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Effect of regioisomeric BODIPY-C_{60} bis-cycloadducts on generation of singlet oxygen

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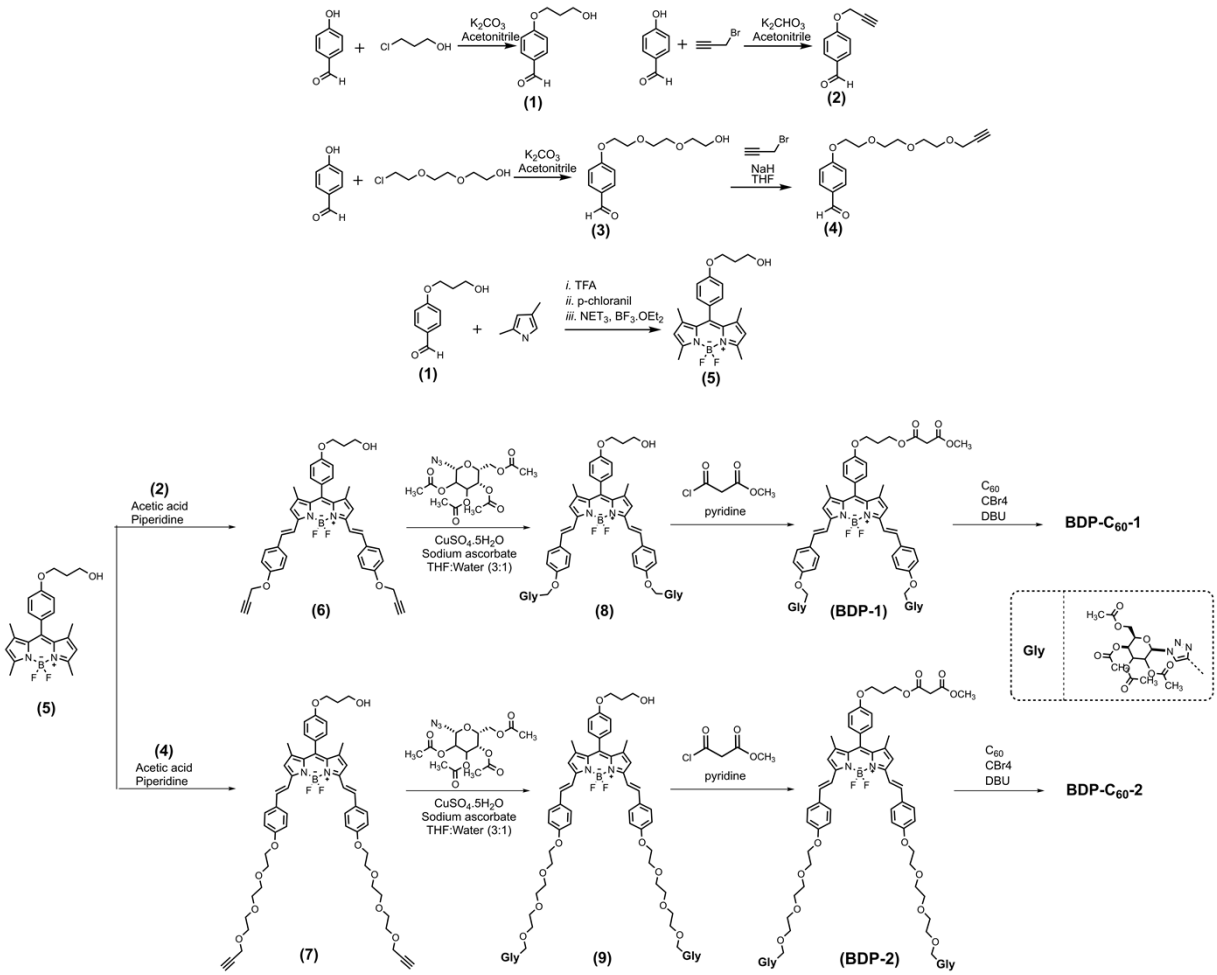
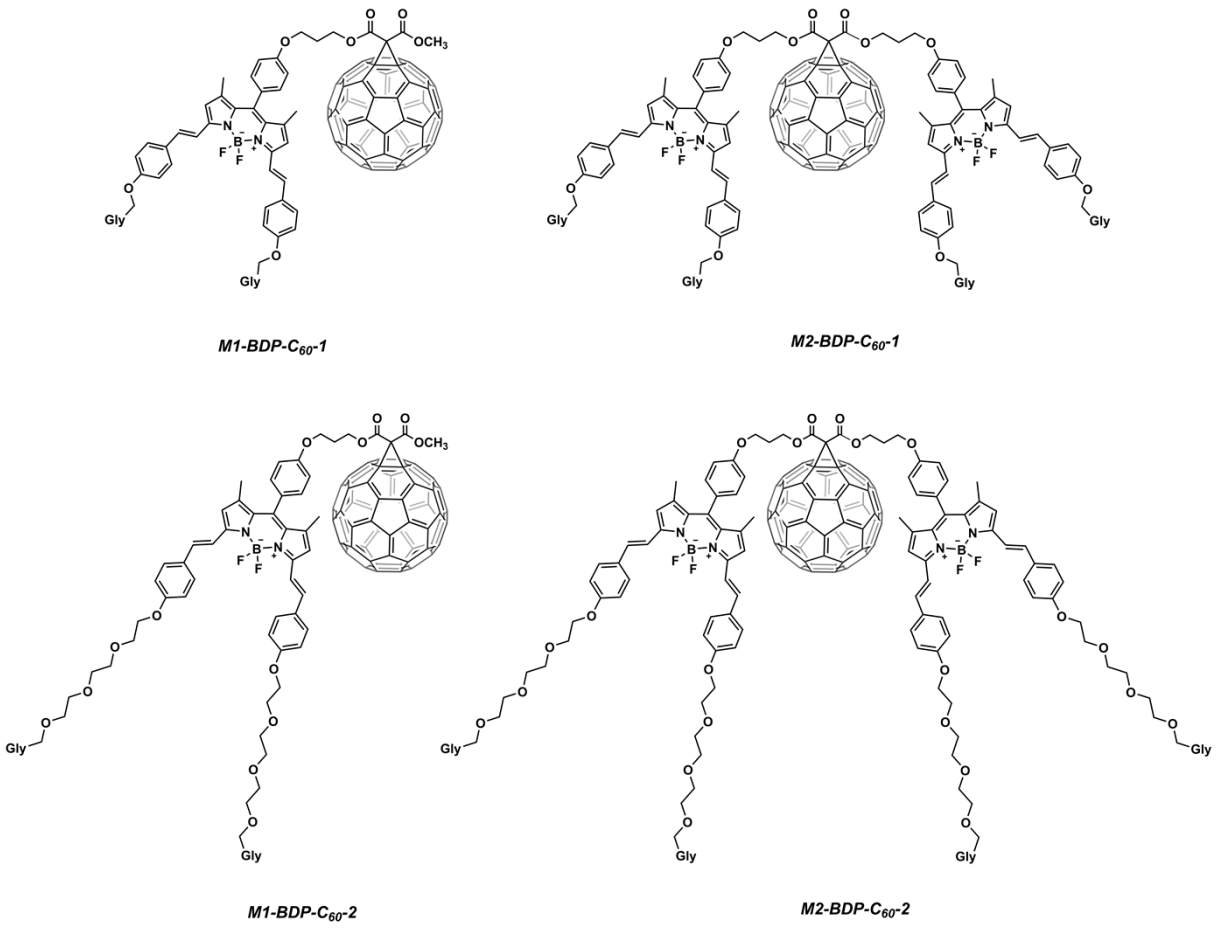


