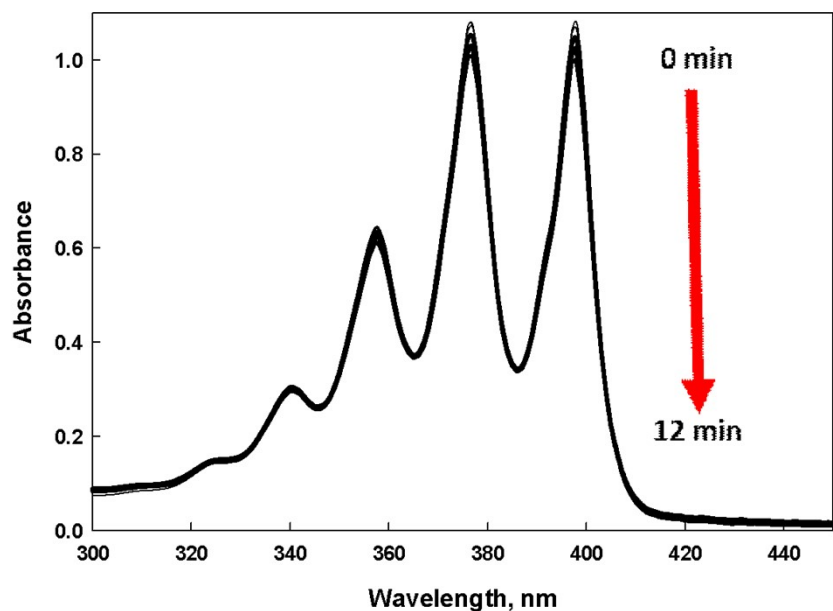


Fig. S6. Electronic spectra of acetonitrile solution of the singlet oxygen scavenger (ABDA) and **BDP-1I** after irradiation with 300 W lamp equipped with a 550 nm long band-pass filter.

BDP-1 ABDA Run 1



BDP-1 ABDA Run 2

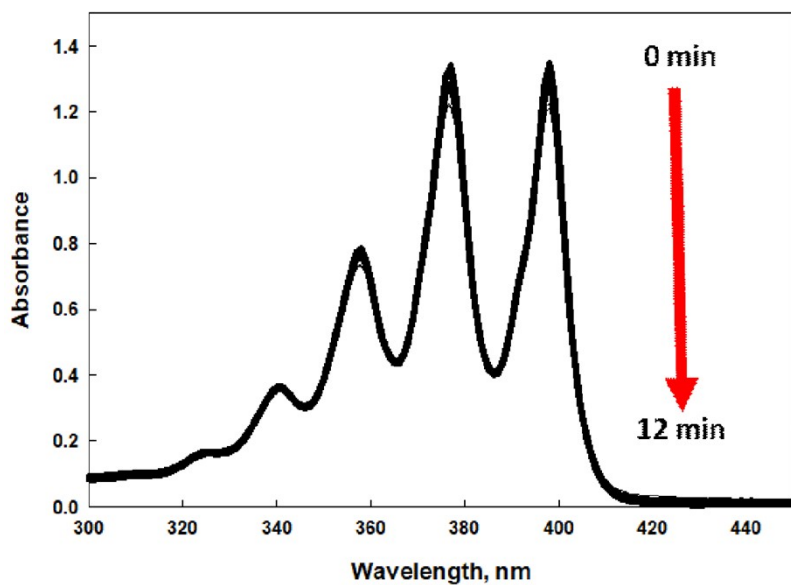


Fig. S7. Electronic spectra of acetonitrile solution of the singlet oxygen scavenger (ABDA) and **BDP-1** after irradiation with 300 W lamp equipped with a 550 nm long band-pass filter.

Procedure for Superoxide Production.

