Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

Novel aggregation-induced emission (AIE)-photosensitizers with built-in capability of mitochondria targeting and glutathione depletion for efficient photodynamic therapy

Sauraj[a], Ji Hee Kang[a], O Hyun Lee, Young Tag Ko*[a]

[a] College of Pharmacy, Gachon Institute of Pharmaceutical Sciences, Gachon University, Incheon, Republic of Korea

*Corresponding author:

Young Tag Ko

College of Pharmacy, Gachon Institute of Pharmaceutical Sciences, Gachon University, Incheon, Republic of Korea 21936

Tel.: +82-32-820-4923; fax:+ 82-32-820-4829

E-mail address: youngtakko@gachon.ac.kr

Synthesis of TPEPy

TPE-Br (496 mg, 1 mmol) and 4-vinylpyridine (496 mg, 1 mmol) were dissolved in 10 ml dry DMF followed by the addition of (22 mg, 0.1 mmol) palladium (II) acetate, and (31mg, 01 mmol) tri (o-tolyl)phosphine. After that, the (0.8 ml) triethylamine was added to reaction mixture and stirred at 110°C temperature for 12 h under argon atmosphere. After cooling down the reaction mixture to room temperature the reaction was quenched by water (30 ml) and the mixture was extracted with ethyl acetate. The collected organic layer was washed by brine, dried over Na_2SO_4 and concentrated under reduced pressure. The desired residue was purified by column chromatography using n-hexane/ethyl acetate (1/1~ 1/2, v/v) as eluent to give the desired product TPEPy as a yellow solid (316 mg, 63.7 %).

^{1}H NMR (600 MHz, CDCl3) δ 8.55 (d, 2H), 7.32 (d, 2H), 7.29 (s, 1H), 7.27 (s, 1H), 7.23-7.19 (m, 1H), 7.14-7.09 (m, 3H), 7.05-7.03 (m, 4H), 6.98-6.91 (m, 5H), 6.69 - 6.61 (m, 4H), 3.75 (s, 3H), 3.74 (s, 3H). ^{13}C NMR (151 MHz, CDCl3) δ 158.4, 158.3, 150.2, 145.3, 145.0, 144.2, 141.0, 138.7, 136.4, 136.3, 133.9, 133.2, 132.8, 132.7, 132.0, 131.6, 127.9, 126.6, 126.4, 125.5, 120.9, 113.3, 55.2. LC-MS, m/z: $[M+H]^+$ calcd 496.2, found 496.2