Scheme S1 Synthesis of bis-adduct BODIPY-C_{60} derivatives



Scheme S2 Molecular structures of M1-BDP-C_{60}-1, M2-BDP-C_{60}-1, M1-BDP-C_{60}-2, M2-BDP-C_{60}-2

Materials

Dichloromethane (DCM), dimethyl sulfoxide (DMSO), benzene, chloroform, acetone, tetrahydrofuran, toluene, methanol (MeOH), acetonitrile, deuterated chloroform ($CDCl_3$), silica gel 60 (0.040-0.063 mm) for column chromatography, silica gel plates with F_{254} indicator (Kieselgel 60 Å, 0.25 mm thickness), *p*-chloranil, trifluoroacetic acid, triethylamine, boron trifluoride diethyl etherate, 3-chloro-1-propanol, 1,3-diphenylisobenzofuran, methylene blue (MB) and sodium hydride were purchased from Merck. 2,4-dimethylpyrrole, acetic acid, propargyl bromide, piperidine, 9,10-anthracenediyl-bis(methylene)dimalonic acid and methyl malonyl chloride were provided from Sigma Aldrich. Following chemicals were obtained from Acros organics; carbon tetrabromide (CBr_4) and 4-hydroxybenzaldehyde. Fullerene, potassium carbonate, and pyridine were provided from Alfa Aesar. 1-Azido-1-deoxy-β-D-glucopyranoside tetraacetate and 1,8-diazabicyclo- [5.4.0]undec-7-ene (DBU) were purchased from ABCR.

Equipment

Analytical thin layer chromatography (TLC) was performed on silica gel plates. Bruker Daltonics Microflex mass spectrometer equipped with a nitrogen UV- Laser operating at 337 nm was employed to provide mass spectra. 500 MHz Bruker Avance Neo NMR was used to obtain ^{1}H and ^{13}C NMR spectra. Electronic absorption spectra were acquired via Shimadzu 2101 UV spectrophotometer in the UV-visible (200-800 nm) region. Varian Eclipse spectrofluorometer was used to record fluorescence emission spectra. The fluorescence lifetime spectra were provided with Horiba- Jobin- Yvon- SPEX Fluorolog 3-2iHR instrument with Fluoro Hub-B Single Photon Counting Controller. Time correlated single photon counting (TCSPC) module was used for signal acquisition during the fluorescence lifetime measurements. Singlet oxygen phosphorescence measurements were carried out via using Horiba Jobin-Yvon Fluoremeter with Hamamatsu NIR PMT 5509 at −80 °C.