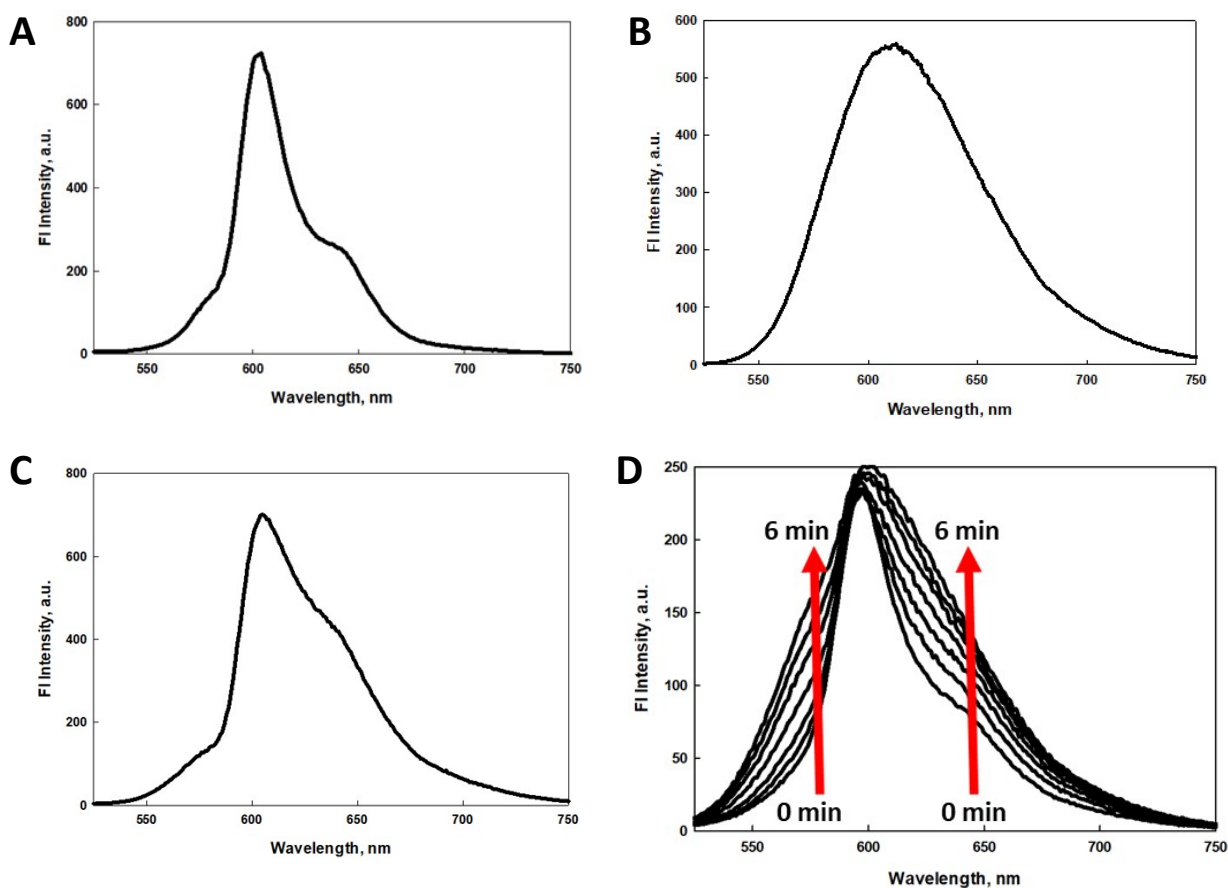
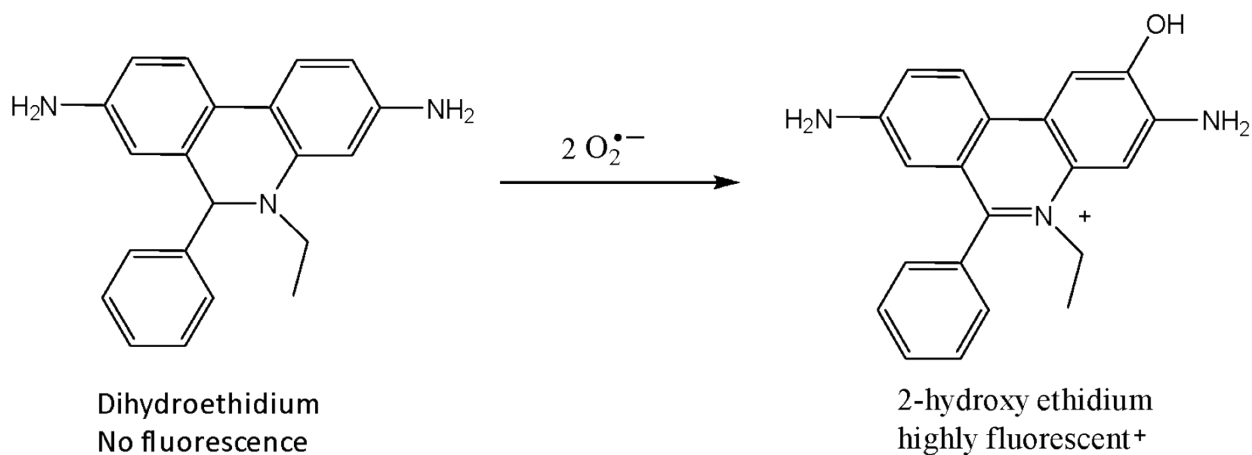


