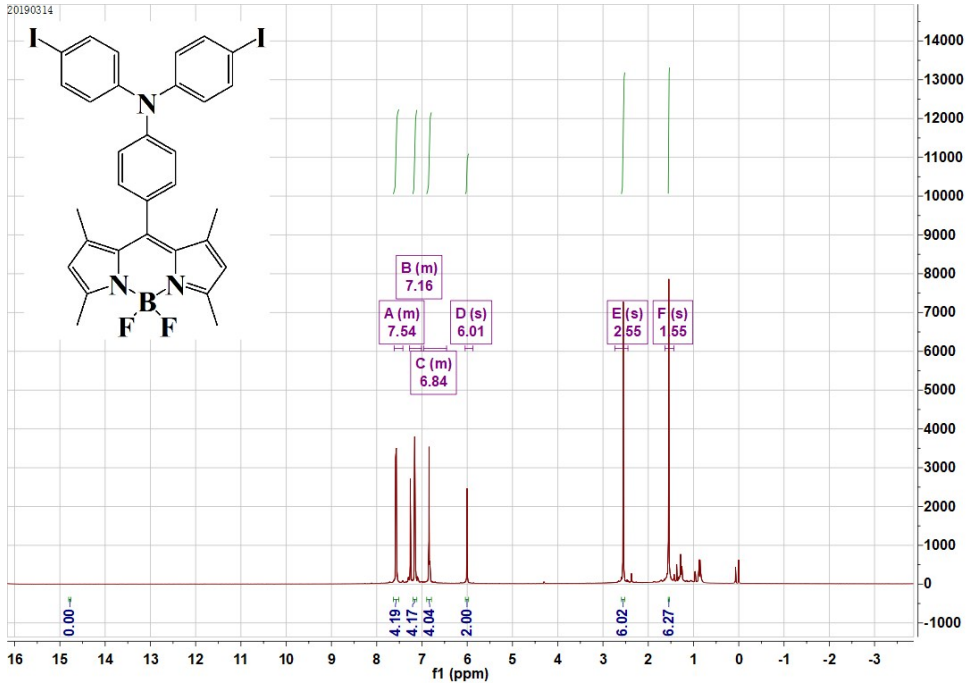
Supporting information

A triphenylamine-BODIPY photosensitizer with D-A configuration and its intracellular simulated photodynamic therapy application

Lingfeng Wang, Jin Bai, Ying Qian *

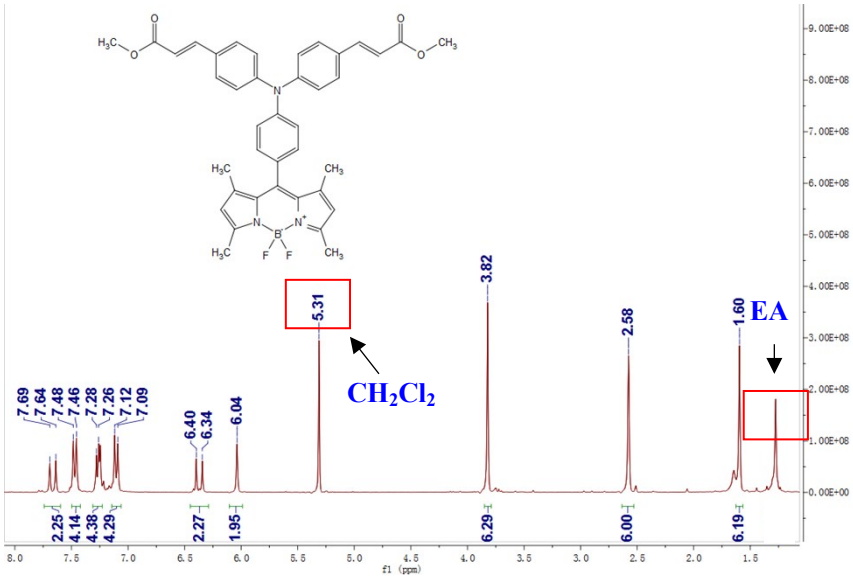
School of Chemistry and Chemical Engineering, Southeast University, Nanjing, Jiangsu 211189, China

Contents:



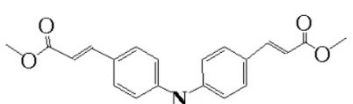
^{1}HNMR ($CDCl_3$, 600MHz) δ:7.54 (m,4H) , δ:7.16 (m,4H), δ:6.84 (m,4H), δ:6.01 (s,2H), δ:2.55 (s,6H), δ:1.55 (s,6H).

Fig. S1. ^{1}H NMR spectra of IPA-BOP in $CDCl_3$.



