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# **Supporting Information**

# Glucose Conjugated Aza-BODIPY for Selective Photodynamic Cancer Therapy

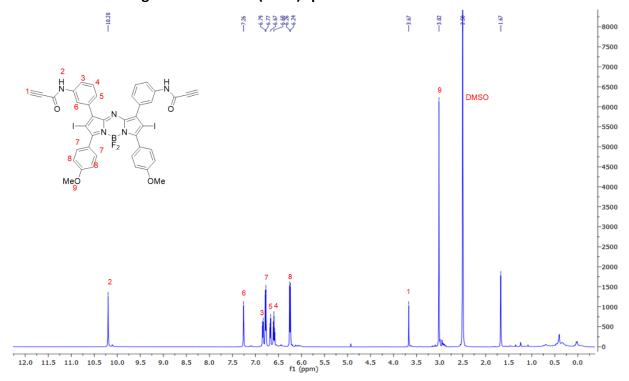
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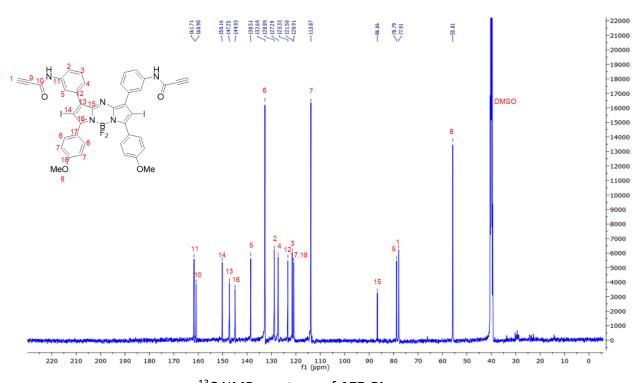
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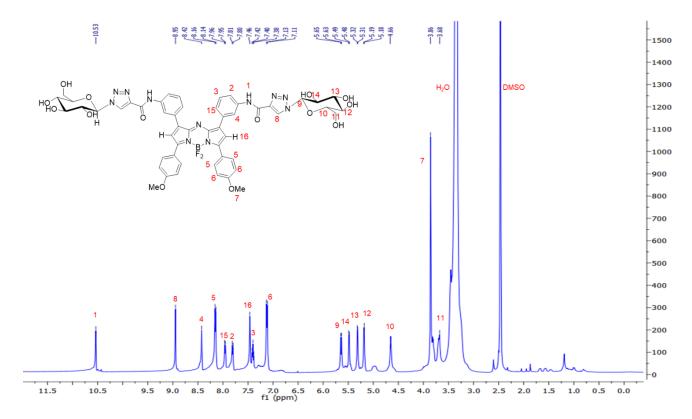
### 1. <sup>1</sup>H and <sup>13</sup>C Nuclear Magnetic resonance (NMR) spectra



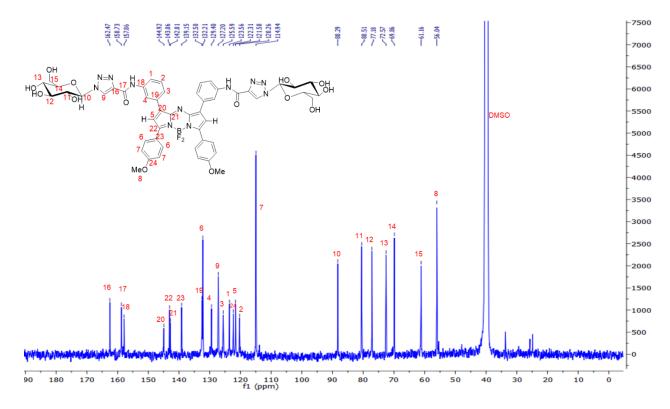
<sup>1</sup>H NMR spectrum of **AZB-PI**.



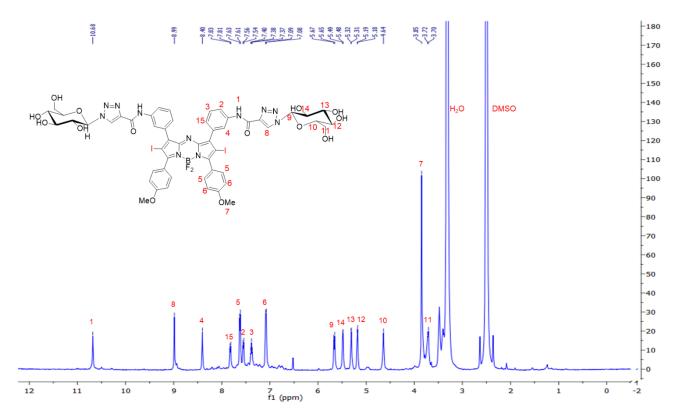
<sup>13</sup>C NMR spectrum of **AZB-PI**.