Fig. S8. **A.** Emission spectra of an acetonitrile solution of **BDP-1I** ($\lambda_{\text{exc}} = 500 \text{ nm}$). **B.** Emission spectra of an acetonitrile solution of ethidium bromide ($\lambda_{\text{exc}} = 500 \text{ nm}$). **C.** Emission spectrum of an acetonitrile solution of ethidium bromide and **BDP-1I** ($\lambda_{\text{exc}} = 500$

nm). **D.** Emission spectra of DHE/**BDP-1** as a function of irradiation with a 300 W mercury arc lamp equipped with a 550 nm long band-pass filter.

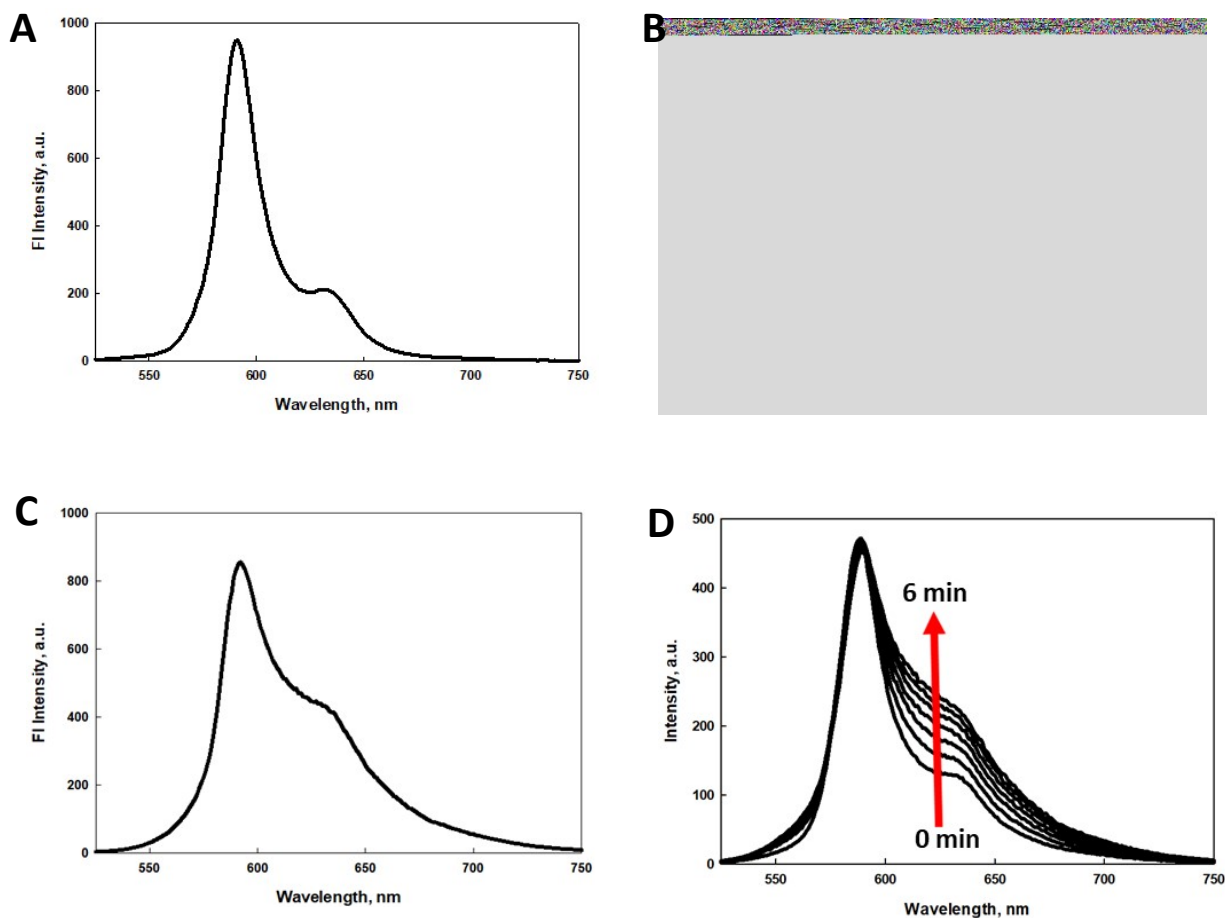