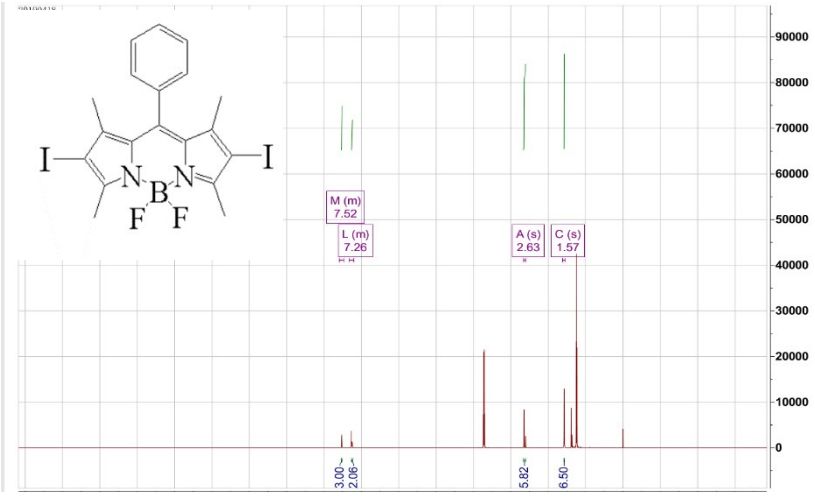
^{1}HNMR ($CDCl_3$, 300MHz) δ: 7.66 (d, J = 15.00 Hz, 2H), δ: 7.47 (d, J = 6.00 Hz, 4H), δ: 7.26 (m, 4H), δ: 7.10 (d, J = 9.00Hz, 4H), δ: 6.37 (d, J = 18.00Hz, 2H) δ: 6.04 (s, 2H), δ: 3.82 (s, 6H), δ: 2.58 (s, 6H), δ: 1.60 (s, 6H).

Fig. S2. ^{1}H NMR spectra of Compound MA-BOP in $CDCl_3$.



HRMS: [M-H$^{\bullet}$] : 658.2803 Obsd: 658.2812

Fig. S3 Mass spectrometry of Compound MA-BOP.



^{1}HNMR ($CDCl_3$, 600MHz) δ:7.52 (m,3H) , δ:7.26 (m,2H), δ:2.63 (s,6H), δ:1.58 (s,6H).

Fig. S4. ^{1}H NMR spectra of Compound I-Ph-BOP (the reference) in $CDCl_3$.

General synthetic method of I-Ph-BOP

A mixture of Ph-BOP and N-Iodosuccinimide (7 equiv) was dissolved in 20 mL dichloromethane solution. Then reaction mixture was mixing at room temperature for 3 h . The color of the solution changes from yellow to bright red gradually and the reaction was monitored by TLC. When the reaction was completed, The solvent was concentrated in vocuo and the residue was purified by silica gel column chromatography to give red solid.

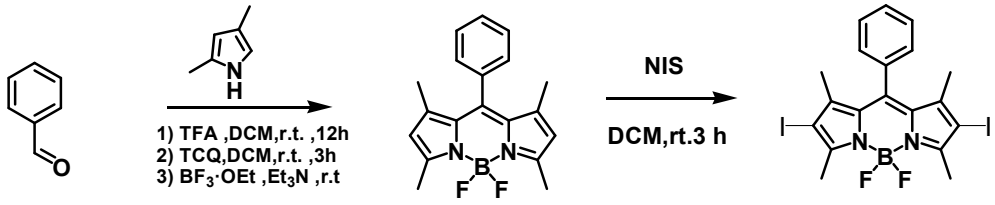


Fig. S5. Method for synthesizing the singlet oxygen reference.

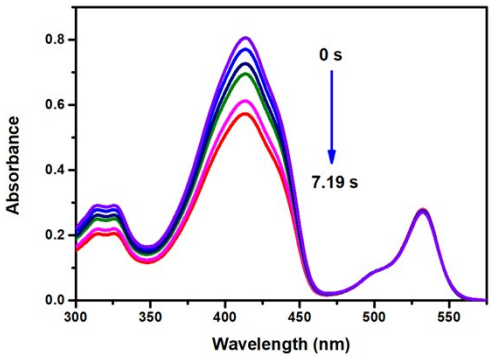


Fig. S6. Absorbance drop of DBPF in a solution of I-Ph-BOP in dichloromethane

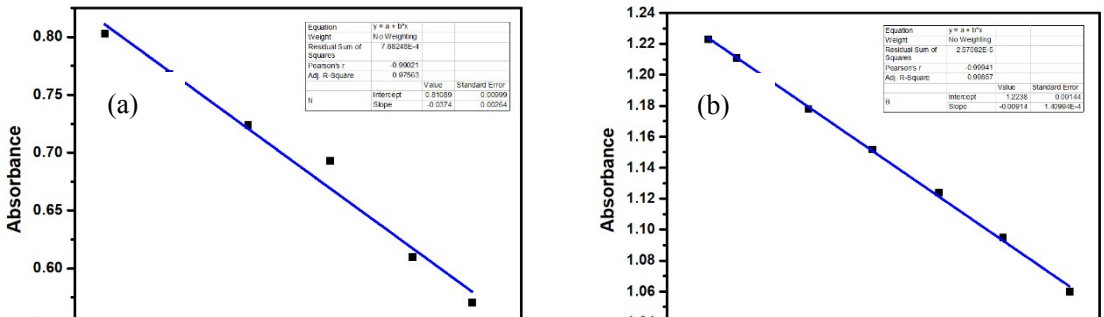


Fig. S7. (a)I-Ph-BOP (b) MA-BOP in linear fit of the value of DBPF absorbance drop versus time .