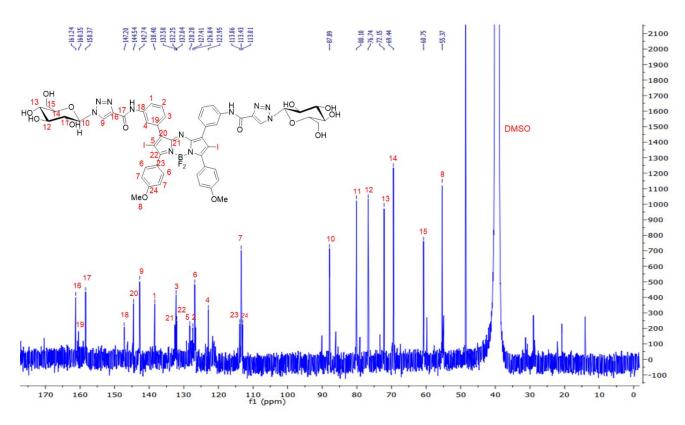
<sup>1</sup>H NMR spectrum of **AZB-Glc**.



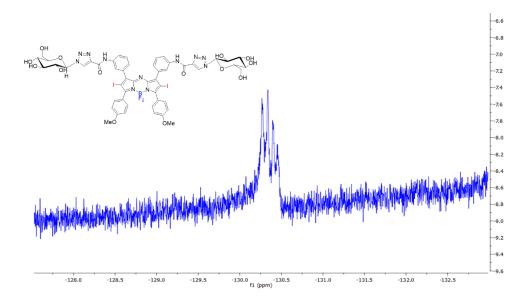
<sup>13</sup>C NMR spectrum of **AZB-Glc**.



<sup>1</sup>H NMR spectrum of **AZB-Glc-I**.

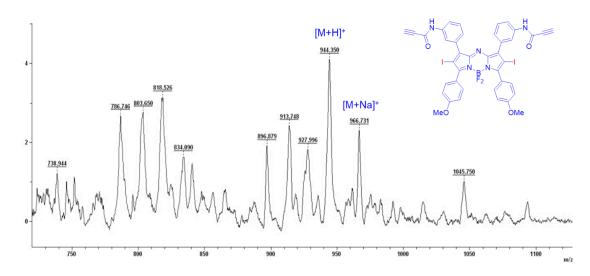


<sup>13</sup>C NMR spectrum of **AZB-Glc-I**.

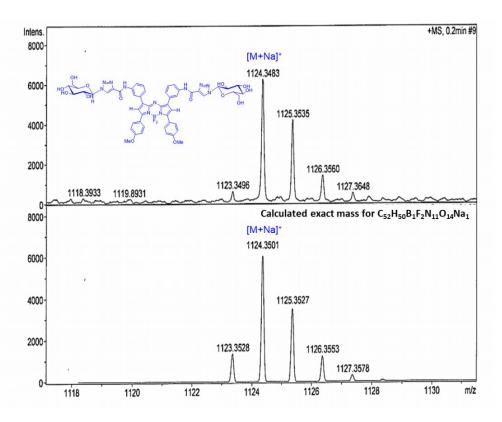


<sup>19</sup>F NMR spectrum of **AZB-Glc-I**.

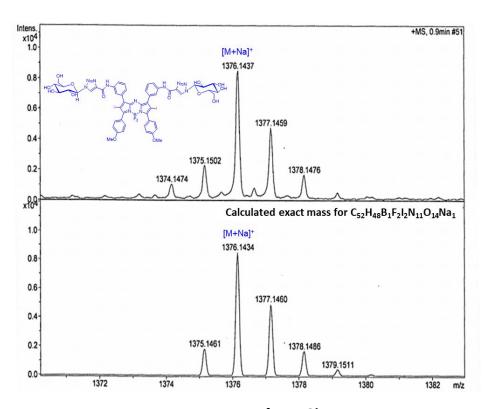
## 2. Mass spectrometry results



Mass spectrum of AZB-PI.