Fig. S9. **A.** Emission spectra of an acetonitrile solution of **BDP-1** ($\lambda_{\text{exc}} = 500$ nm). **B.** Emission spectra of an acetonitrile solution of ethidium bromide ($\lambda_{\text{exc}} = 500$ nm). **C.** Emission spectrum of an acetonitrile solution of ethidium bromide and **BDP-1** ($\lambda_{\text{exc}} = 500$ nm). **D.** Emission spectra of DHE/**BDP-1** as a function of irradiation with a 300 W mercury arc lamp equipped with a 550 nm long band-pass filter.

S5 Cell Studies

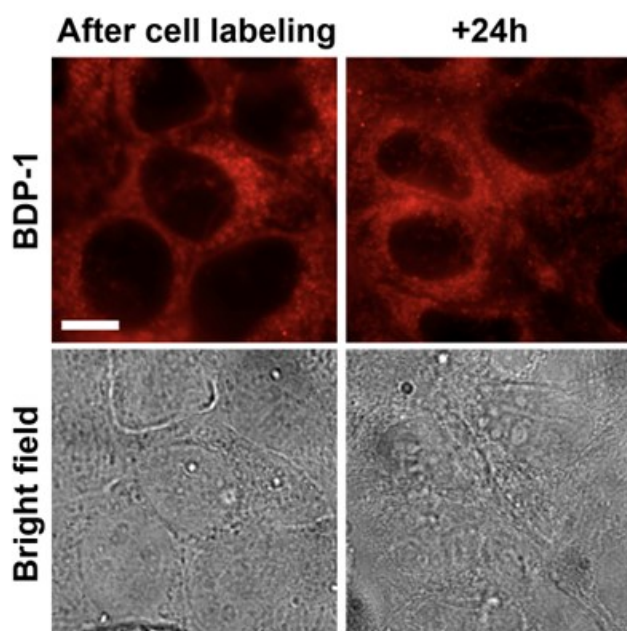


Fig. S10. BDP-1 staining is retained in breast epithelial cells. Scale bar, 10 μm .