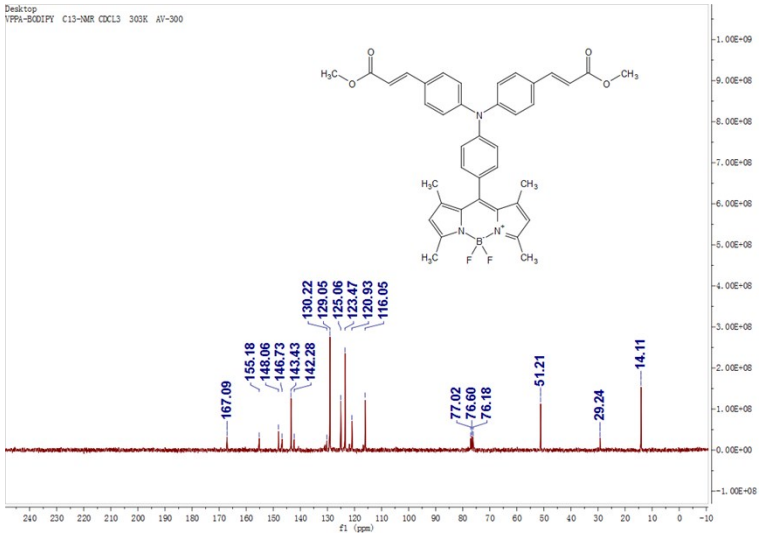


Fig. S8. ^{13}C NMR spectra of Compound MA-BOP in $CDCl_3$.

^{13}CNMR ($CDCl_3$, 300MHz) δ:167.09, 155.18, 148.06, 146.73, 143.43, 142.28, 130.22, 129.24, 125.06, 123.47, 120.93, 116.05, 52.21, 29.24, 14.11.

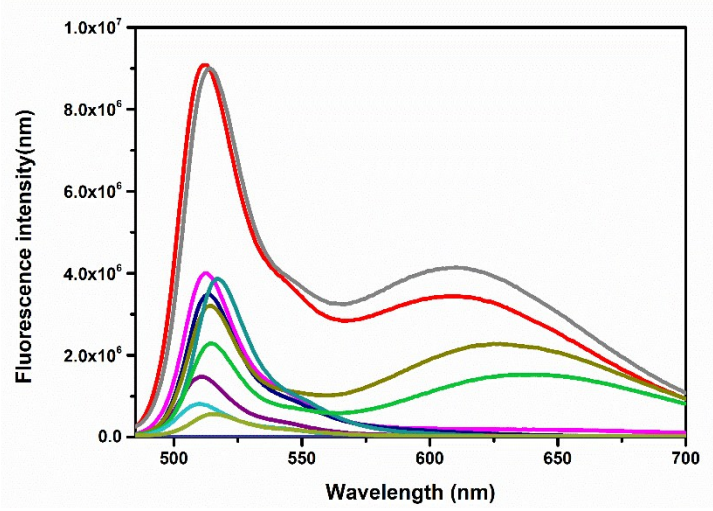


Fig S9. Fluorescence spectra of MA-BOP in different polarity solvents (Solvent: THF, DCM, CH_3CN, $CH_3CH_2Cl_2$, EtOH,MeOH,DMSO,EA.Slit:5/5 nm,Excited wavelength:470 nm. Solvent: benzene, 1,4 dioxane. Slit: 2/2 nm,Excited wavelength:470 nm.)

Table S1 : Photophysical parameters of MA-BOP.

	$\lambda_{abs}{}^{max}$/nm	$\varepsilon_{max}/10^5 M^{-1}cm^{-1}$	$\lambda_{em}{}^{max}$/nm	Stokes Shift/nm	$\Phi_{Fluorescence\ quantum\ yield}$ /(%)	$\Phi_{\Delta\ singlet\ oxygen}$ /(%)	I/Io
MA-BOP	502	0.62	515/625	123	5.69	20.12	0.71

(I/Io : Ratio of fluorescence intensity between CT states emission peak with LE states emission peak, ΦFluorescence quantum yield /(%) was refers to the fluorescence quantum yield in the long-wave direction. The ethanol solution of Rhodamine B (ΦF=0.98) was selected as the fluorescence reference16.)