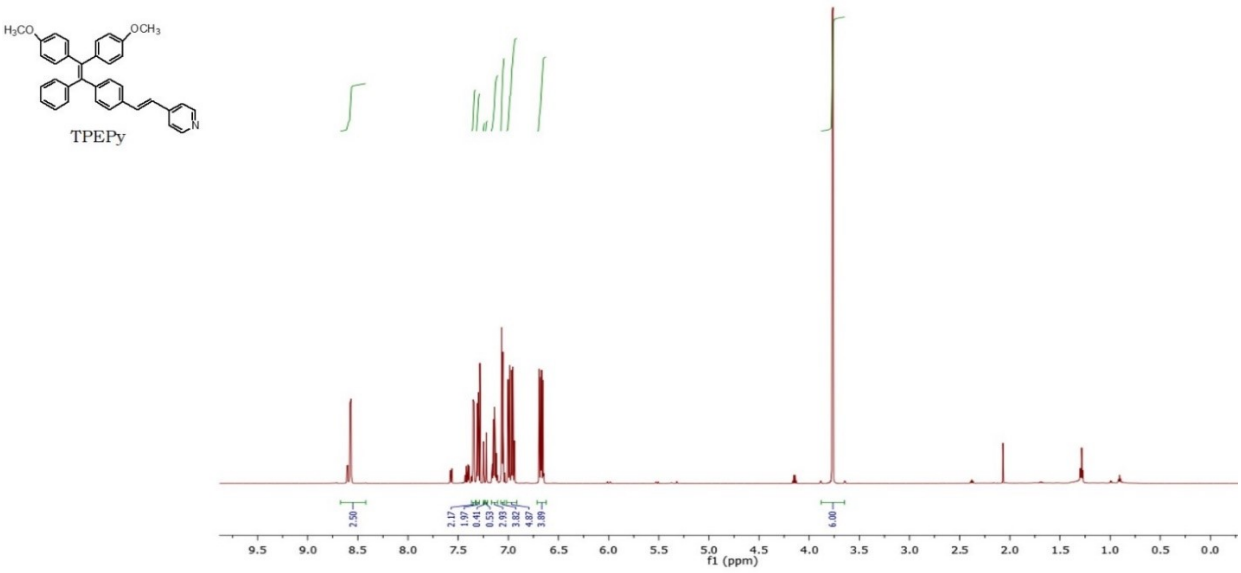

Fig. S1. (a) ^{1}HNMR spectrum of TPEPy

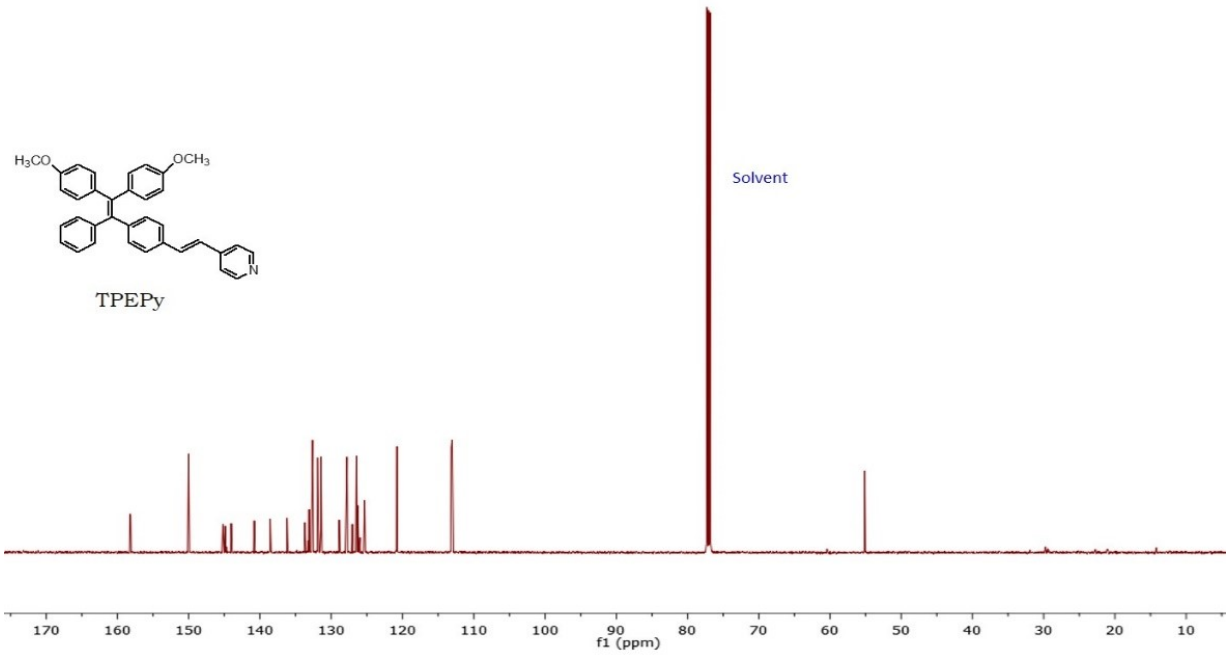

Fig. S2. ^{13}C NMR spectrum of TPEPy

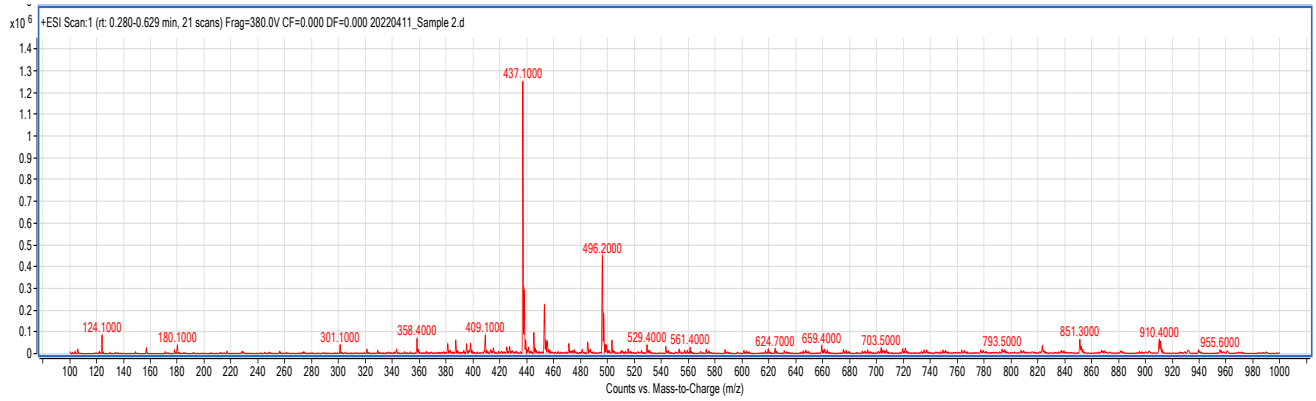

Fig. S3. LC-MS chromatograph of TPEPy in the positive mode of ionization (ESI+/[M+H]+)