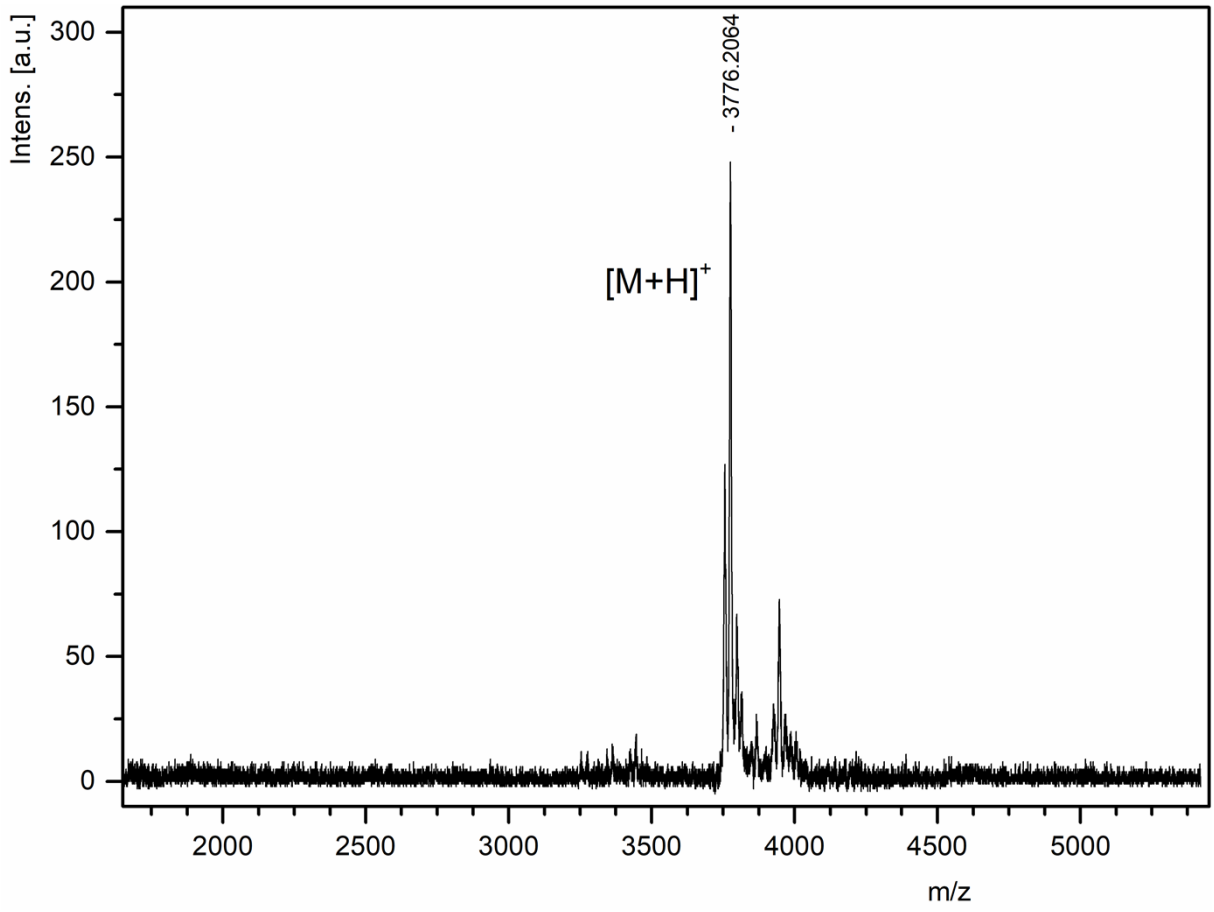


Fig. S1 MALDI-MS spectra of compound **BDP-C_{60}-1**

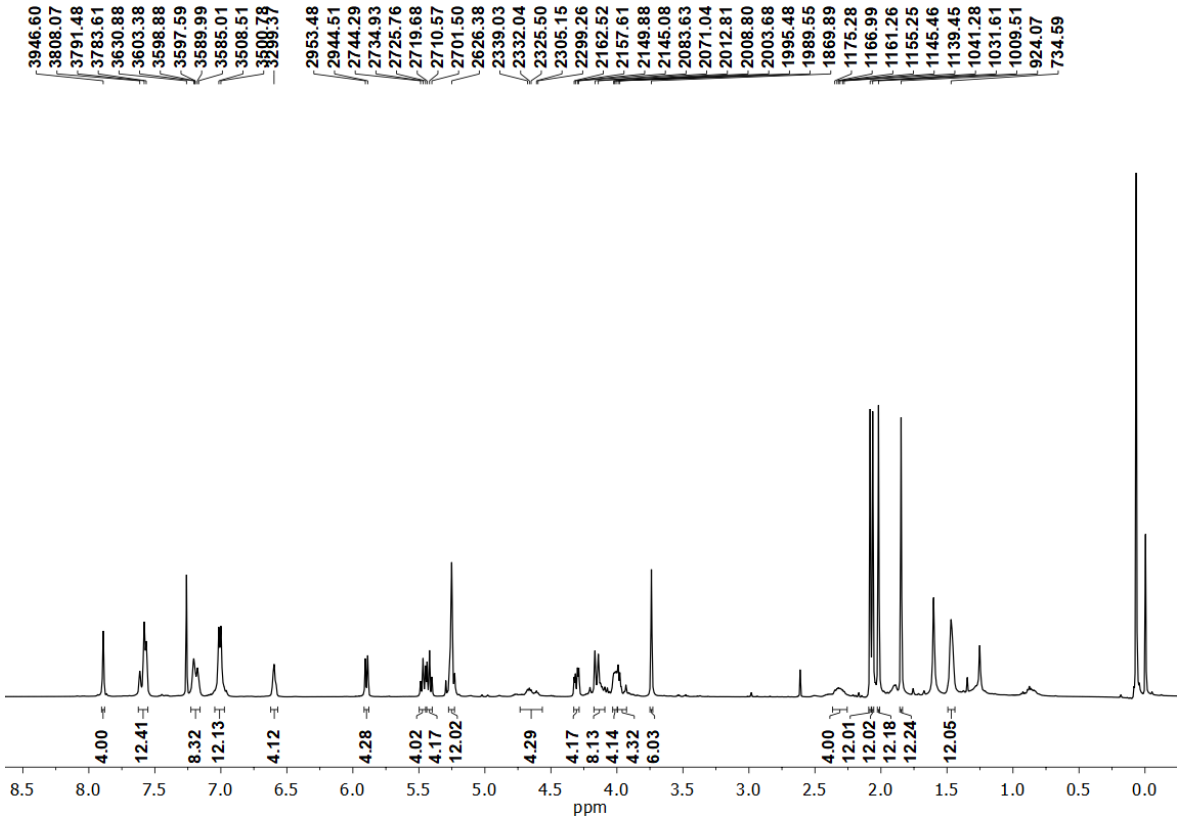


Fig. S2 ^{1}H- NMR spectra of compound **BDP-C_{60}-1** in $CDCl_3$

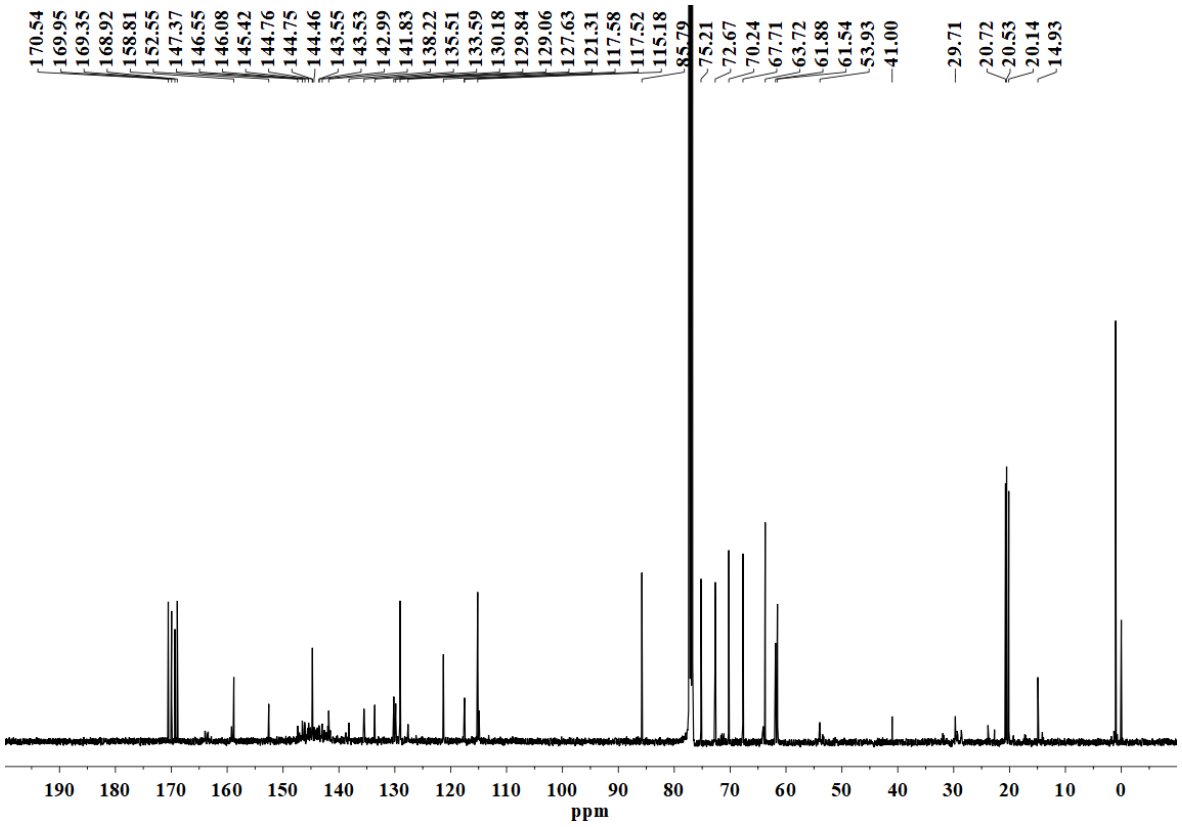