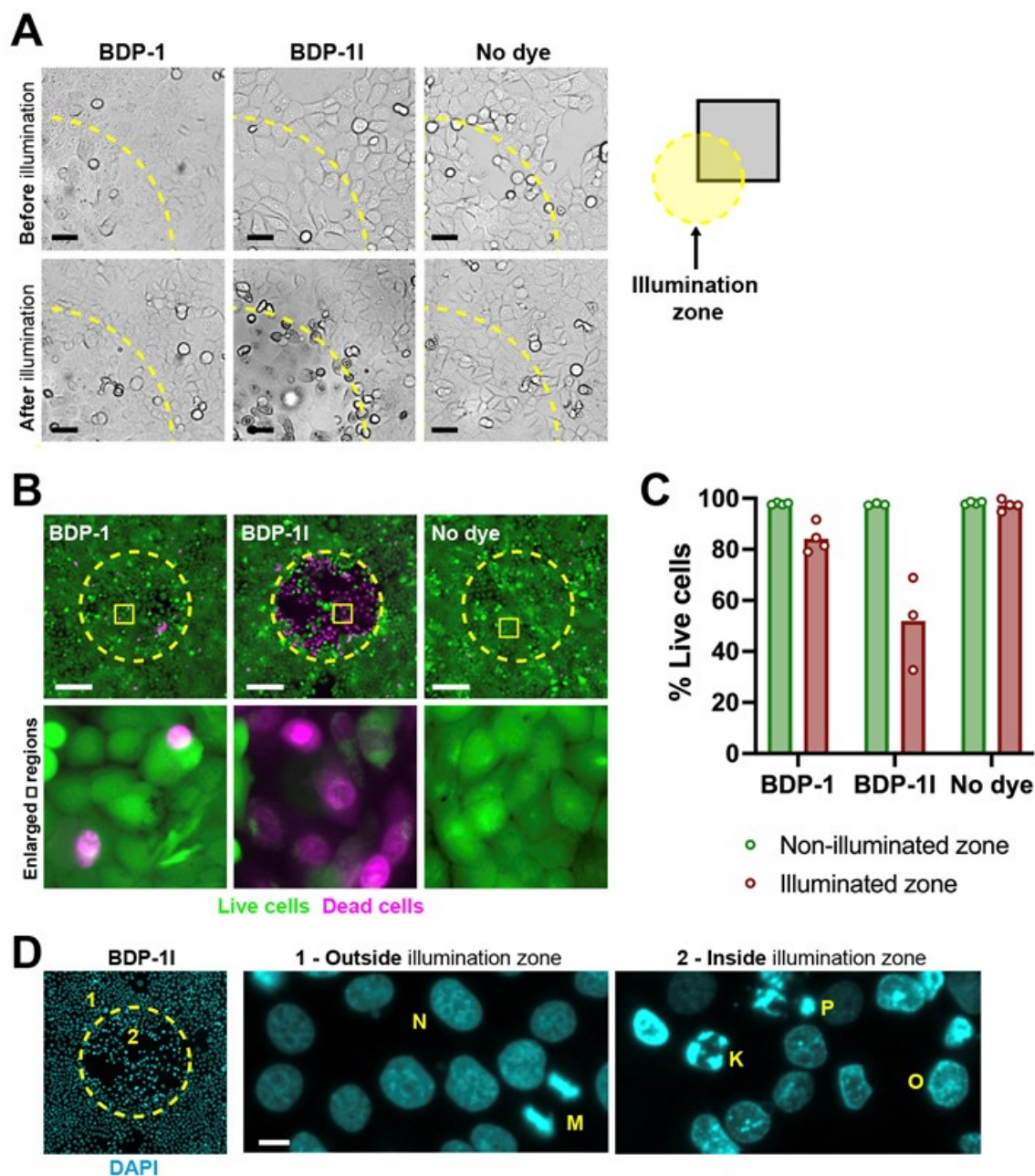


Fig. S11. **A** Bright field images of HMT3522-T4 breast cancer cells stained with **BDP-1** or **BDP-1I**, inside and outside the illumination zone. Scale bar, 50 μm . Illumination zones are indicated with dashed lines. **B** Calcein AM (live cells, green) and SYTOX (dead cells, purple) staining of cells treated with **BDP-1**, or **BDP-1I**, or without dye. Scale bar, 200 μm . **C** Quantification of cell viability. Imaging fields had 3000-5000 cells. Each symbol represents an independent illumination zone. **D** Nuclear morphology (DAPI) post-irradiation in cells photosensitized with **BPD-1I**. N, normal interphase nucleus; M, mitotic cell; O, chromatin marginalization; P, pyknosis; K, karyorrhexis. Scale bar, 10 μm .