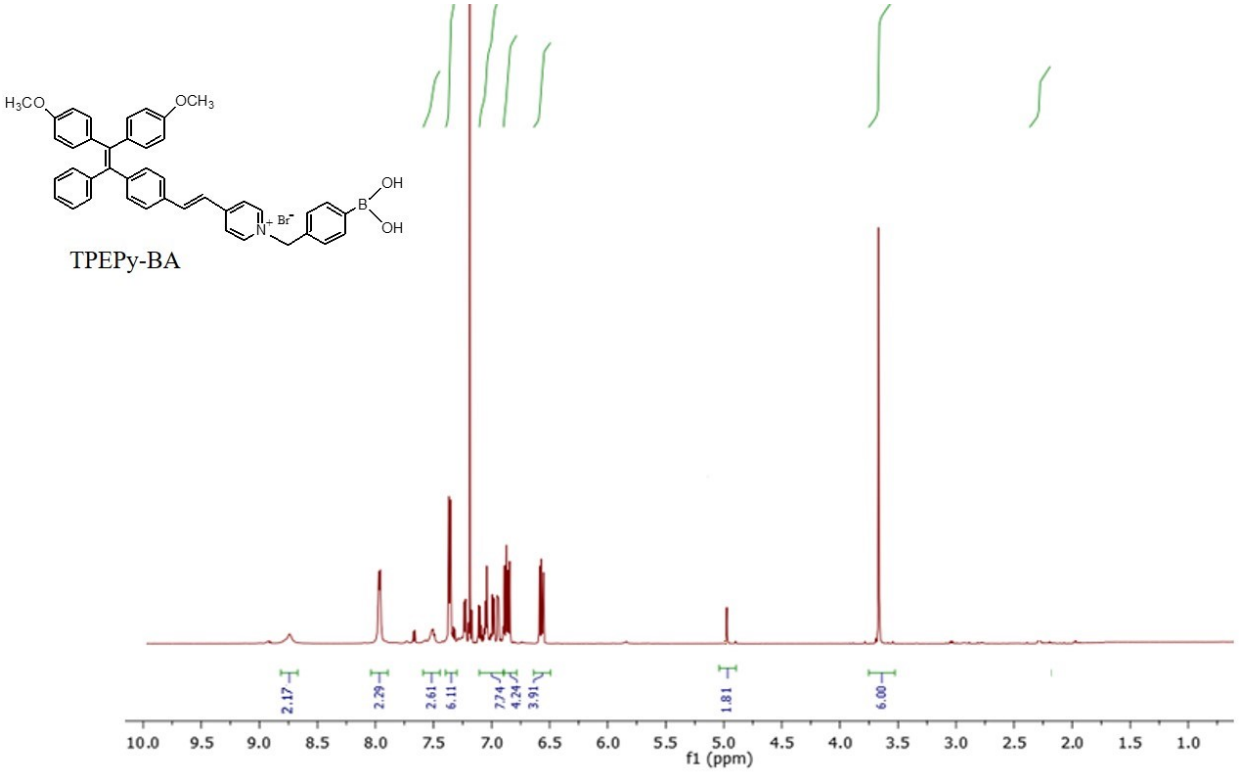

Fig. S4. ^{1}H NMR spectrum of TPEPy-BA

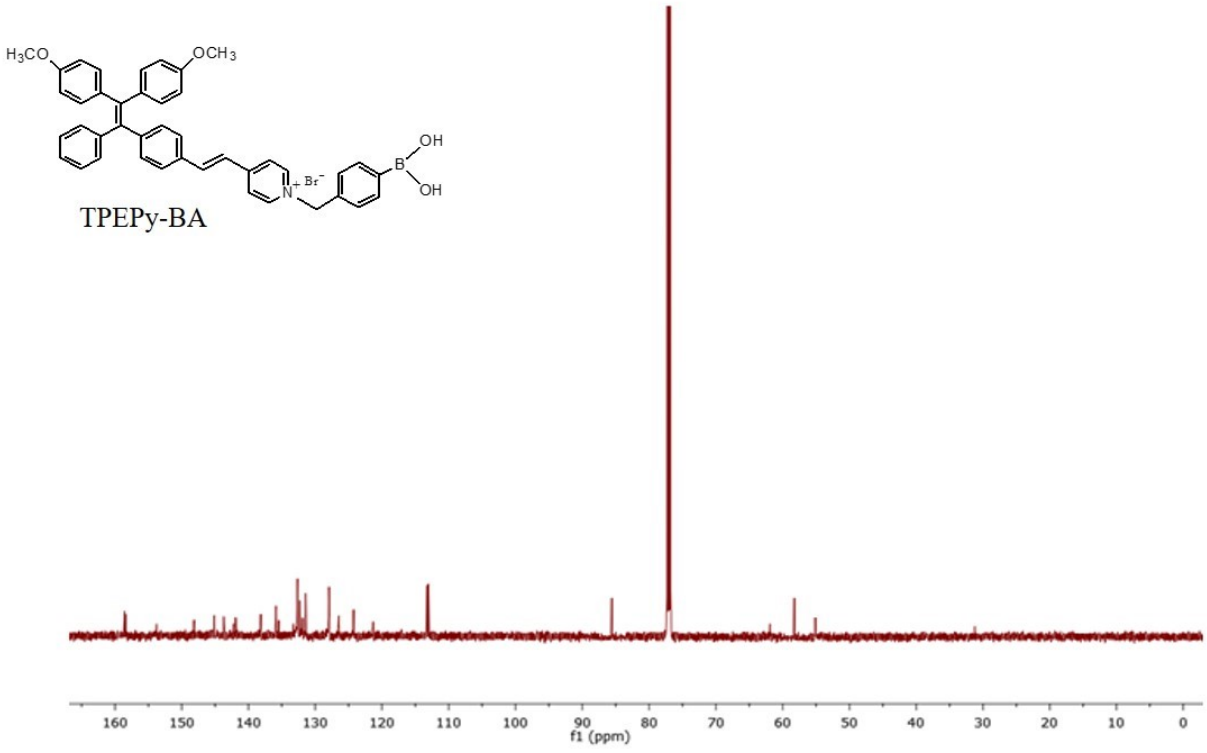

Fig. S5. ^{13}C NMR spectrum TPEPy-BA