Fig. S3 ^{13}C- NMR spectra of compound **BDP-C_{60}-1** in $CDCl_3$

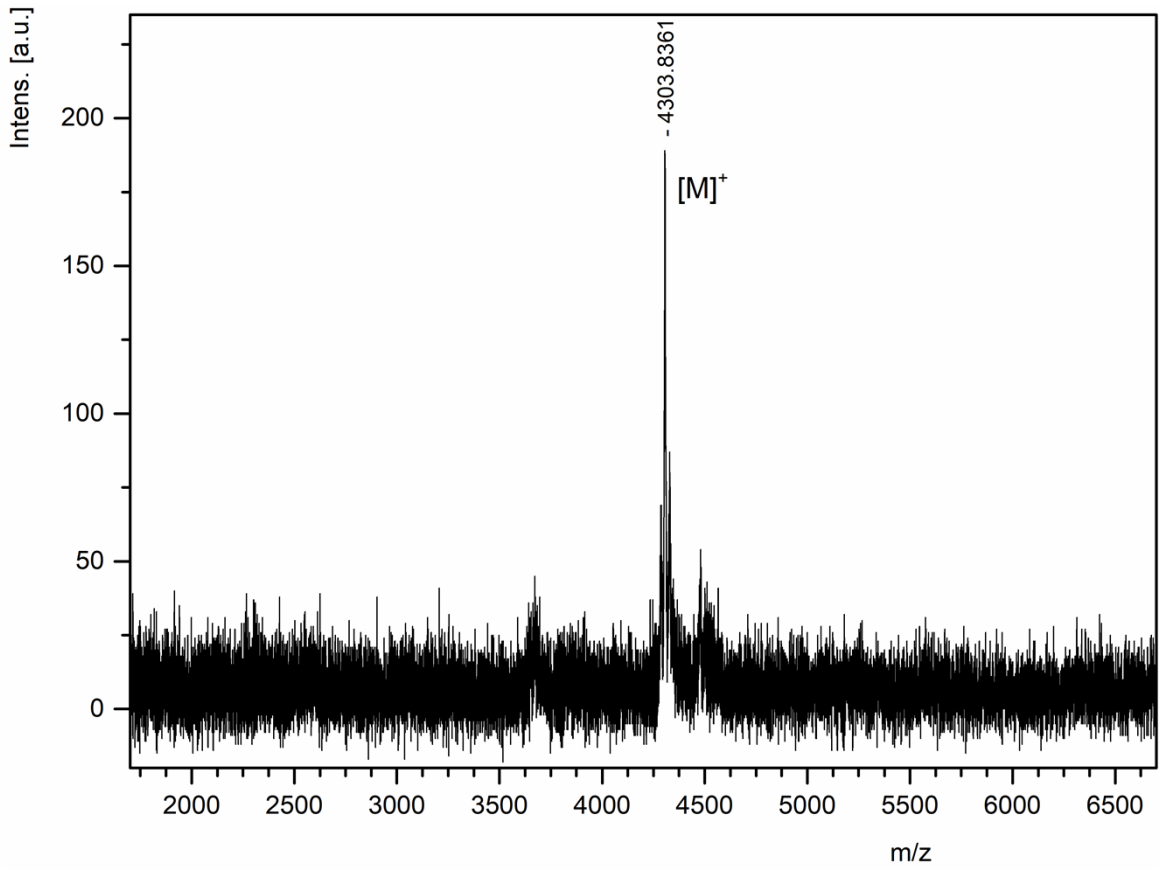


Fig. S4 MALDI-MS spectra of compound **BDP-C_{60}-2**

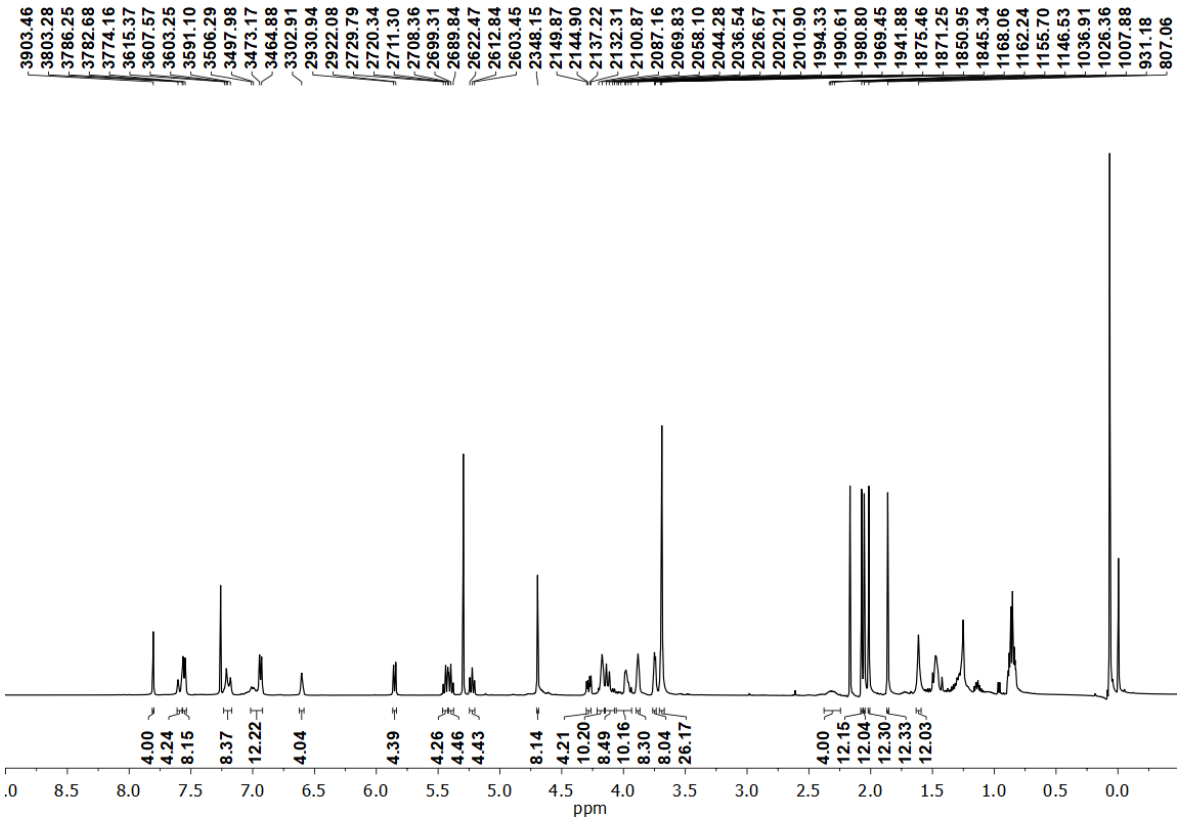


Fig. S5 ^{1}H- NMR spectra of compound **BDP-C_{60}-2** in $CDCl_3$