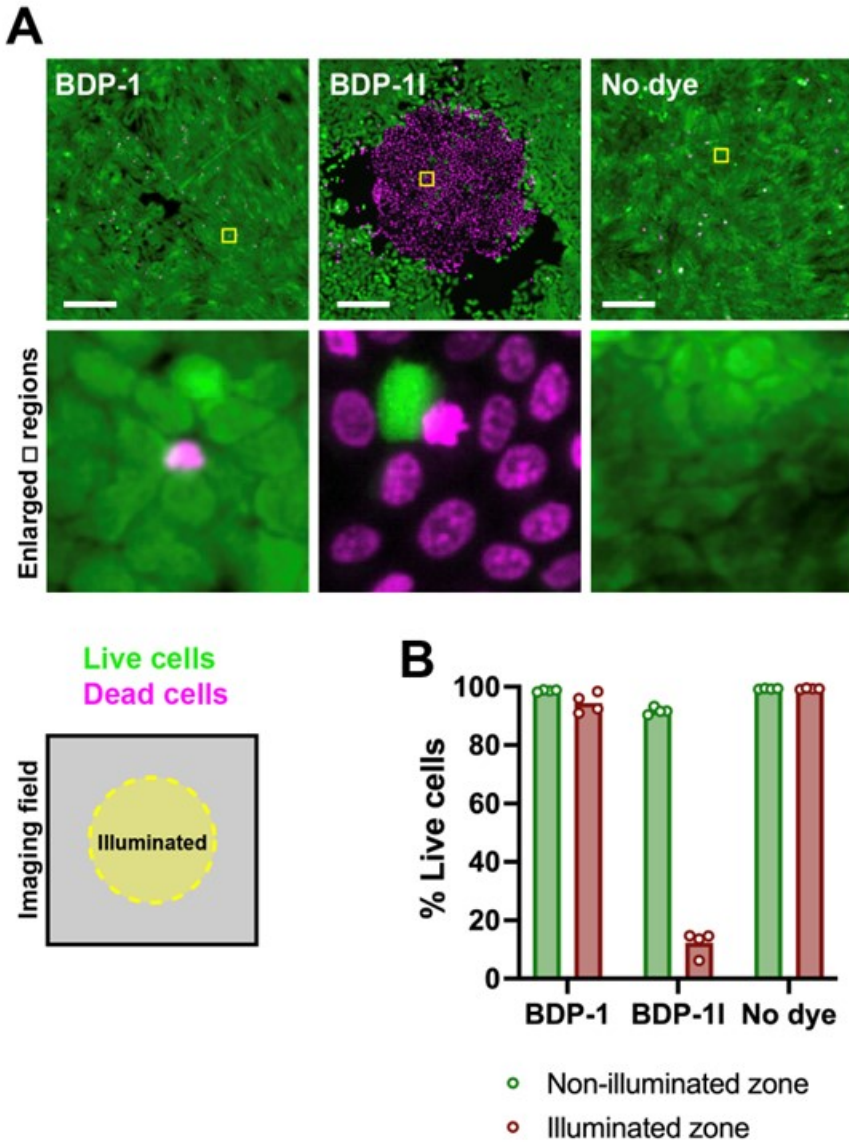


Fig. S12. A Images of calcein AM (live cells, green) and SYTOX (dead cells) fluorescence in non-cancerous HMT3522-S1 cells treated with **BDP-1**, or **BDP-1I**, or without dye. Localization of the illumination zone is shown in the schematic. Scale bar, 200 μm . **B** Quantification of cell viability. Imaging fields had 8000-14000 cells. Each symbol represents an independent illumination zone.