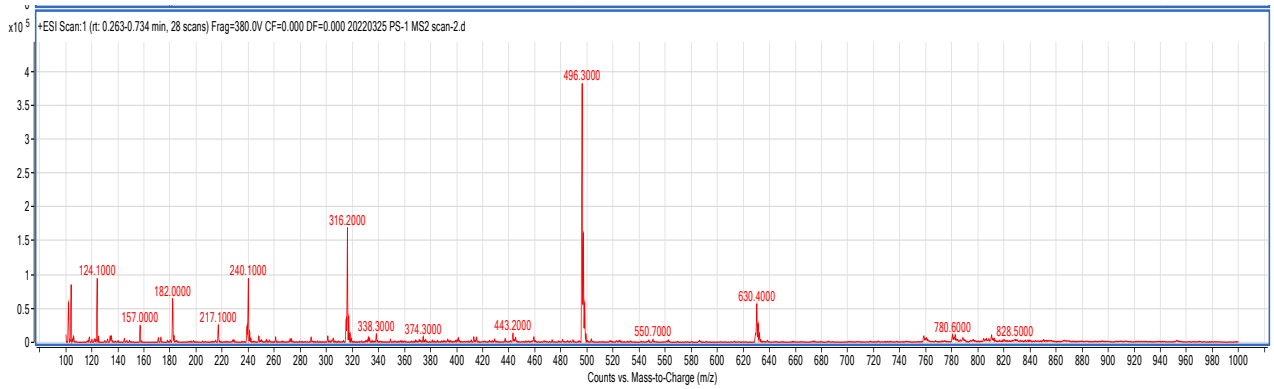

Fig. S6. LC-MS chromatograph of TPEPy-BA in in the positive mode of ionization (ESI+/[M+H]+)