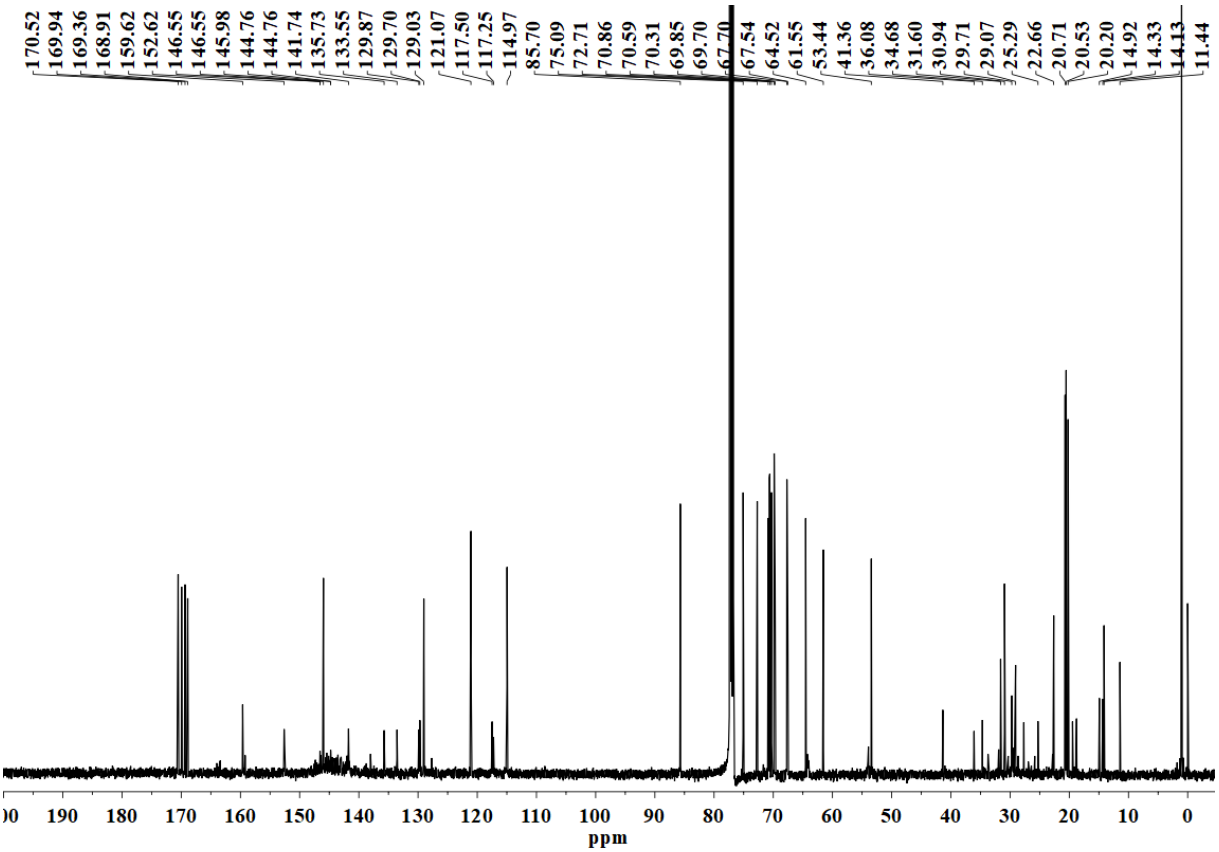


Fig. S6 ^{13}C- NMR spectra of compound **BDP-C_{60}-2** in $CDCl_3$

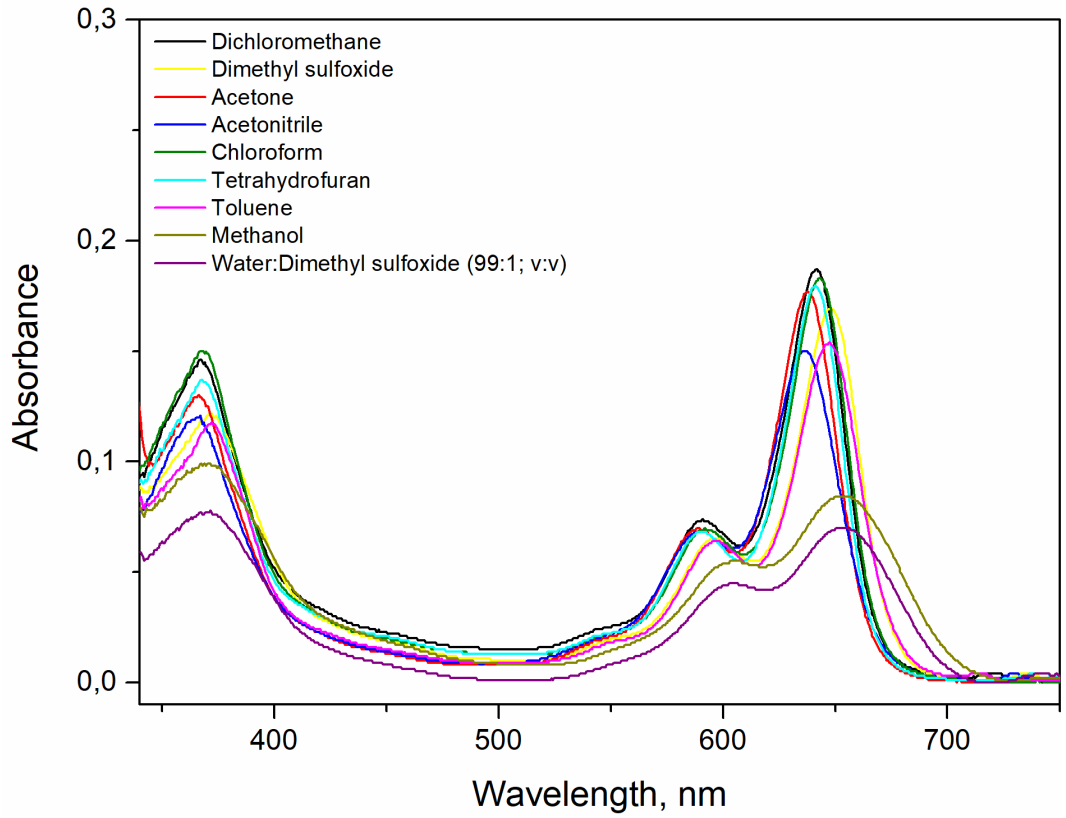


Fig. S7 Absorption spectra of compound **BDP-C_{60}-1** in different solvents