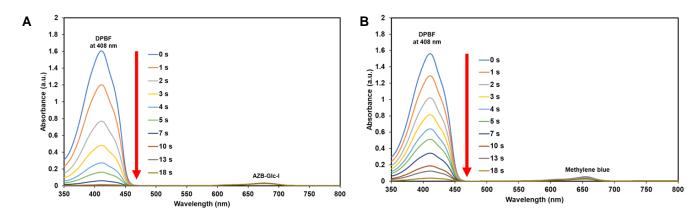


Mass spectrum of AZB-Glc.



Mass spectrum of AZB-Glc-I.

#### 3. Singlet oxygen generation of AZB-Glc-I



**Figure S1**. DPBF absorbance changes at 408 nm under being exposed to NIR light in the presence of A) **AZB-Glc-I** B) Methylene blue in ethanol.

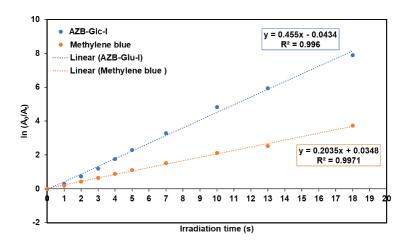
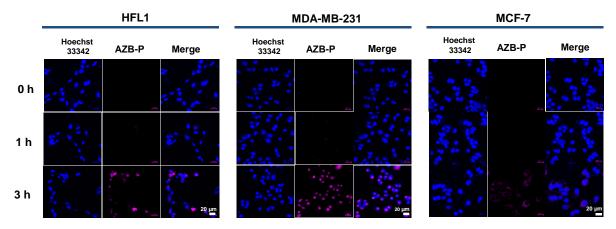


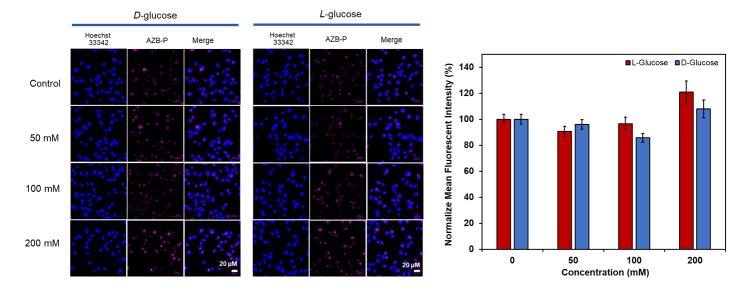
Figure S2. The first order kinetic plot of DPBF absorbance at 408 nm vs irradiation times.

#### 4. Time dependent internalization of AZB-P in cancer cells



**Figure S3**. Time dependent internalization of **AZB-P** (5  $\mu$ M) in HFL1, MDA-MB-231 and MCF-7 cells in various incubation times. Scale bars = 20  $\mu$ m.

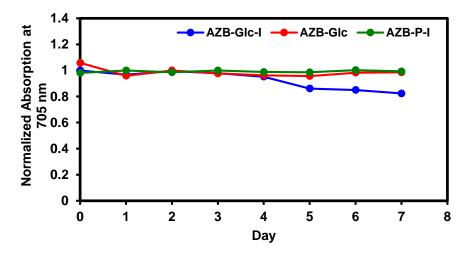
#### 5. Competition assay between D-/L-Glucose and AZB-P



**Figure S4**. Glucose competition assay of **AZB-P** (5  $\mu$ M) in MDA-MB-231 cells in the presence of various concentrations of *D*- Glucose and *L*-Glucose for 30 min. The fluorescence intensities of the images were quantified using Image J and data are presented as means  $\pm$  SD (n = 40) in the bar graph. Scale bars = 20  $\mu$ m.

#### 6. Stability of AZB-Glc-I, AZB-Glc, and AZB-P-I stock solutions

Solutions of AZB-Glc-I, AZB-Glc, and AZB-P-I were made as 1.5 mM stocks in DMSO and stored at 20 °C. Before measuring absorbance spectra, all compounds were diluted in DMEM (to mimic the cell assay condition) to a final concentration of 5  $\mu$ M. The NIR absorption of AZB-Glc-I, AZB-Glc, and AZB-P-I were measured by UV-VIS spectrometer (Thermo Scientific/MultiskanGO) in three independent experiments, every day for 7 days. The absorbance at 705 nm was normalized relative to the freshly prepared stock solutions.



**Figure S5**. Normalized absorption at 705 nm of **AZB-Glc-I**, **AZB-Glc**, and **AZB-P-I** stock solutions in DMSO measured every day for 7 days.