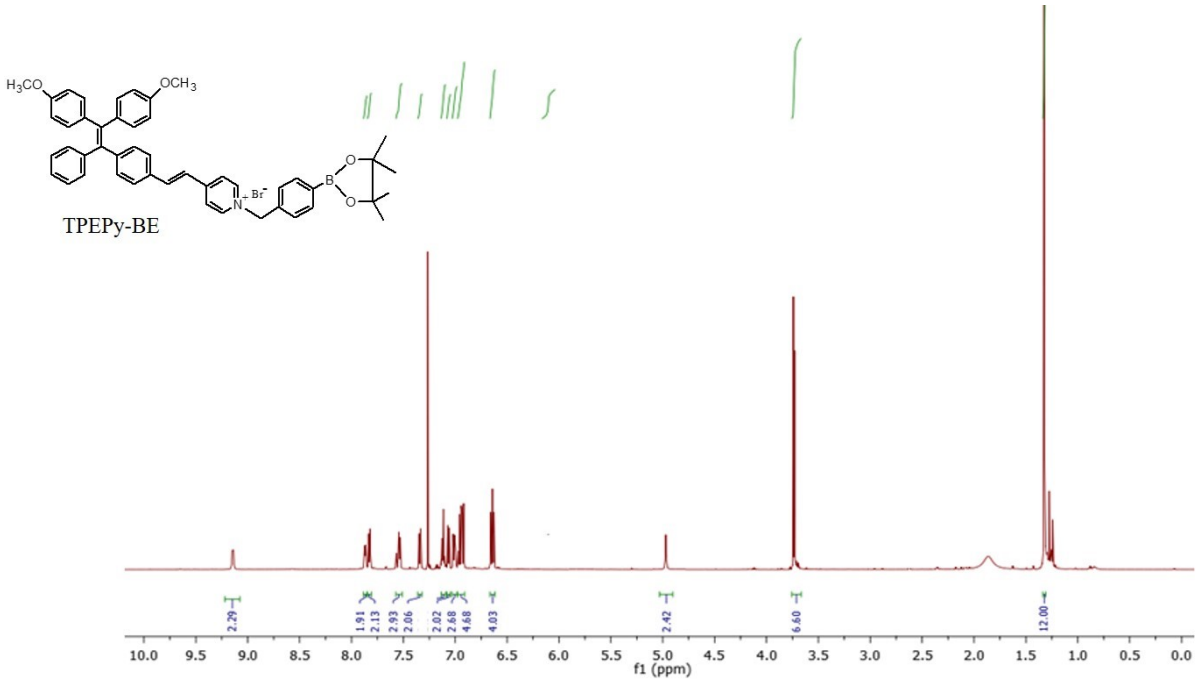

Fig. S7. ^{1}H NMR spectrum of TPEPy-BE

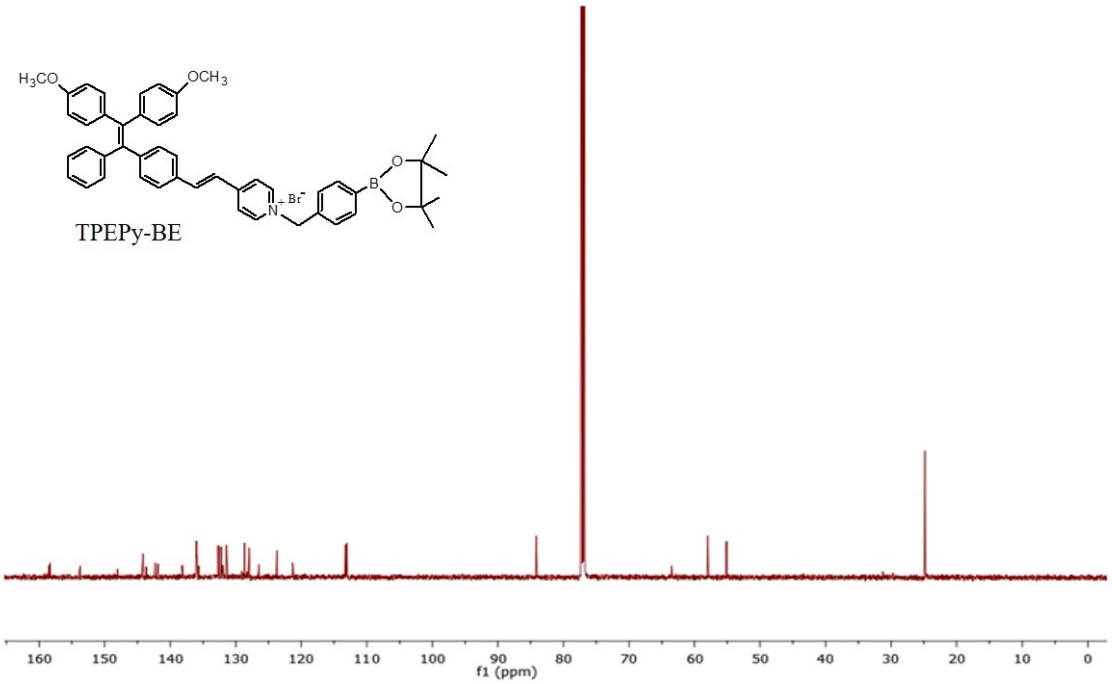

Fig. S8. ^{13}C NMR spectrum of TPEPy-BE

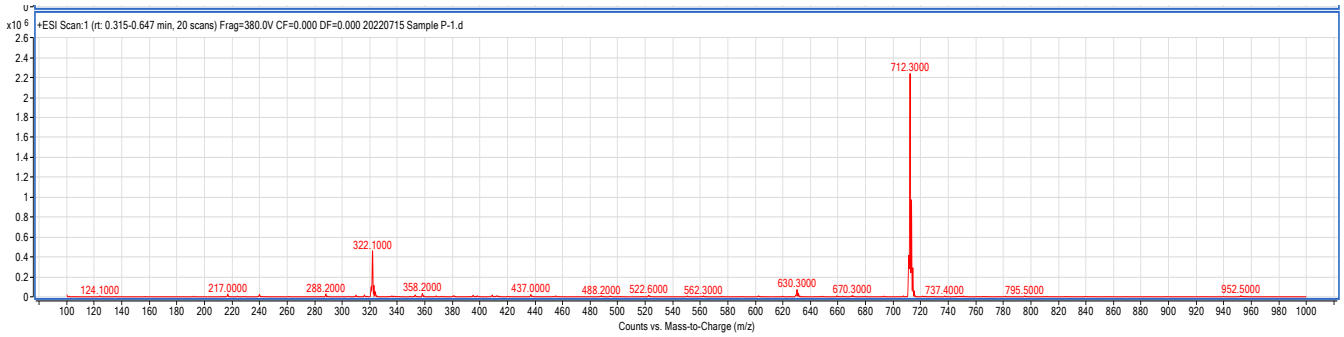

Fig. S9. LC-MS chromatograph of TPEPy-BE in the positive mode of ionization (ESI+/[M+H]+)