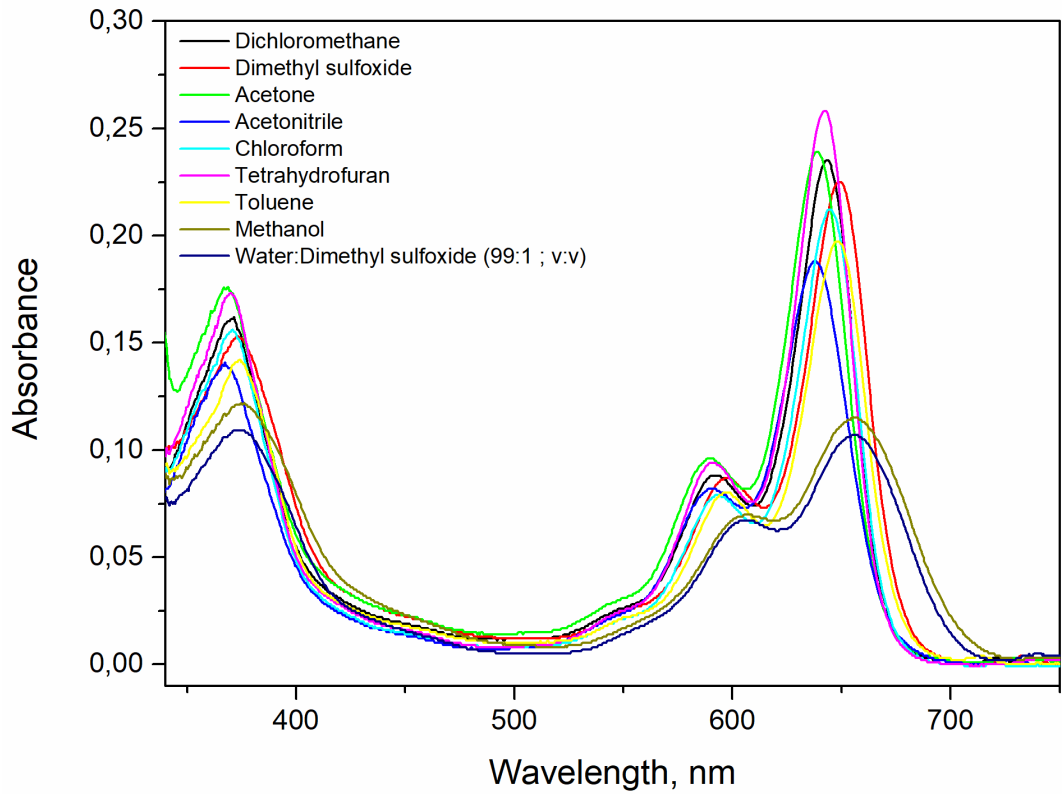


Fig. S8 Absorption spectra of compound **BDP-C_{60}-2** in different solvents

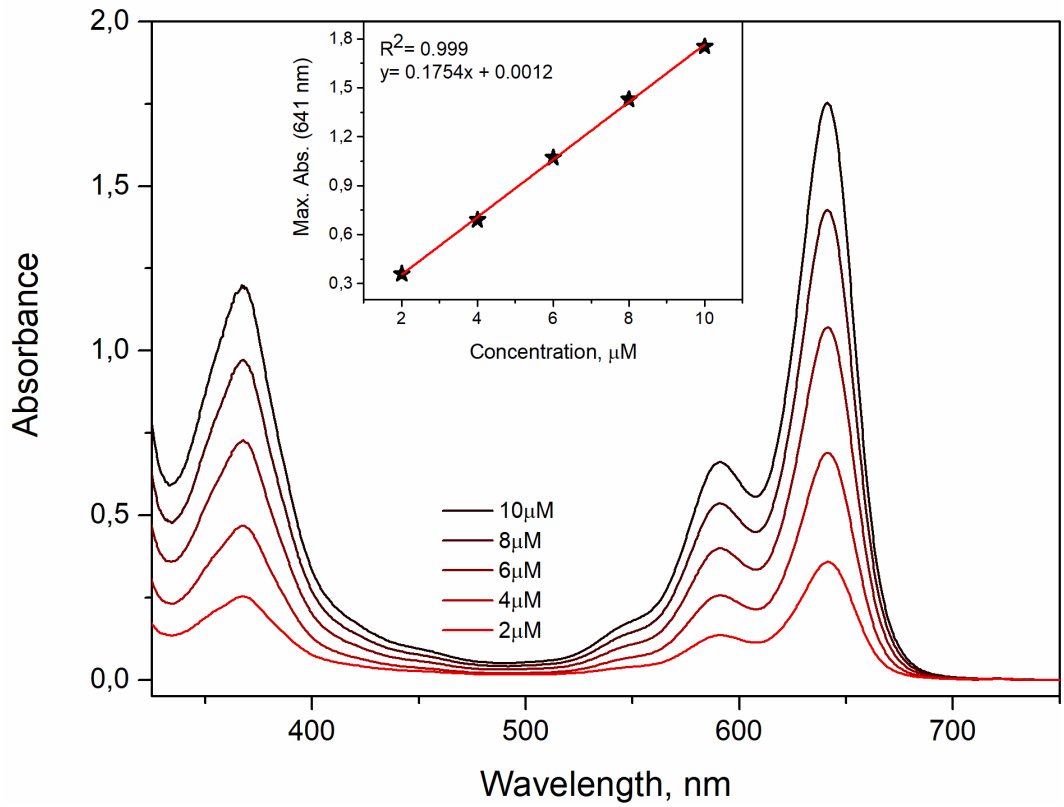


Fig. S9 Absorption spectra of compound **BDP-C_{60}-1** in DCM at different concentrations