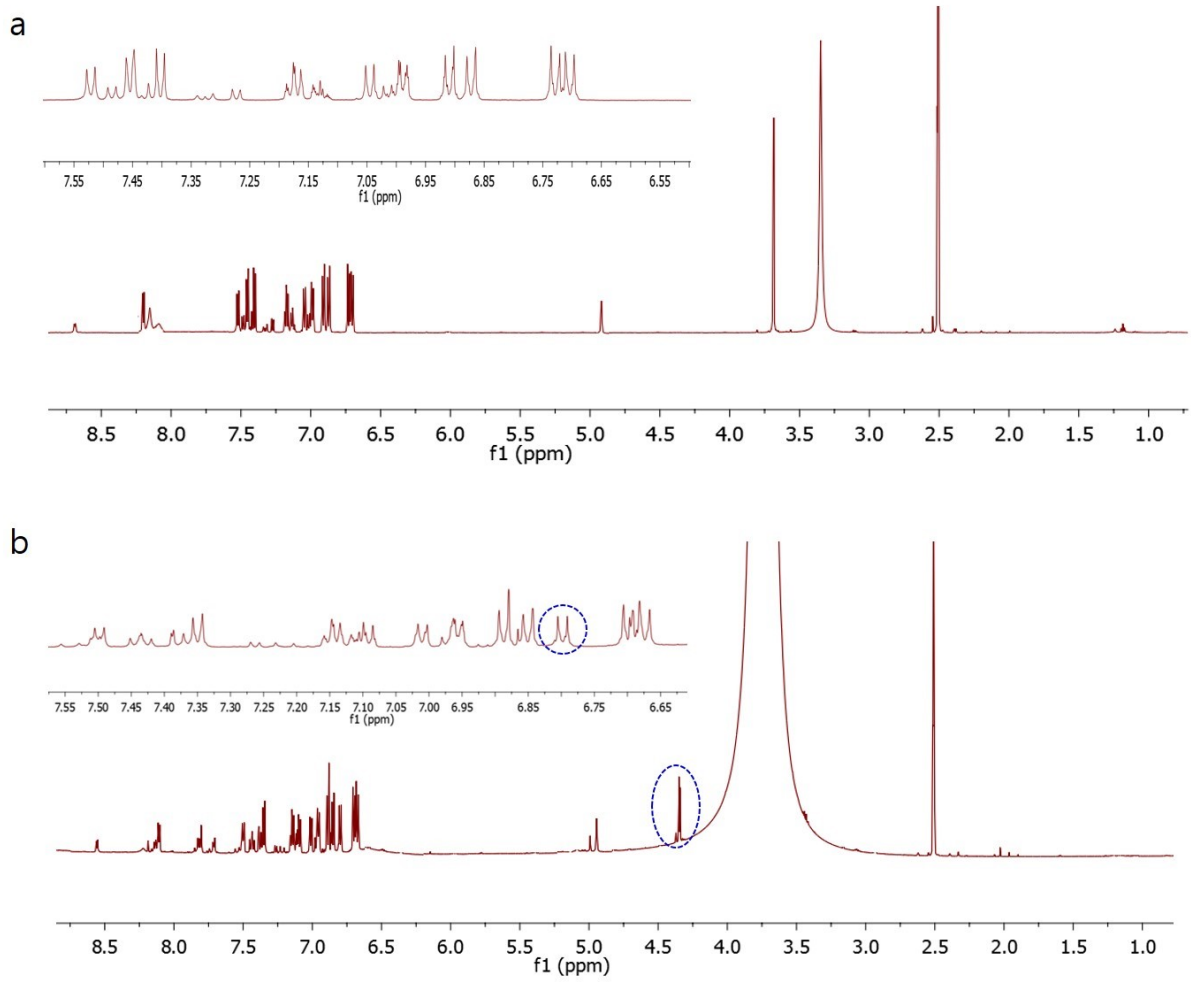

Fig. S10. (a) ^{1}H NMR spectrum of TPEPy-BA before and after hydrolysis in presence of (100 µM) H_2O_2.