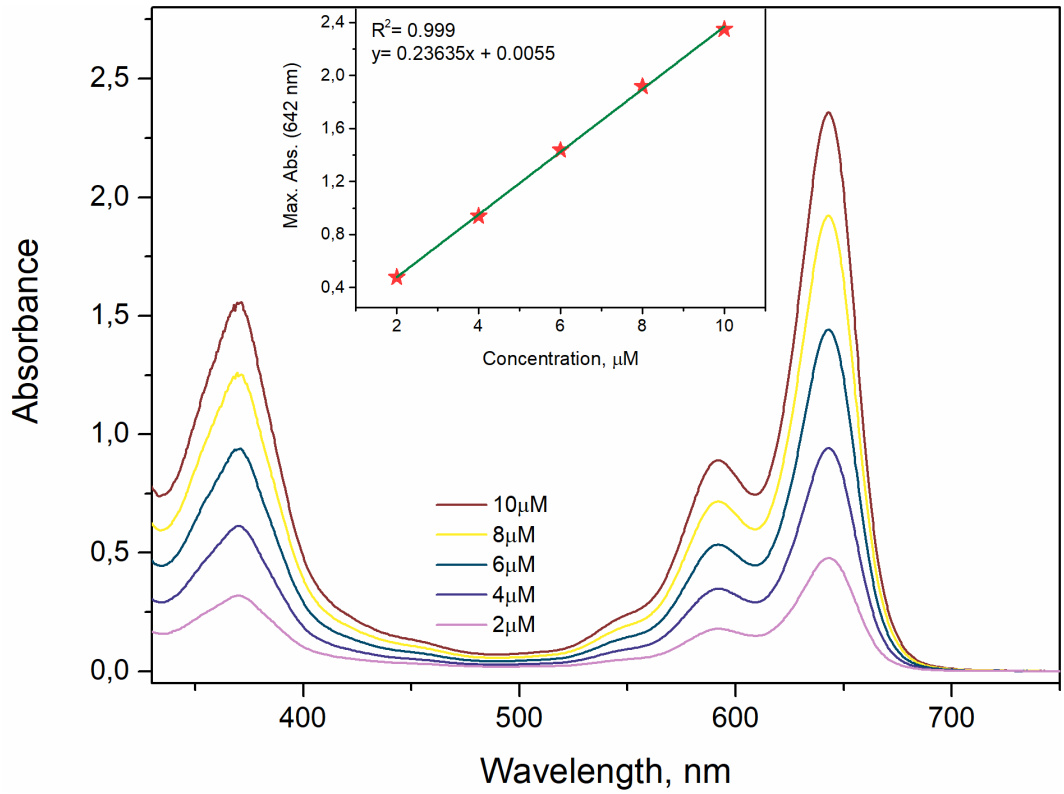


Fig. S10 Absorption spectra of compound **BDP-C_{60}-2**in DCM at different concentrations

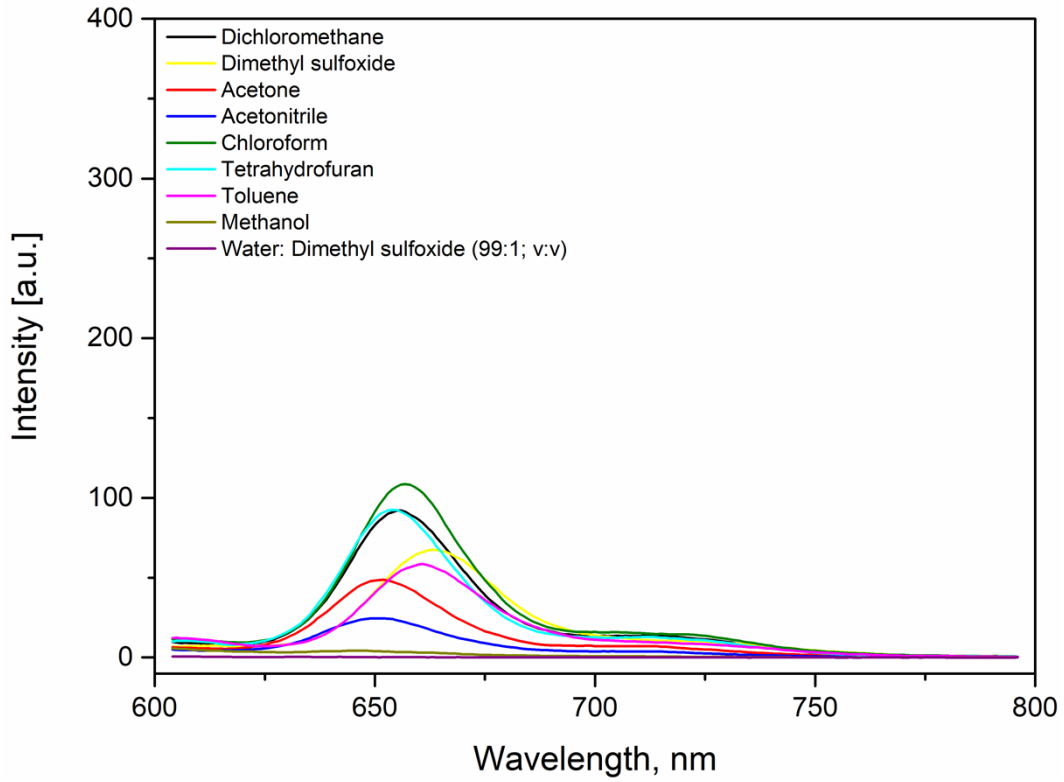


Fig. S11 Fluorescence emission spectra of compound **BDP-C_{60}-1** in different solvents (1μM; λ_{ex}:590 nm)

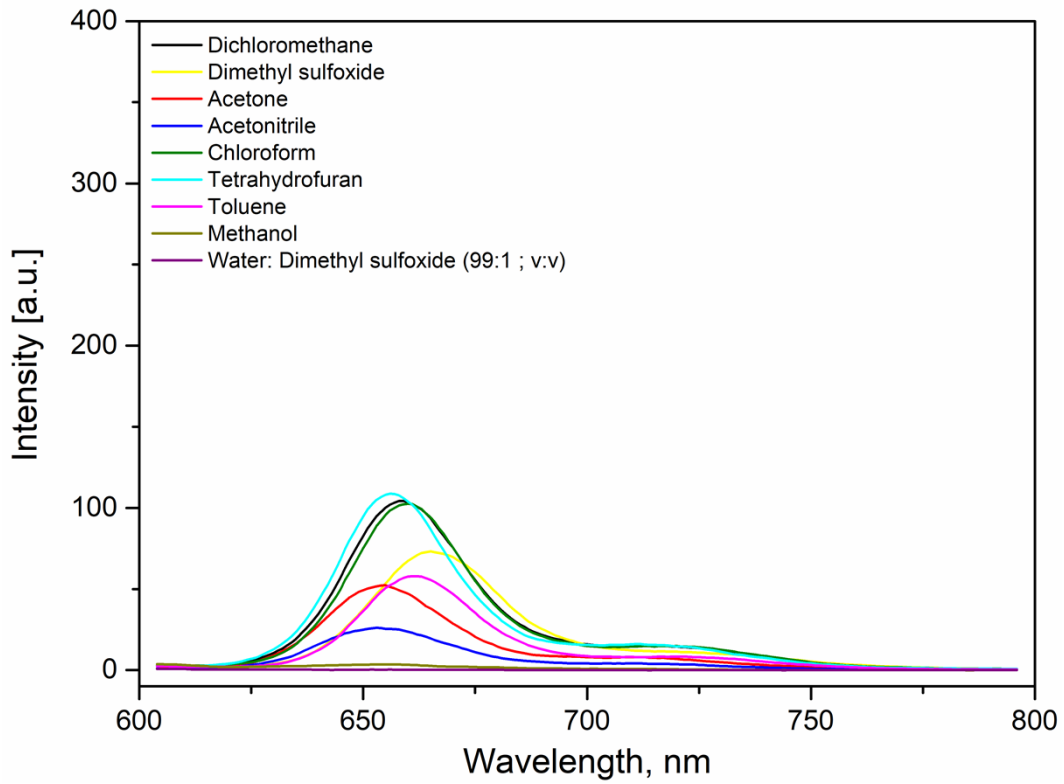


Fig. S12 Fluorescence emission spectra of compound **BDP-C_{60}-2** in different solvents (1µM; λ_{ex}:590 nm)

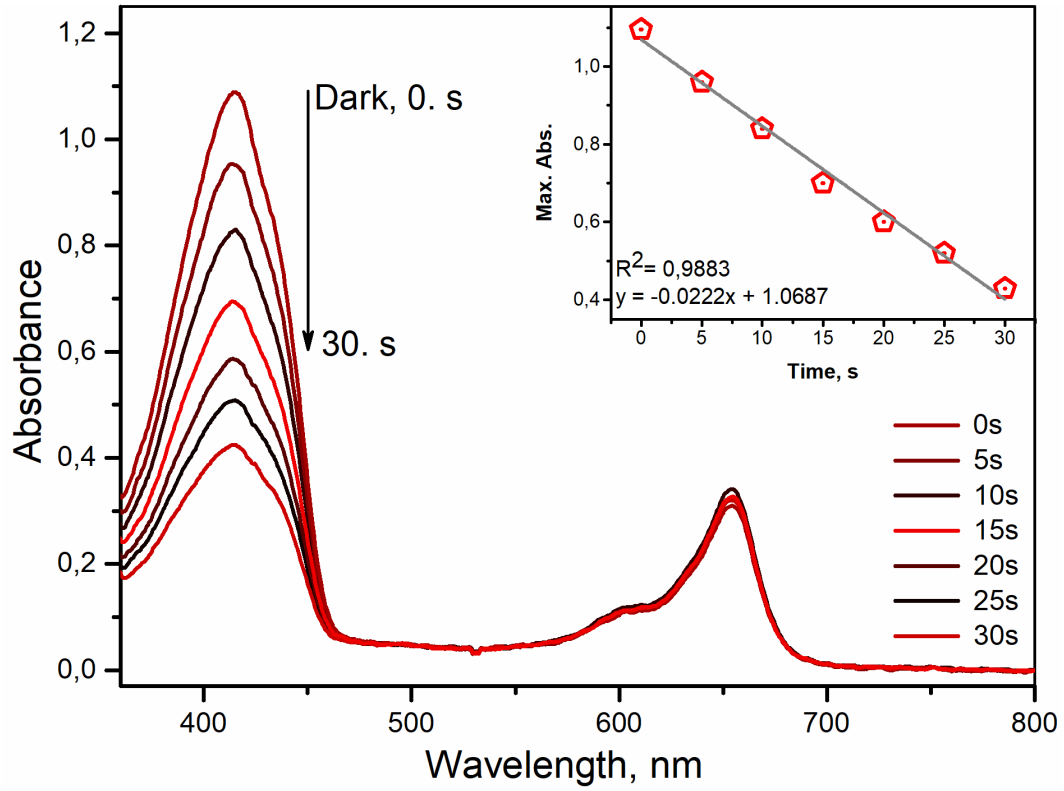


Fig. S13 Decrease the absorbance of DPBF at 414 nm in the presence 2 µM MB

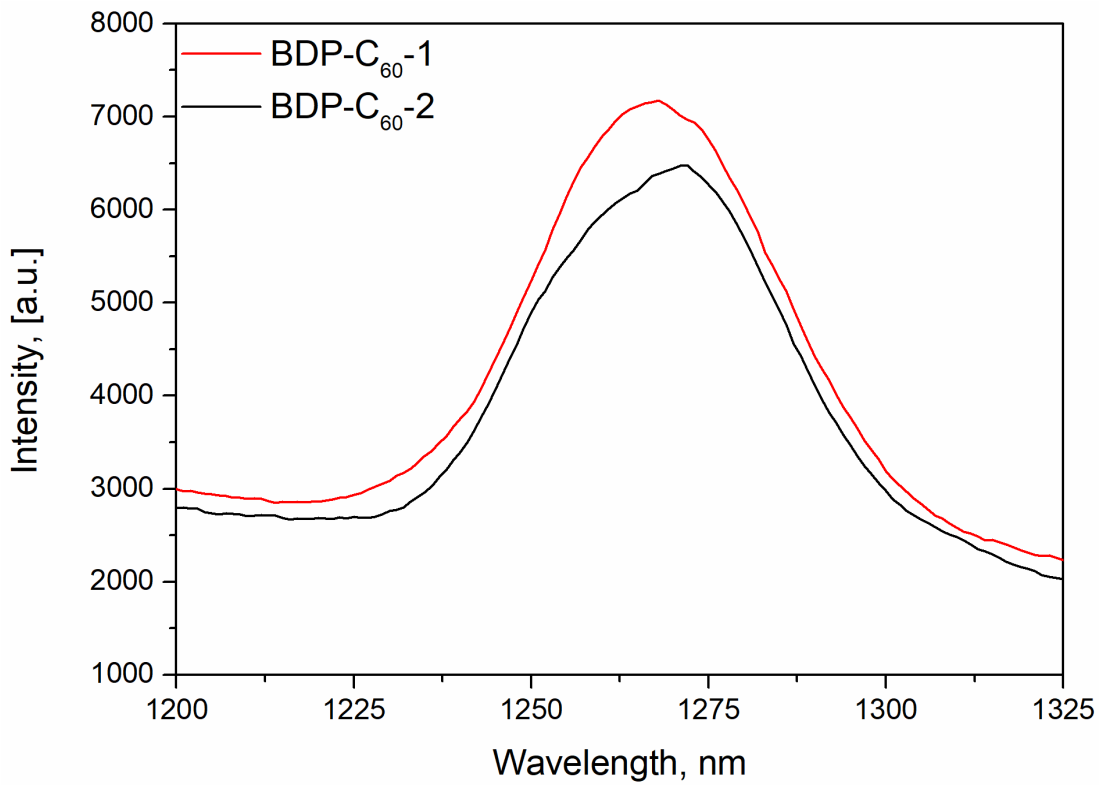


Fig. S14 Singlet oxygen phosphorescence of **BDP-C_{60}-1** and **BDP-C_{60}-2** in DCM (maximum absorptions were set to 0.2 for comparison)