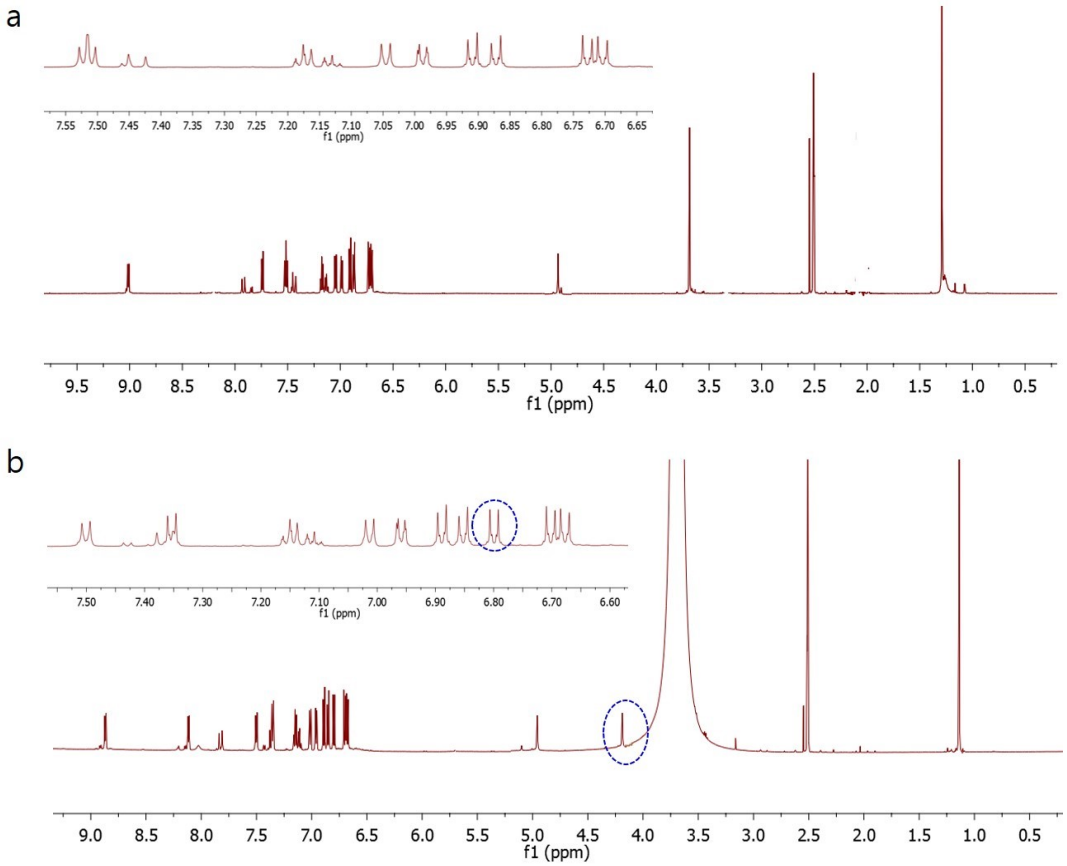

Fig. S11. (a) ^{1}H NMR spectrum of TPEPy-BE before and after hydrolysis in presence of (100 µM) H_2O_2.

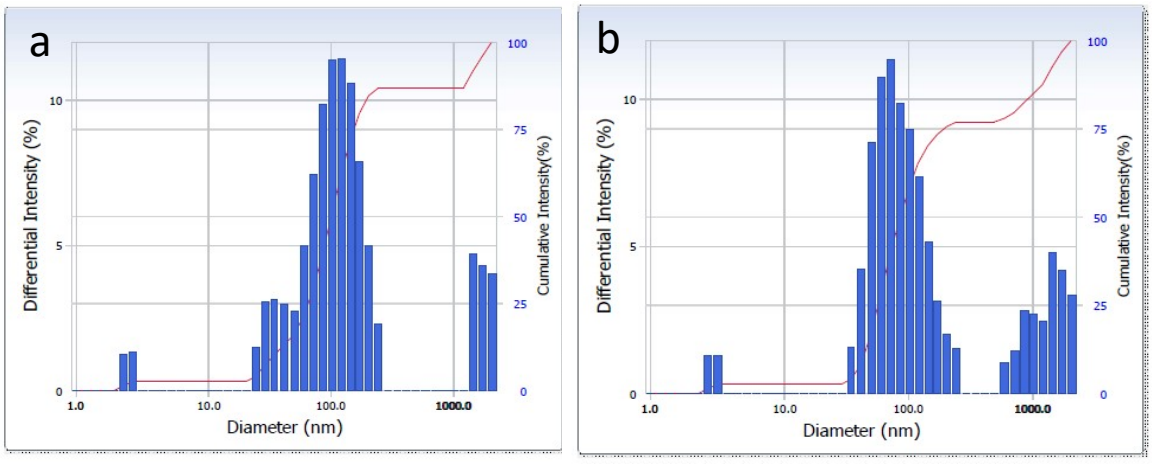

Fig. S12. (a) Average particle size of TPEPy-BA NPs, and (b) TPEPy-BE NPs in PBS (7.4).

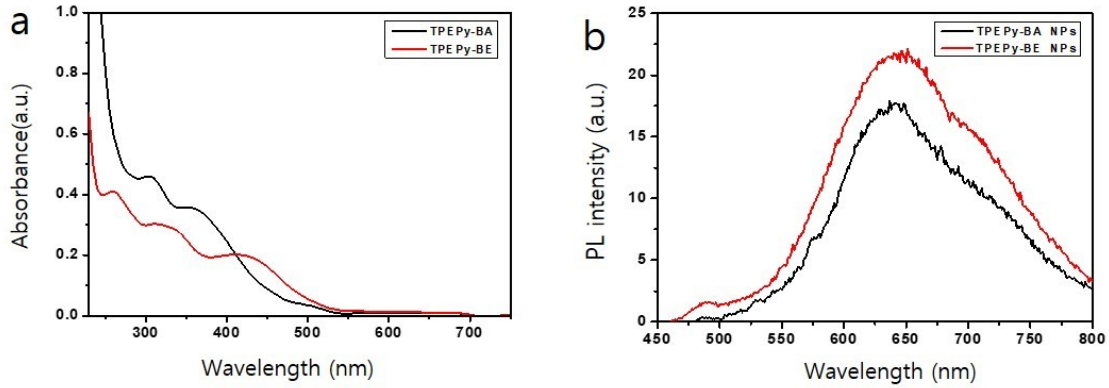

Fig. S13. (a) Absorbance spectra of TPEPy-BA NPs and TPEPy-BE NPs in PBS (7.4) and (b) Photoluminescence (PL) spectra of TPEPy-BA NPs and TPEPy-BE NPs in PBS (7.4).

Table S1. Characterization of AIE-PSs NPs

Sample	Size (nm)	PDI	ΦF
TPEPy-BA NPs	108.3±42	0.311 ± 0.2	0.14
TPEPy-BE NPs	118.3±61	0.316 ± 0.1	0.17

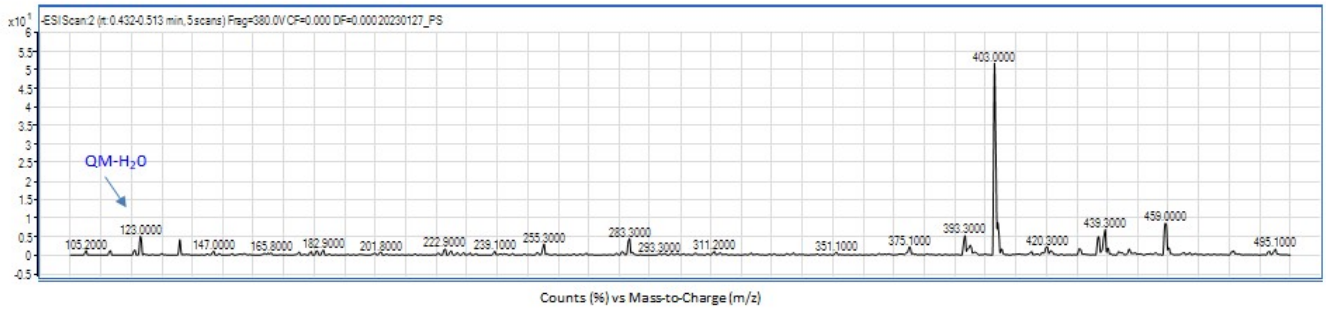

Fig. S14. LC-MS spectrum of TPEPy-BA treated with (100 μM) H_2O_2. QM-H_2O were products of nucleophilic addition between quinone methide and H_2O.

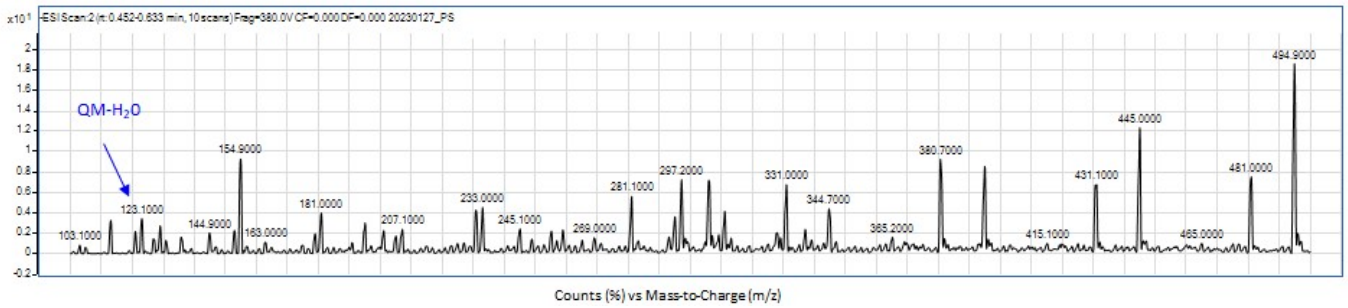

Fig. S15. LC-MS spectrum of TPEPy-BE treated with (100 μM) H_2O_2. QM-H_2O were products of nucleophilic addition between quinone methide and H_2O.

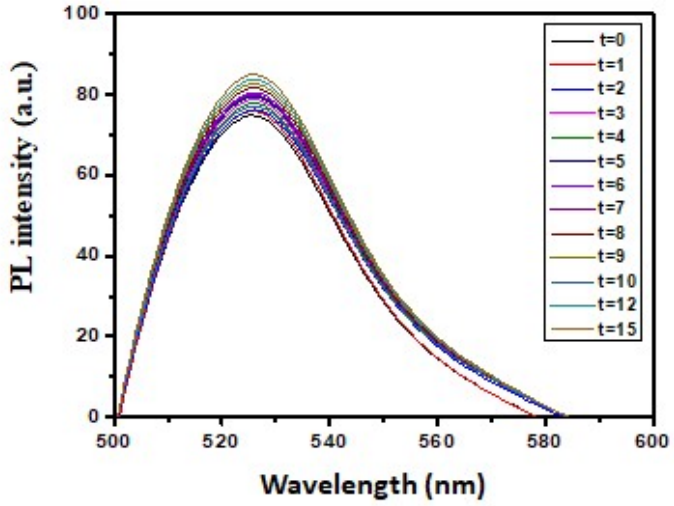

Fig. S16. Fluorescence spectrum of DHR123 irradiation with white light (200 mW/cm^2) for 15 min.